

**On the Failure of Correlating Partitioned Electrostatic
Surface Potentials Using Bader's Atoms-in-Molecules
Theory to Impact Sensitivities**

by Edward F. C. Byrd

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14. ABSTRACT U.S. Army Research Laboratory researchers applied Bader's atoms-in-molecules theory by partitioning the electrostatic surface potential, and associated Politzer parameters, into atom-specific areas with the resultant data correlated to impact sensitivity. Although we determined many correlations, we found no quantitative correlations for aromatic compounds, with several correlations exhibiting limited predictive capability. Attempts at using area-weighted parameters yielded negligible differences compared to the nonweighted parameters. Ultimately, we found no useful correlations with atom- or group-partitioned electrostatic surface potentials; one should refer to the associated supplemental material in the appendix of this report for the host of unsuccessful correlations and related Politzer parameters.					
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1. Introduction

Recent advances in theoretical models and computational power have vastly improved the capability to predict performance properties of energetic materials (EMs), thus allowing researchers to efficiently and safely screen candidate materials and focus synthesis efforts on the most promising compounds. While theoretical models predicting properties important to the prediction of performance, such as heats of formation (1, 2) and crystal densities (3), have shown significant successes, there is a paucity of effective models for sensitivity to impact ($h_{50\%}$).

Many different methodologies have been employed in attempts to find correlations between molecular properties and impact sensitivity, with varying degrees of success. Researchers have attempted correlations ranging from oxygen balance (4), Mulliken charges (5–7), normal mode analysis (8), dissociation energies (9), and, most recently, distributed multipole analysis (10). Based off of Murray et al.’s efforts (11, 12), ARL researchers Rice and Hare (13) explored correlations between an EM’s electrostatic surface potential (ESP) mapped onto the $\rho_{0.001}$ electron density isosurface to its sensitivity to impact (14). While Rice and Hare were unable to determine an accurate quantitative correlation, they did identify a qualitative visual relationship between patterns of charge on the isodensity surface and impact sensitivity. This qualitative mapping of charge to impact sensitivity illustrated regions of localized electron deficiency over covalent bonds for sensitive materials.

In a different attempt, Yau et al. (15) employed the AIMPAC software package (16) to calculate atoms-in-molecules (AIM) (17) properties from a Kohn-Sham density functional theory (KS-DFT) wave function in order to correlate specific regions of the electronic density with impact sensitivity. It was thought that the ability of AIM to probe these regions and to assign properties to specific nuclei and intermolecular “bonds” would yield a more quantitative predictive tool than those developed by Rice and Hare. However, Yau et al. determined that the number of these “critical points” was variable depending on the DFT and basis set used, thus negating the feasibility of using data gathered from these critical points for sensitivity prediction.

In this report, we explore another facet of Bader’s AIM methodology, chiefly that of partitioning the electron density into “atomic basins” (18–20). The atomic basin is defined as the volume bounded by a zero flux surface, i.e., the surface bounding the atom not crossed by any gradients of the density ($\nabla\rho$). This can be stated mathematically as

$$\nabla\rho \cdot \vec{n} = 0 \tag{1}$$

for every point on the surface, with $\vec{n}$ denoting unit vectors normal to the surface. Using this concept of atomic basins, we shall map and assign every point on the $\rho_{0.001}$ isosurface to a specific atom and attempt to derive correlations based off of the atom-specific Politzer electrostatic statistics.

2. Computational Methods

In this study, we chose 21 aromatic and nonaromatic compounds, spanning the range of experimental drop hammer impact sensitivities. Of these 21 compounds, 11 were chosen to populate the training (fitting) set (table 1), while the other 10 compounds were reserved for the test set (table 2). The molecules explored in this study include nitroaromatics, nitrate esters, polynitroanilines, nitramines, nitrotriazoles, and nitroaliphatics. For all of the molecules in this study, we generated spin-restricted KS-DFT electron densities using the B3LYP (21–24) and PBE (25, 26) potentials with either the 6-31G* or 6-31G** Pople gaussian basis sets (27–29). The geometries employed were the experimental crystal structures contained in the Cambridge Structural Database (30, 31). All calculations to determine the electronic densities and ESPs were performed with the Gaussian09 program package (32). A program developed in-house was used to assign density and ESP points to individual atoms. A second in-house code was employed to determine the Politzer statistics.

Table 1. Training set of 11 aromatic and nonaromatic molecules.

Molecule	Acronym	Experimental $h_{50\%}$ (cm)
hexanitrobenzene	HNB	11 (33)
2,4,6,8,10,12-hexanitrohexaazaisowurtzitane (ϵ -polymorph)	CL20	12 (34)
tetranitrate pentaerythritol	PETN	13 (35)
pentanitroaniline	PNA	22 (33)
hexahydro-1,3,5-trinitro-1,3,5-triazine	RDX	28 (36)
1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane	HMX	29 (37)
<i>N,N'</i> -dinitro-1,2-ethanediamine	EDNA	34 (37)
2,4,6-trinitrotoluene	TNT	98 (33)
1,1-diamino-2,2-dinitro-ethylene	FOX-7	126 (38)
nitroguanidine	NQ	320 (35)
1,3,5-triamino-2,4,6-trinitrobenzene	TATB	490 (37)

Table 2. Test set of 10 aromatic and nonaromatic molecules.

Molecule	Acronym	Experimental $h_{50\%}$ (cm)
azidopentanitrobenzene	CL16	17 (33)
2-azido-1,3,5-trinitrobenzene	Picryl azide	19 (33)
<i>N</i> ³ , <i>N</i> ⁶ -bis(2,2,2-trinitroethyl)-1,2,4,5-tetrazine-3,6-diamine	BTAT	22 (39)
<i>N</i> -methyl- <i>N</i> ,2,4,6-tetranitroaniline	Tetryl	25 (33)
2,4,6-trinitroresorcinol	Styphnic acid	43 (37)
2,2',4,4',6,6'-hexanitrostilbene	HNS	54 (36)
2,4,5-trinitroimidazole	Tri245	68 (37)
4,6-dinitrobenzofuroxan	DNBF	76 (33)
2-methoxy-1,3,5-trinitrobenzene	Methyl picrate	192 (37)
3-nitro-1,2,4-triazole-5-one	NTO	291 (37)

3. Results and Discussion

Inspired by the work of Murray et al. (12) and Rice et al. (13), this report shall follow a similar convention for the definitions of the electrostatic properties. These electrostatic properties are global properties across the 0.001 electron/bohr (3) isosurface of electronic density. The ESP V is defined as

$$V(\mathbf{r}) = \sum_i \frac{Z_i}{|\mathbf{R}_i - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}') d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|}, \quad (2)$$

where Z_i and $\mathbf{R}_i$ represent the charge and position of atom i and $\rho(\mathbf{r})$ is the electronic density. Regions of negative V indicate a large electron density (i.e., electron rich), while a region with a positive V is electron poor (i.e. has a low electron density).

In addition to the mapping of ESP, Murray et al. (11, 12) developed statistical tools to analyze the distribution of charge across the density isosurface. The statistical quantities examined in this report are the surface area, the average ESP (Σ), the average deviation of ESP (Π), the variance of ESP (σ^2), and the balance parameter (v). These are defined as

$$\Sigma^x = \frac{1}{n} \sum_{i=1}^n V^x(r_i), \quad (3)$$

$$\Pi = \frac{1}{n} \sum_{i=1}^n |V(r_i) - \Sigma^{tot}|, \quad (4)$$

$$\sigma_x^2 = \frac{1}{n} \sum_{i=1}^n |V^x(r_i) - \Sigma^x|^2, \quad (5)$$

$$\sigma_{tot}^2 = \sigma_+^2 + \sigma_-^2, \quad (6)$$

$$v = \frac{\sigma_+^2 \sigma_-^2}{[\sigma_{tot}^2]^2}, \quad (7)$$

where $V(r_i)$ is the value of the ESP at r_i . To further partition the data, the average ESP (Σ) and the variance of ESP (σ^2) were computed for the positive (Σ^+ , σ_+^2), negative (Σ^- , σ_-^2), and total (Σ^{tot} , σ_{tot}^2) portions of the ESP; in equations 3 and 5 these are denoted by the superscript or subscript x ; equation 6 defines σ_{tot}^2 . The surface area is defined as the simple addition of the surface quadrature points.

The partitioning employed herein is not limited to atoms but can also be used for any combination of atoms. Of particular interest are the nitro (NO_2) and amine (NH_2) groups and the atoms to which they are connected (either carbon [C], nitrogen [N], or oxygen [O]). As shall be discussed, correlations were sought with either the pure nitro or amine group or with the explicit X-N group of the nitro group (where X is either C, N, or O). Correlations were also explored

with additive ($a + b$) and differences ($a - b$) between the X and nitro N atoms. In addition, we have determined and attempted to correlate the mean (average), the maximum, and the minimum of each of the Politzer values for each atom or group type per molecule. All told, this yielded a gargantuan number of parameters; however, there were few differences between the different DFT functionals and basis sets, and thus we focused on the PBE/6-31G** values. Refer to the appendix for a tabulation of all computed and calculated statistical values.

Additionally, in an effort to establish whether the surface area of each region affected the statistics to any measurable degree, we also calculated the area-weighted Politzer statistics (see appendix for relevant data). Inspection of the resultant parameters showed minimal differences, and therefore we will restrict our discussion to the non-area-weighted parameters.

In the course of this study, little to no correlation was found for most of the atom-specific Politzer parameters (see appendix for all relevant graphs and tables). The parameters for which even slight correlations were found typically involved the nitrogens in the nitro groups (nitro nitrogens, N_{nitro}), either singly or in conjunction with associated bonded atoms, with the best correlations involving the average ESP and/or the maximum value of the ESP. We found no universal correlation for both aromatic and nonaromatic species. Therefore, we attempted to ascertain whether individual correlations could be realized for aromatic and nonaromatic species.

A sample correlation is shown in figure 1, where the average of the average positive ESP for the nitro nitrogens (for nonaromatics) and average Σ^+ for the nitro nitrogens *plus* the average Σ^+ for the aromatic carbons (for aromatics) are correlated to impact sensitivity (methods A and B). In this fit, a simple exponential fit ($y = a * e^{bx}$) is used to determine the correlation parameters. Figure 2 illustrates the same data, with the inclusion of the test set data. The sole nonaromatic test point (BTAT) agrees well with the nonaromatic fit, while the aromatic test data displays a large error for this particular fit. As stated previously, this trend of poor predictive capability for the aromatic compounds holds true for every fit attempted in this study regardless of Politzer parameter or atom/group type (see the appendix). The two best nonaromatic fits are listed in table 3, where both fits are based off of average Σ^{tot} values (either nitro nitrogen or the entire nitro group). With the large deviations from fitting occurring with the aromatic compounds, the remainder of this report shall focus on these.

Similar to table 3, table 4 contains fits for nonaromatic species, with simple exponential fits ($y = a * e^{bx}$) of the average Σ^{tot} values for the nitro nitrogen or the entire nitro group (*plus* the average Σ^{tot} values for the associated aromatic carbon) compared to experiment methods C and D). The modification to the full nitro group in method D substantially worsens the error for the training set molecules relative to method C, with an approximate 30- to 40-cm increase in mean and absolute mean errors. However, the absolute mean errors for the test set molecules are in closer agreement, with method C exhibiting a 43-cm absolute error vs. a 36-cm absolute error for method D. In general, both methods underpredict the impact sensitivities vs. experimental values.

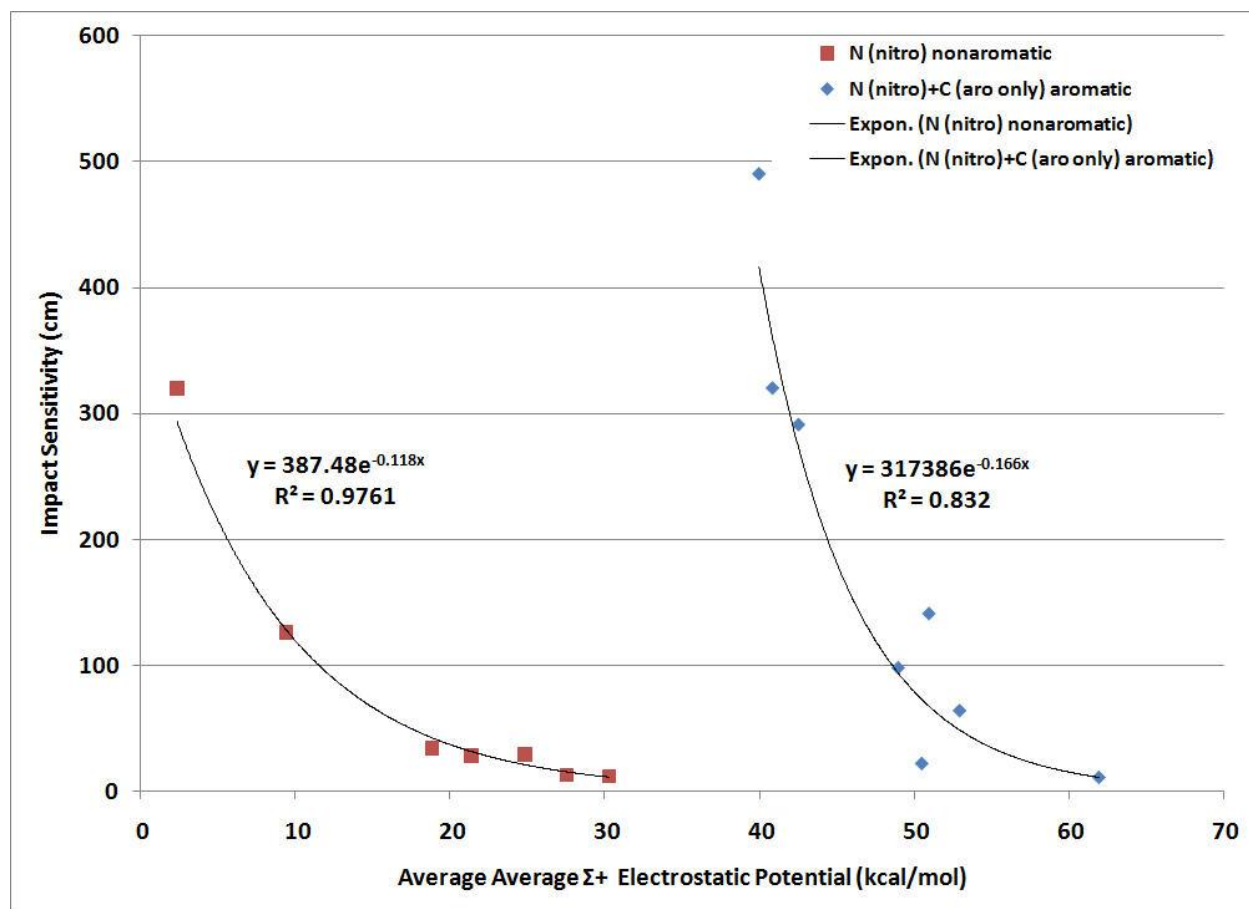


Figure 1. Impact sensitivity (cm) vs. average average Σ+ ESP (kcal/mol) for (1) nitro nitrogens for nonaromatic species and (2) nitro nitrogen plus associated aromatic carbons for aromatic species for PBE/6-31G**. Exponential fits with associated R^2 factors included.

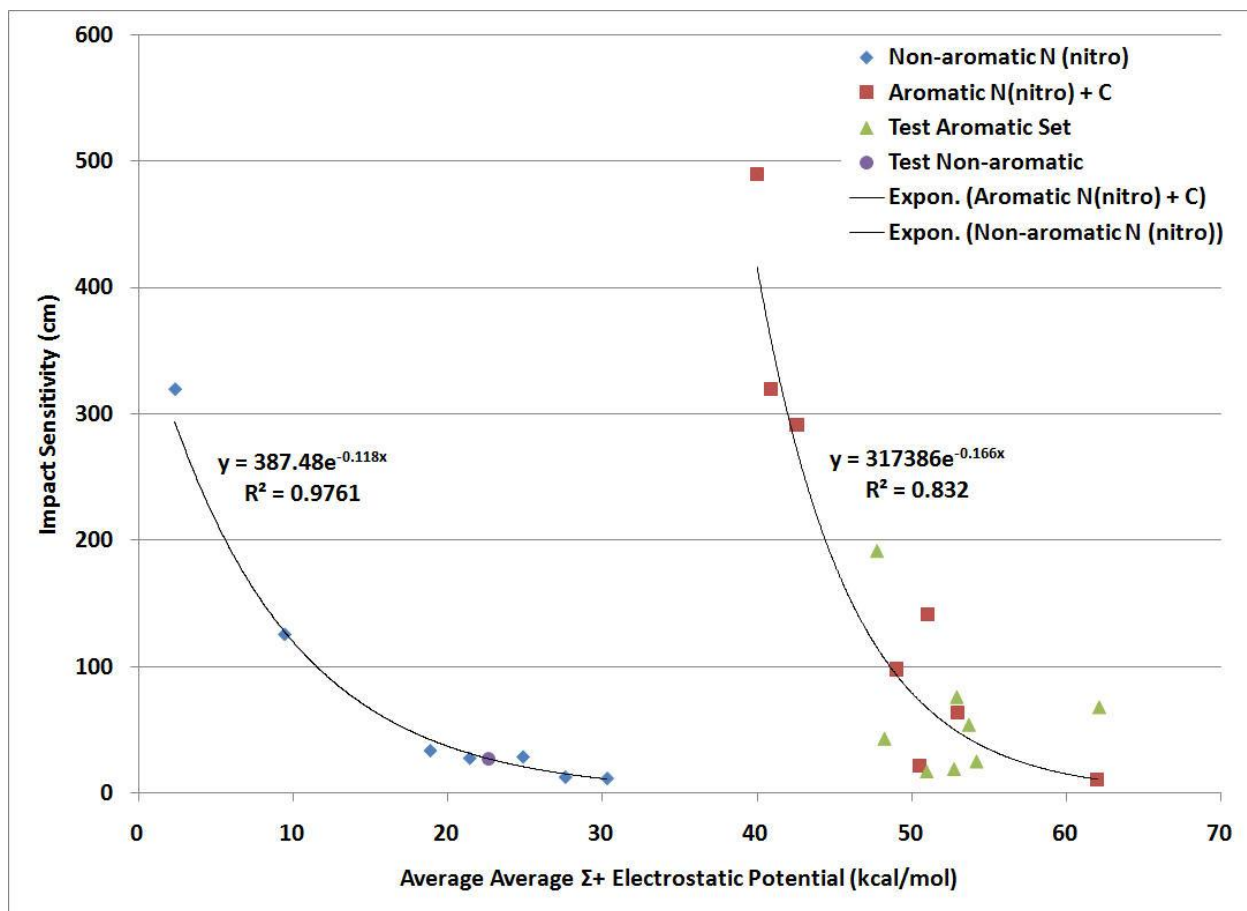


Figure 2. Impact sensitivity (cm) vs. average average Σ^+ ESP (kcal/mol) for (1) nitro nitrogens for nonaromatic species and (2) nitro nitrogen plus associated aromatic carbons for aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

Table 3. Comparison of predicted-to-experiment impact sensitivities for nonaromatic species (derived from PBE/6-31G** data).

Molecule	Experimental Sensitivity (cm)	Method A Predicted Sensitivity (cm)	Method A Error (% Error)	Method B Predicted Sensitivity (cm)	Method B Error (% Error)
Training Set					
FOX7	126	110.3	-15.7 (-12.4)	106.7	-19.3 (-15.4)
HMX	29	21.7	-7.3 (-25.1)	21.4	-7.6 (-26.0)
PETN	13	15.2	2.2 (17.0)	12.7	-0.3 (-2.7)
EDNA	34	38.2	4.2 (12.3)	44.9	10.9 (32.0)
NQ	320	343.5	23.5 (7.4)	309.2	-10.8 (-3.4)
RDX	28	29.5	1.5 (5.2)	36.6	8.6 (30.7)
CL20	12	12.0	0.01 (0.08)	11.9	-0.1 (-1.0)
Test Set					
BTAT	22.1	26.9	4.8 (21.6)	13.1	-9.0 (-40.7)

Notes: Method A: Predicted sensitivity = $189.57 \cdot e^{-0.092x}$, where x is the average average Σ_{tot} for nitro nitrogens.

Method B: Predicted sensitivity = $14.117 \cdot e^{-0.109x}$, where x is the average average Σ_{tot} for nitro groups.

Table 4. Comparison of one-parameter predicted-to-experiment impact sensitivities for aromatic species (derived from PBE/6-31G** data) for nitro nitrogens and nitro groups (both plus associated aromatic carbon).

Molecule	Experimental Sensitivity (cm)	Method C Predicted Sensitivity (cm)	Method C Error (% error)	Method D Predicted Sensitivity (cm)	Method D Error (% Error)
Training Set					
HNB	11	9.3	-1.7 (-15.2)	34.0	23.0 (209.5)
PNA	22	72.7	50.7 (230.3)	137.1	115.2 (523.4)
Picric acid	64	42.8	-21.2 (-33.1)	31.3	-32.6 (-51.0)
TNT	98	88.2	-9.8 (-10.0)	39.3	-58.6 (-59.8)
TNA	141	122.6	-18.4 (-13.1)	126.7	-14.3 (-10.1)
NTO	291	255.2	-35.8 (-12.3)	228.2	-62.8 (-21.6)
DATB	320	337.9	17.9 (5.6)	184.2	-135.8 (-42.4)
TATB	490	395.3	-94.7 (-19.3)	325.9	-164.1 (-33.5)
Mean	—	—	-14.1	—	-41.2
Absolute mean	—	—	31.3	—	75.8
Standard dev.	—	—	42.1	—	88.0
Test Set					
CL16	17	74.9	57.2 (340.7)	7.6	-9.4 (-55.1)
Picryl azide	19	52.9	33.9 (178.2)	32.7	13.7 (71.9)
Tetryl	25	49.1	24.1 (96.5)	12.0	-13.0 (-52.1)
Styphnic acid	43	113.7	70.7 (164.4)	39.3	-3.7 (-8.6)
HNS	54	45.5	-8.4 (-15.6)	32.4	-21.6 (-39.9)
Tri245	68	11.3	-56.7 (-83.4)	6.3	-61.6 (-90.7)
DNBF	76	54.5	-21.5 (-28.3)	31.5	-44.5 (-58.5)
Methyl picrate	192	123.6	-68.4 (-35.6)	67.4	-124.6 (-64.9)
Mean	—	—	3.9	—	-33.1
Absolute mean	—	—	42.6	—	36.5
Standard dev.	—	—	51.1	—	43.9

Notes: Method C: Predicted sensitivity = $284413 \cdot e^{-0.167x}$, where x is the average average Σ_{tot} for nitro nitrogens plus associated aromatic carbon.

Method D: Predicted sensitivity = $3280.6 \cdot e^{-0.186x}$, where x is the average average Σ_{tot} for nitro groups plus associated aromatic carbon.

Marginally improved predictive capability can be obtained with correlations derived from the explicit X-N (from the nitro group) subgroup Politzer statistics as illustrated in table 5. Four one-parameter methods are explored, using the forms $y = a * e^{bx}$, $y = y_0 + a * e^{bx}$, $y = a * b / (b + x)$, and $y = y_0 + a * b / (b + x)$. All four fits use the average Σ^{tot} values for the X-N_{nitro} as the x parameter, with the sensitivity indicated by y . Each fit has similar R^2 values for both the fitting (0.92, 0.93, 0.91, 0.93) and test sets (0.55, 0.56, 0.52, 0.49). For each of the four methods in table 5, the mean errors for the fitting set were all uniformly small (~6 cm or less), with absolute errors ranging from 36 to 40 cm. Method E performed the best for the test set, both within this series of methods as well as overall, with a mean error of 4 cm and a mean absolute error of 29 cm. Method F was almost as good a predictor for the test suite, with a mean error and absolute mean error of 6 and 30 cm, respectively. The two hyperbolic functions (methods G and H) did not perform as well, with larger errors displayed for the test set. Additionally, because of their functional form, hyperbolic functions can result in values less than zero. Method H suffers from such a failure of the functional form with a -2 cm predicted sensitivity value for HNB.

Finally, to improve upon these correlations, fits involving two parameters were attempted. Table 6 illustrates the three fits essayed, with the forms $y = y_0 + a * e^{bx} + c * e^{dz}$, $y = y_0 + a * b / (b + x) + c * d / (d + z)$, and $y = a * b / (b + x) + c * d / (d + z)$. Each of the two parameter fits used the average Σ^{tot} values for the X-N_{nitro} as the x parameter and the maximum V^+ for the X-N_{nitro} as the z parameter. The two hyperbolic functions (methods J and K) yielded marginally better R^2 values (0.97 for the fitting set and 0.53 for the training set for both) than the exponential fit (method I) (0.93 and 0.38 for the fitting and test sets, respectively). While the three methods exhibited small statistical errors in the training set, two displayed significant overall issues.

In a similar manner to method H, method J failed as a predictive tool because of the hyperbolic functional form. However, method J failed most spectacularly with a predicted *infinite* impact value for NTO (experimental value of 291 cm). In addition to potential negative values stated previously, the hyperbolic functional form is suspect to catastrophic failure as the denominator approaches zero. For NTO, the maximum V^+ for the explicit X-N_{nitro} is of the exact same magnitude as the d parameter (29.7509). This causes the ruinous predicted infinite value for NTO. Another potential failure for two parameter additive functions, dependant on the signs of the parameters, is the possibility of obtaining negative impact sensitivities; this possibility is seen in method I (the two-parameter exponential fit), which predicted an impact value of -60 cm for CL16 (experimental value of 17 cm). Of the three two-parameter fits discussed here, only method K yielded a “viable” correlation. However, it suffers the same potential fate as method J—chiefly, apocalyptic failure due to its hyperbolic form.

Table 5. Comparison of one-parameter predicted-to-experiment impact sensitivities for aromatic species (derived from PBE/6-31G** data) for explicit X-N of nitro groups.

Molecule	Experimental Sensitivity (cm)	Method E Predicted Sensitivity (cm)	Method E Error (% Error)	Method F Predicted Sensitivity (cm)	Method F Error (% Error)	Method G Predicted Sensitivity (cm)	Method G Error (% Error)	Method H Predicted Sensitivity (cm)	Method H Error (% Error)
Training Set									
HNB	11	3.4	-7.6 (-69.2)	10.5	-0.5 (-4.8)	40.3	29.3 (266.4)	-1.6	-12.6 (-114.4)
PNA	22	36.4	14.3 (65.2)	39.7	17.7 (80.5)	72.5	50.5 (229.7)	50.6	28.6 (130.1)
Picric acid	64	66.8	2.8 (4.3)	68.1	4.1 (6.4)	91.2	27.2 (42.5)	79.0	15.0 (23.4)
TNT	98	161.1	63.1 (64.4)	159.3	61.3 (62.6)	145.6	47.6 (48.6)	154.4	56.4 (57.6)
TNA	141	91.2	-49.8 (-35.3)	91.4	-49.6 (-35.2)	105.1	-35.9 (-25.4)	99.2	-41.8 (-29.6)
NTD	291	234.6	-56.4 (-19.4)	232.2	-58.8 (-20.2)	195.2	-95.8 (-32.9)	215.4	-75.6 (-26.0)
DATB	320	383.1	63.1 (19.7)	382.7	62.7 (19.6)	351.7	31.7 (9.9)	370.4	50.4 (15.7)
TATB	490	452.8	-37.2 (-7.6)	454.4	-35.6 (-7.3)	483.9	-6.1 (-1.2)	469.6	-20.4 (-4.2)
Mean	—	—	-1.0	—	0.2	—	6.1	—	-0.001
Absolute mean	—	—	36.8	—	36.3	—	40.5	—	37.6
Standard dev.	—	—	46.7	—	46.6	—	50.2	—	46.0
Test Set									
CL16	17	38.9	21.9 (128.7)	42.0	25.0 (147.2)	74.2	57.2 (336.5)	53.2	36.2 (213.1)
Picryl azide	19	71.3	52.3 (275.4)	72.4	53.4 (281.0)	93.8	74.8 (393.9)	82.9	63.9 (336.1)
Tetryl	25	33.7	8.7 (34.91)	37.3	12.3 (49.2)	70.7	45.7 (183.0)	47.8	22.8 (91.4)
Styphic acid	43	91.9	48.9 (113.6)	92.0	49.0 (113.9)	105.5	62.5 (145.3)	99.7	56.7 (132.0)
HNS	54	55.0	1.0 (1.9)	57.0	3.0 (5.6)	84.3	30.3 (56.1)	68.6	14.6 (27.1)
tri245	68	21.6	-46.4 (-68.3)	26.3	-41.7 (-61.4)	61.7	-6.3 (-9.3)	33.5	-34.5 (-50.7)
DNBF	76	77.5	1.5 (2.0)	78.3	2.3 (3.0)	97.4	21.4 (28.2)	88.1	12.1 (15.9)
Methyl picrate	192	140.1	-51.9 (-27.0)	138.7	-53.3 (-27.8)	133.0	-59.0 (-30.7)	137.8	-54.2 (-28.2)
Mean	—	—	4.5	—	6.2	—	28.3	—	14.7
Absolute mean	—	—	29.1	—	30.0	—	44.7	—	36.8
Standard dev.	—	—	38.5	—	38.4	—	43.7	—	41.2

Notes: Method E: Predicted sensitivity = $106086.8513e^{-0.2749x}$, where x is the average average Σ_{tot} for the explicit X-N subgroups of the nitro groups.

Method F: Predicted sensitivity = $7.8043 + 134622.3047e^{-0.2876x}$, where x is the average average Σ_{tot} for the explicit X-N subgroups of the nitro groups.

Method G: Predicted sensitivity = $a*b/(b+x)$ as the form of the equation and with $a = -42.9343$ and $b = -18.2317$, where x is the average average Σ_{tot} for the explicit X-N subgroups of the nitro groups.

Method H: Predicted sensitivity = $y_0 + a*b/(b+x)$ as the form of the equation and with $y_0 = -73.5168$, $a = -86.1842$, and $b = -17.1309$, where x is the average average Σ_{tot} for the explicit X-N subgroups of the nitro groups.

Table 6. Comparison of two-parameter predicted-to-experiment impact sensitivities for aromatic species (derived from PBE/6-31G** data) for explicit X-N of nitro groups.

Molecule	Experimental Sensitivity (cm)	Method I Predicted Sensitivity (cm)	Method I Error (% Error)	Method J Predicted Sensitivity (cm)	Method J Error (% Error)	Method K Predicted Sensitivity (cm)	Method K Error (% Error)
Training Set							
HNB	11	0.2	-10.8 (-97.8)	20.5	9.5 (86.4)	29.8	18.8 (171.1)
PNA	22	18.1	-3.9 (-17.5)	49.1	27.1 (123.1)	54.7	32.7 (148.8)
Picric acid	64	116.6	52.6 (82.2)	66.0	2.0 (3.1)	69.7	5.7 (8.8)
TNT	98	115.4	17.4 (17.7)	116.5	18.5 (18.9)	115.1	17.1 (17.4)
TNA	141	89.7	-51.3 (-36.4)	78.7	-62.3 (-44.2)	81.0	-60.0 (-42.6)
NTO	291	224.3	-66.7 (-22.9)	NaN	NaN	248.7	-42.3 (-14.6)
DATB	320	370.8	50.8 (15.9)	329.2	9.2 (2.9)	320.8	0.8 (0.3)
TATB	490	461.7	-28.3 (-5.8)	486.0	-4.0 (-0.8)	489.7	-0.3 (-0.1)
Mean	—	—	-5.0	—	-.0002	—	-3.4
Absolute mean	—	—	35.2	—	18.9	—	22.2
Standard dev.	—	—	43.8	—	29.3	—	31.8
Test Set							
CL16	17	-59.6	-76.6 (-450.7)	50.6	33.6 (197.6)	56.1	39.1 (229.8)
Picryl azide	19	24.2	5.2 (27.1)	68.4	49.4 (259.9)	71.8	52.8 (277.8)
Tetryl	25	74.6	49.6 (198.4)	47.5	22.5 (89.9)	53.3	28.3 (113.3)
Stylphic acid	43	152.4	109.4 (254.5)	79.0	36.0 (83.8)	81.3	38.3 (89.0)
HNS	54	130.5	76.5 (141.8)	59.7	5.7 (10.6)	64.1	10.1 (18.7)
tri245	68	64.0	-4.0 (-5.9)	39.4	-28.6 (-42.1)	46.2	-21.8 (-32.0)
DNBF	76	165.6	89.6 (117.8)	71.6	-4.4 (-5.8)	74.7	-1.3 (-1.8)
Methyl picrate	192	169.4	-22.6 (-11.8)	104.6	-87.4 (-45.5)	104.3	-87.7 (-45.7)
Mean	—	—	28.4	—	3.3	—	7.2
Absolute mean	—	—	54.2	—	33.4	—	34.9
Standard dev.	—	—	63.6	—	44.4	—	45.4

Method I: Predicted sensitivity = $y_0 + a \cdot \exp(-b \cdot x) + c \cdot \exp(-d \cdot z)$ as the form of the equation and with $y_0 = -4643.0357$, $a = 57070071804.3329$, $b = 0.9694$, $c = 5124.2966$, and $d = 0.0019$, where x is the average average Σ_{tot} and z is the maximum $V+$ for the explicit X-N subgroups of the nitro groups.

Method J: Predicted sensitivity = $y_0 + a \cdot b / (b + x) + c \cdot d / (d + z)$ as the form of the equation and with $y_0 = -14.28$, $a = -35.9446$, $b = -18.5189$, $c = 0.0001$, and $d = -29.7509$, where x is the average average Σ_{tot} and z is the maximum $V+$ for the explicit X-N subgroups of the nitro groups.

Method K: Predicted sensitivity = $a \cdot b / (b + x) + c \cdot d / (d + z)$ as the form of the equation and with $a = -30.2474$, $b = -18.6947$, $c = 0.0003$, and $d = -29.751$, where x is the average average Σ_{tot} and z is the maximum $V+$ for the explicit X-N subgroups of the nitro groups.

Of the nine correlations determined for aromatic species, methods E and F yielded the most accurate fits. Both methods are single parameter fits of the average Σ^{tot} values for the explicit X-N_{nitro} using an exponential fit. Though these two methods yielded the most accurate fits, they both exhibited prohibitively large errors, underestimating the sensitivity of several sensitive compounds by ~50 cm on experimental values of 19 and 43 cm (picryl azide and styphnic acid) while overestimating the $h_{50\%}$ of tri245, with a predicted $h_{50\%}$ of 22 and 26 cm (methods E and F, respectively) vs. an experimental value of 68 cm. While errors on the order of 5–10 cm would have been acceptable, errors of 20–50 cm are not. All methods reported here and in the appendix did not yield any correlation that achieved such desired accuracy.

4. Conclusions

In this article, we applied the concept of Bader’s atoms-in-molecules atomic basins in an attempt to partition the ESP into atom-specific areas and correlate the resultant data to impact sensitivity. While many correlations were attempted, no accurate quantitative correlations were found for aromatic compounds. Several approximate correlations were determined, but all exhibited limited predictive capability. Attempts at using area-weighted parameters yielded negligible differences compared to the nonweighted parameters. While atom-centered partitioning has not yielded accurate correlations, an emerging theory of irreducible bundles by Dr. Eberhart could potentially offer a partitioning scheme producing viable correlations of electrostatic parameters with impact sensitivities (40–42). Irreducible bundles have the attractive property of describing the electron densities centered on bonds vs. the Bader atom description studied in this work, which is centered on atoms. The ability to correlate sensitivity directly to the properties of the bonds could yield a viable methodology to predict sensitivity of energetic materials.

5. References

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**Appendix. Supplemental Figures and Tables Documenting Descriptors and
Attempted Correlations to Impact Sensitivity**

The following figures document for archival purposes:

- the atomic designation,
- the atom or group Politzer descriptors derived from partitioned Bader AIM atomic basins,
- the additive or difference of said Politzer parameters, and
- the most successful correlations found to impact sensitivity.

The data is broken up into training set and test set molecules for both graphs (at aid in visual determination of potential correlations) as well as in table format.

A.1 Training Set Molecules

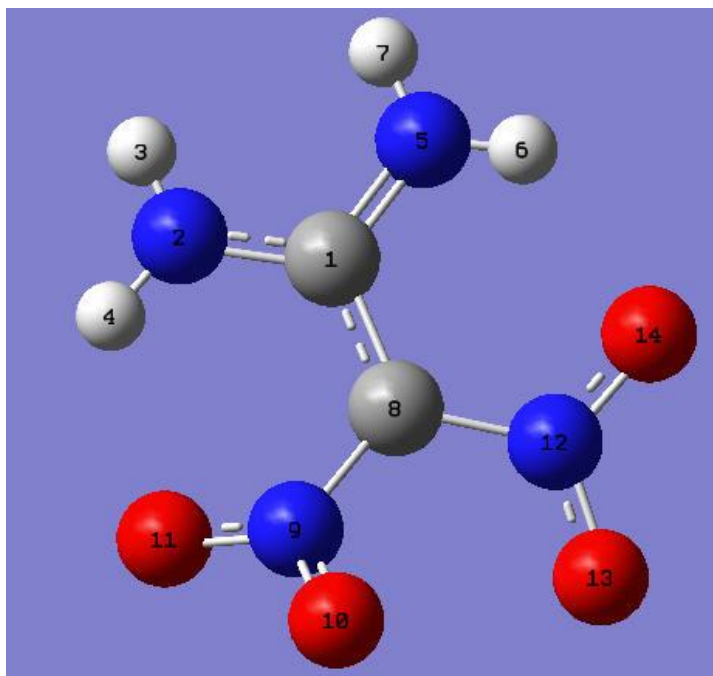


Figure A-1. FOX-7 with atoms labeled.

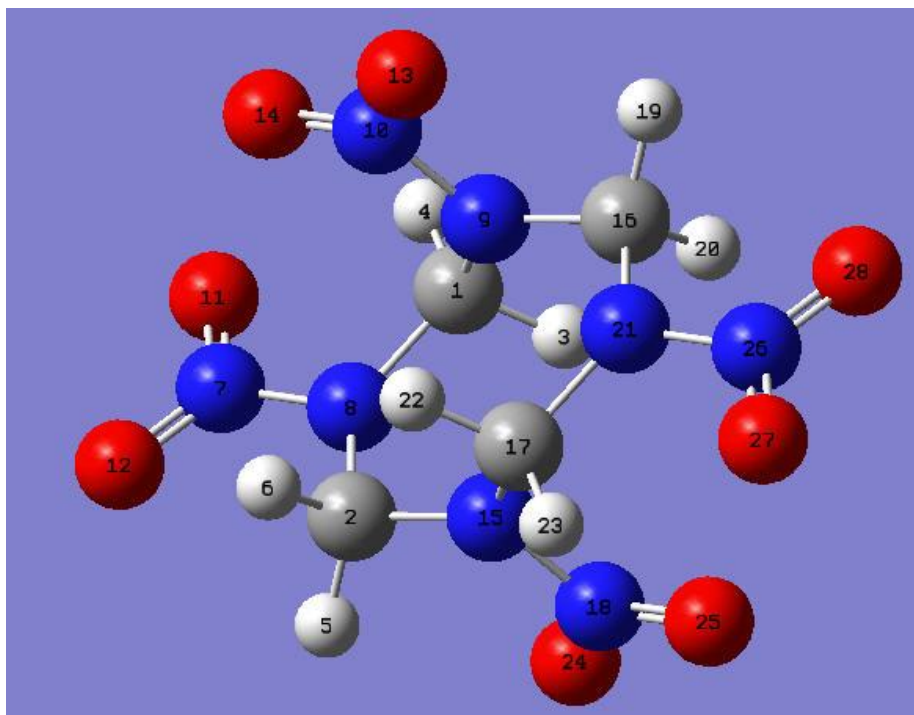


Figure A-2. HMX with atoms labeled.

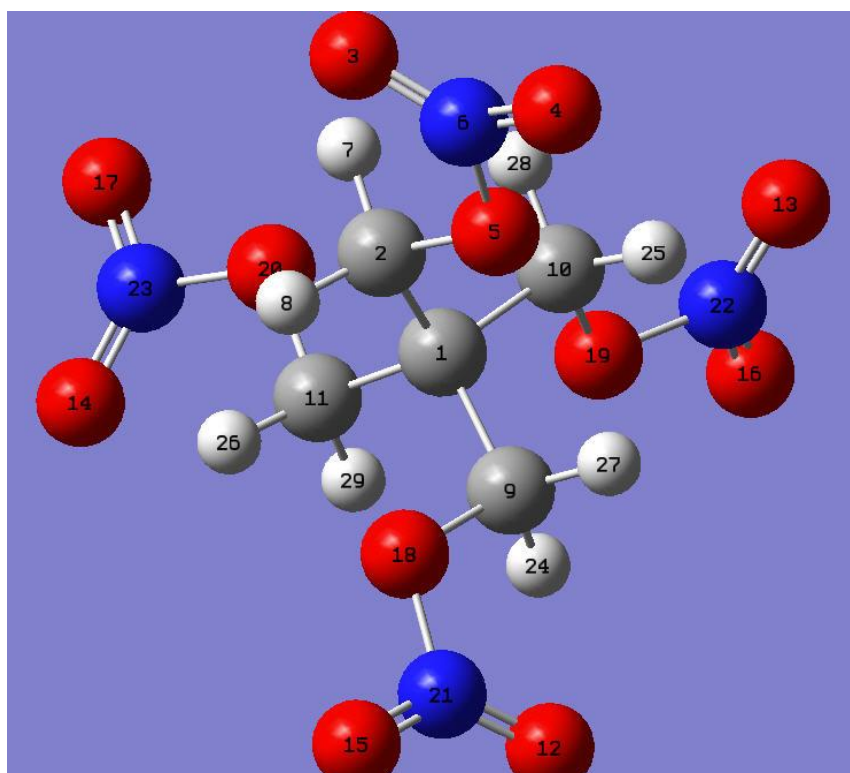


Figure A-3. PETN with atoms labeled.

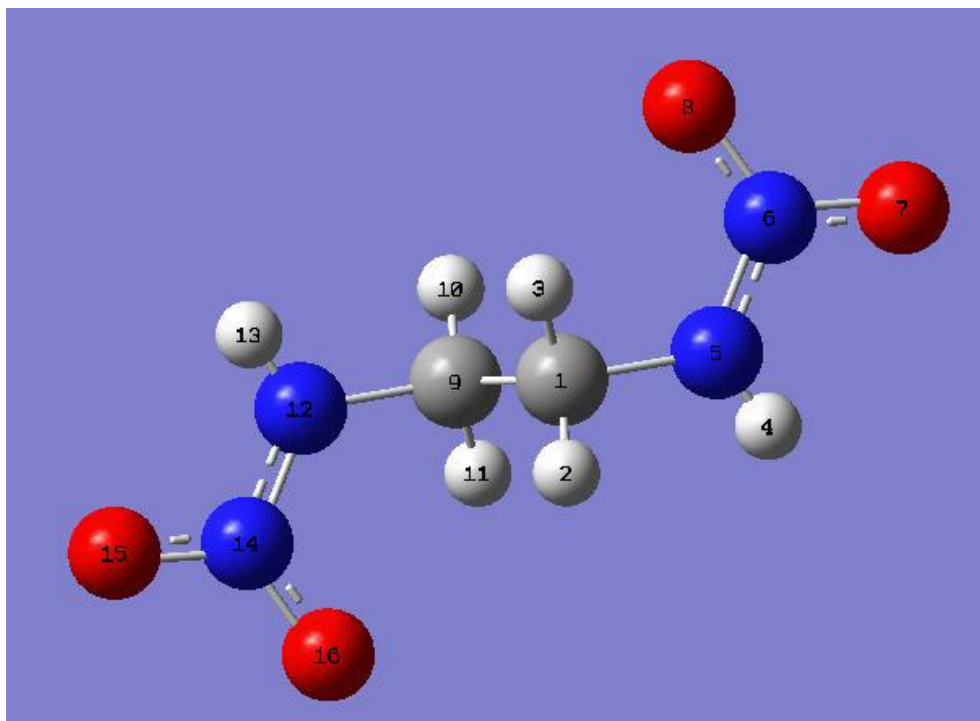


Figure A-4. EDNA with atoms labeled.

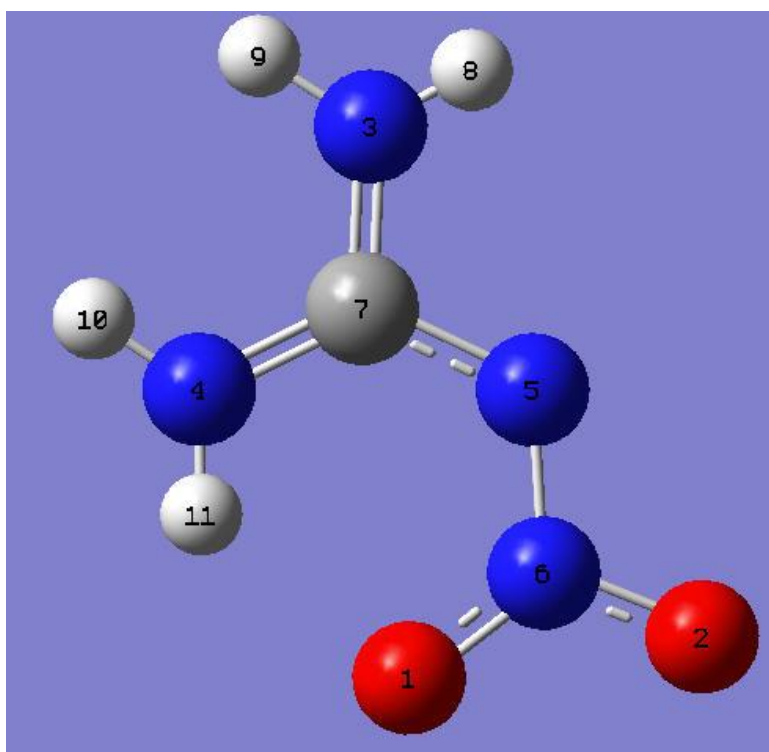


Figure A-5. NQ with atoms labeled.

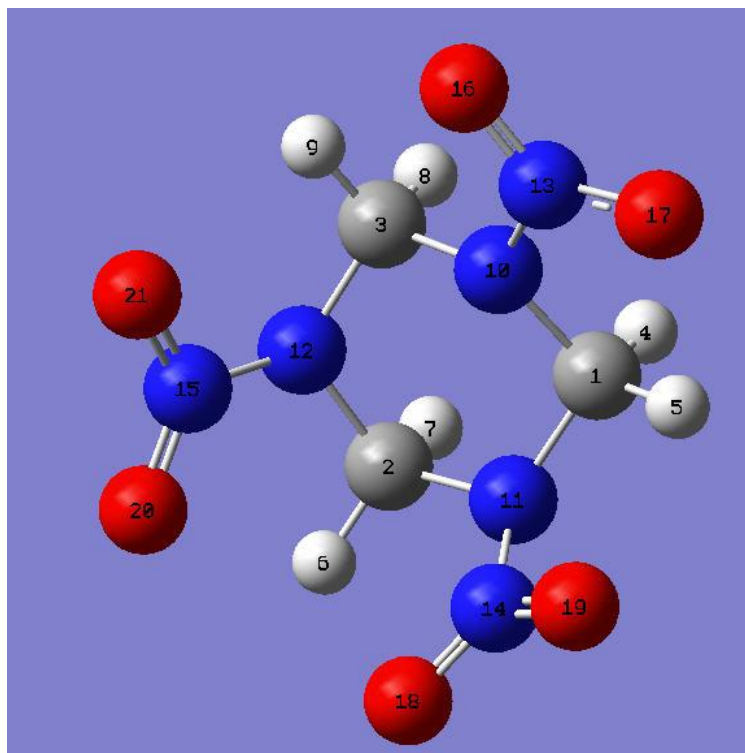


Figure A-6. RDX with atoms labeled.

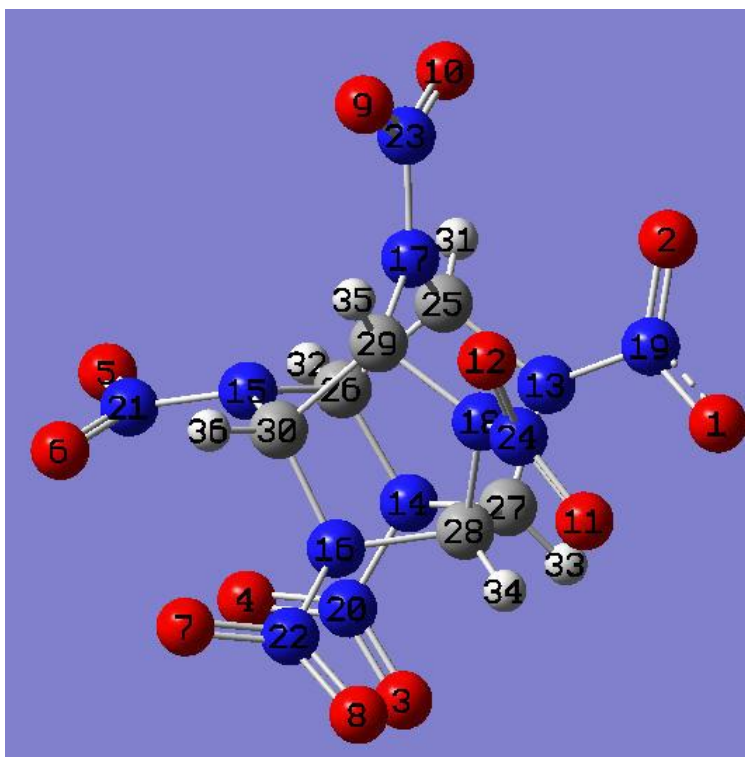


Figure A-7. CL20 with atoms labeled.

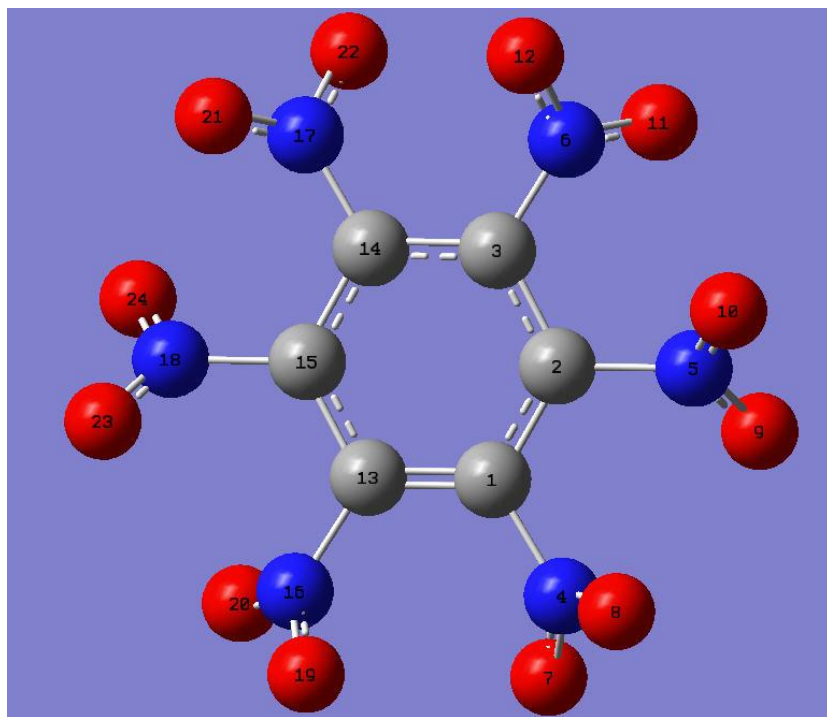


Figure A-8. HNB with atoms labeled.

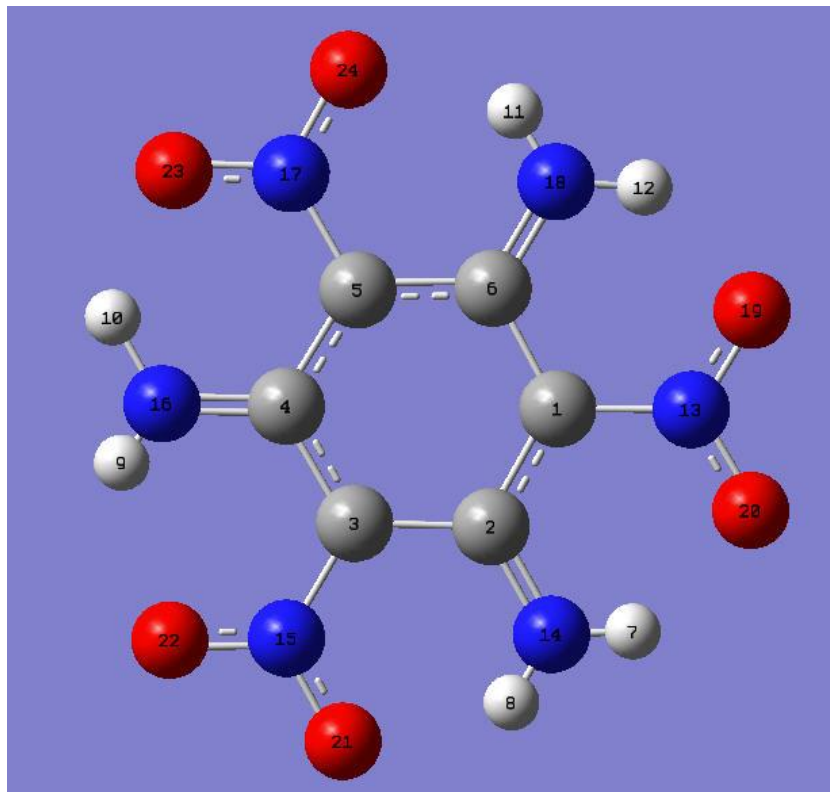


Figure A-9. TATB with atoms labeled.

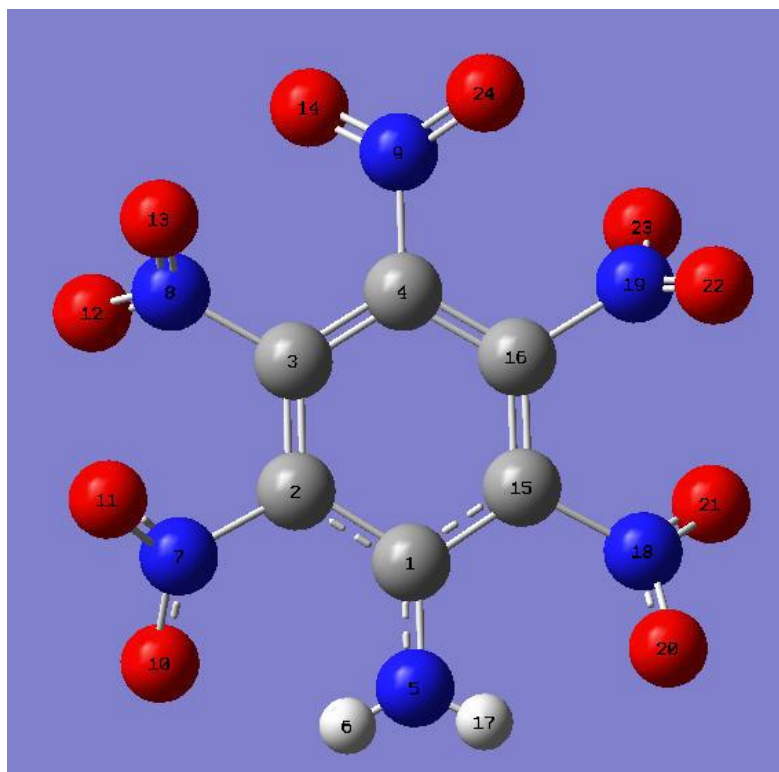


Figure A-10. PNA with atoms labeled.

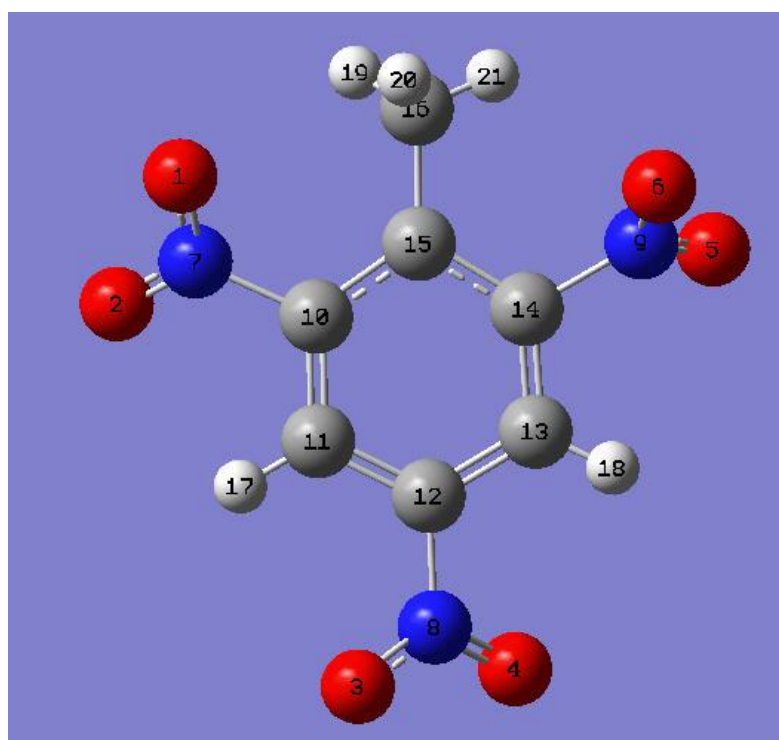


Figure A-11. TNT with atoms labeled.

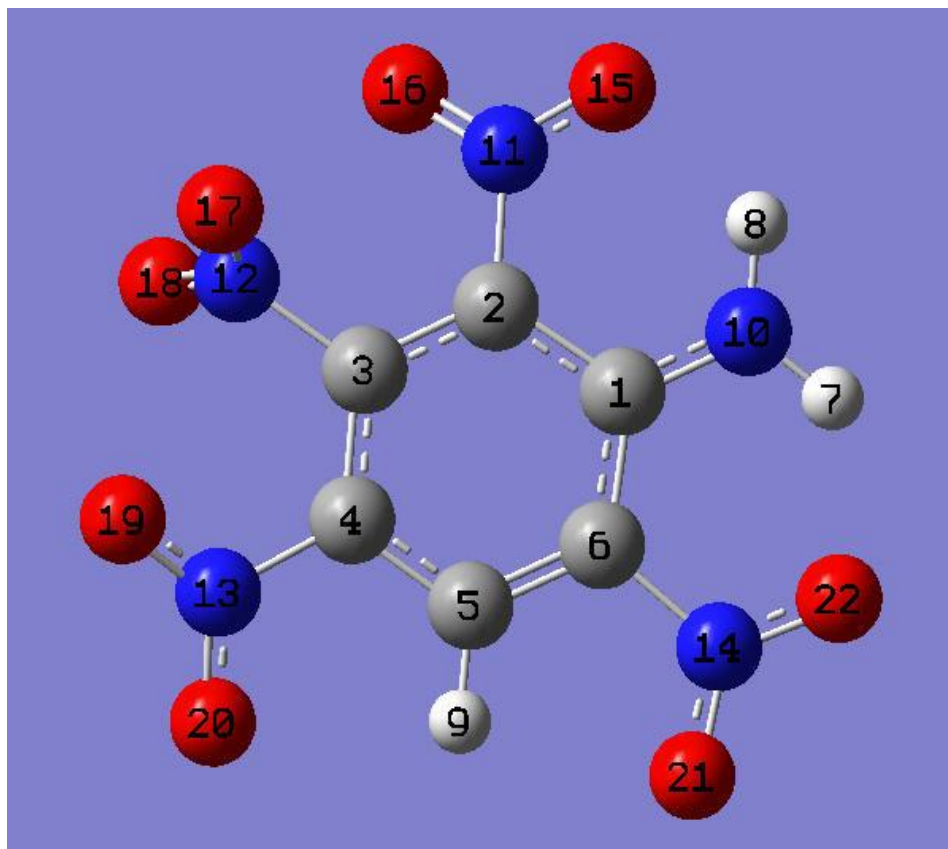


Figure A-12. TNA with atoms labeled.

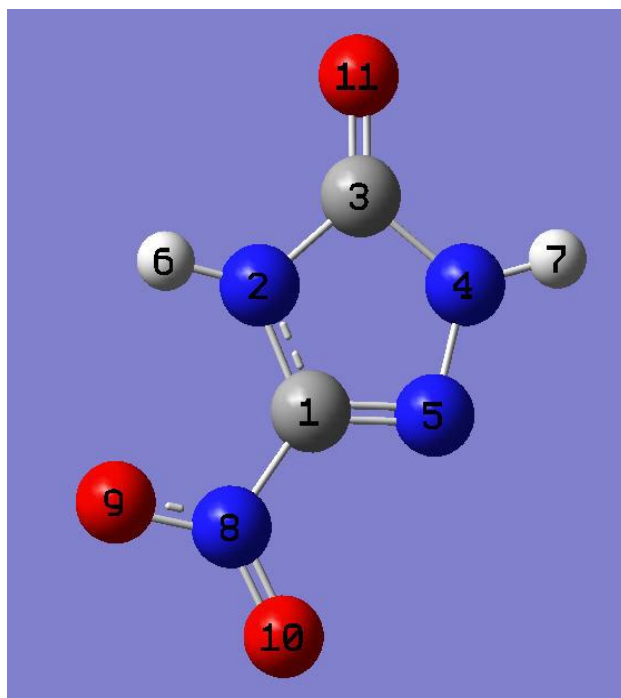


Figure A-13. NTO with atoms labeled.

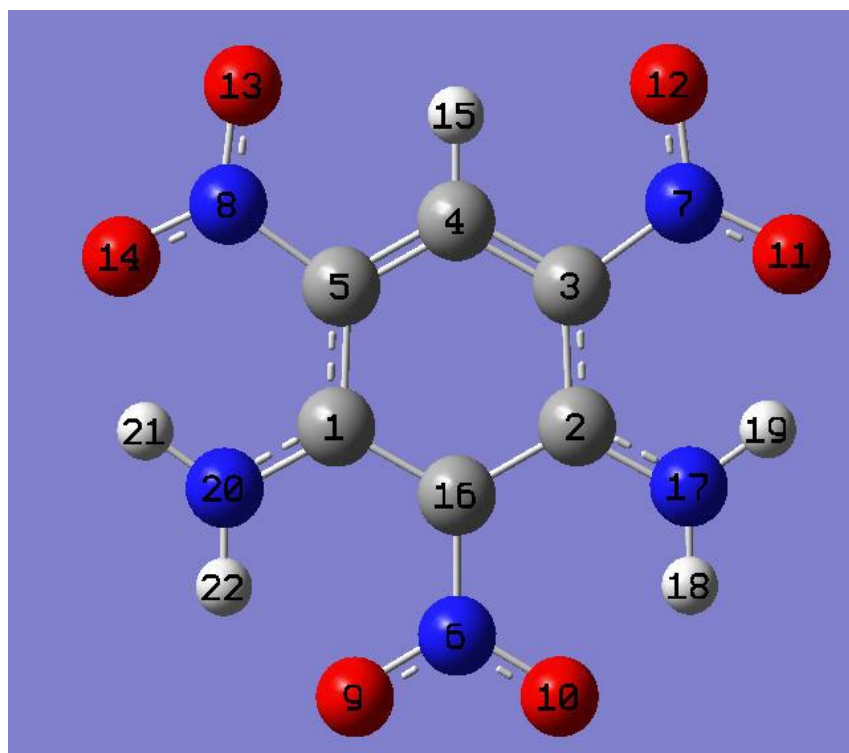


Figure A-14. DATB with atoms labeled.

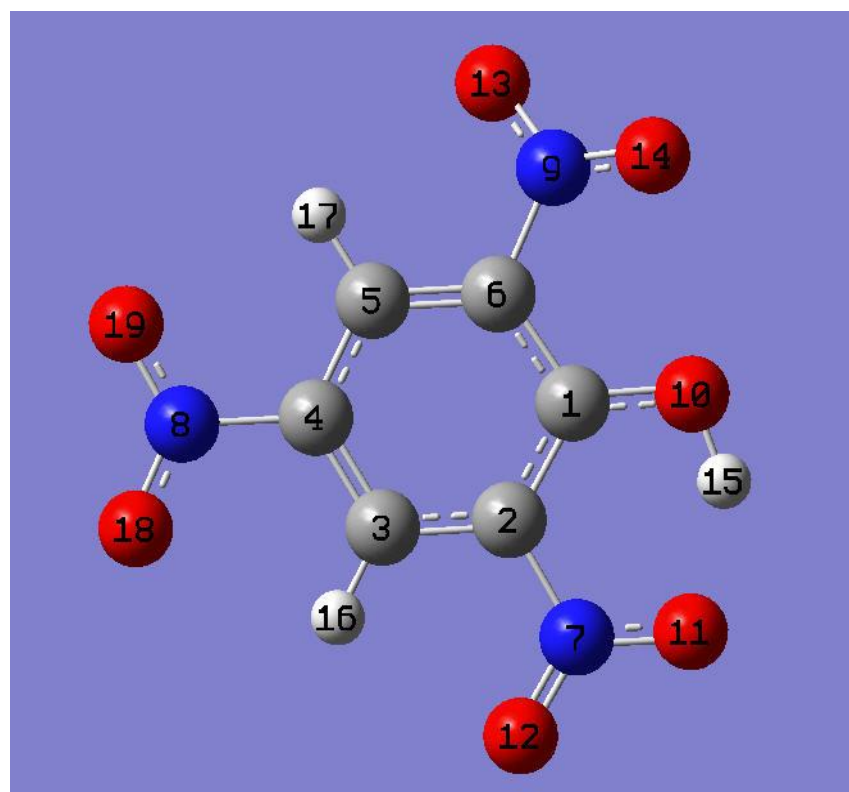


Figure A-15. Picric acid with atoms labeled.

A.2 Test Set Molecules

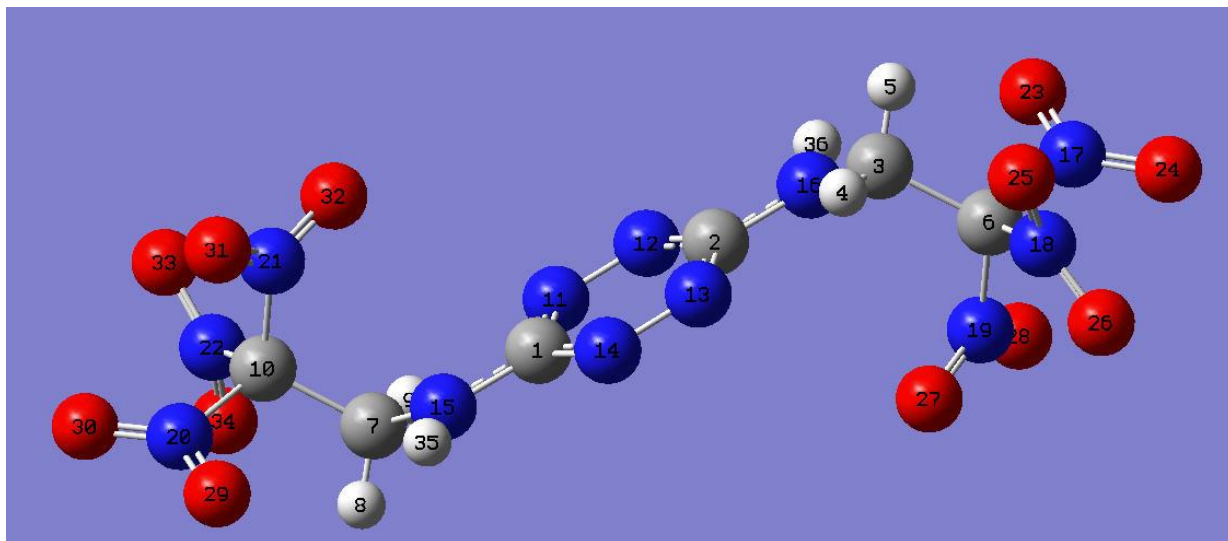


Figure A-16. BTAT with atoms labeled.

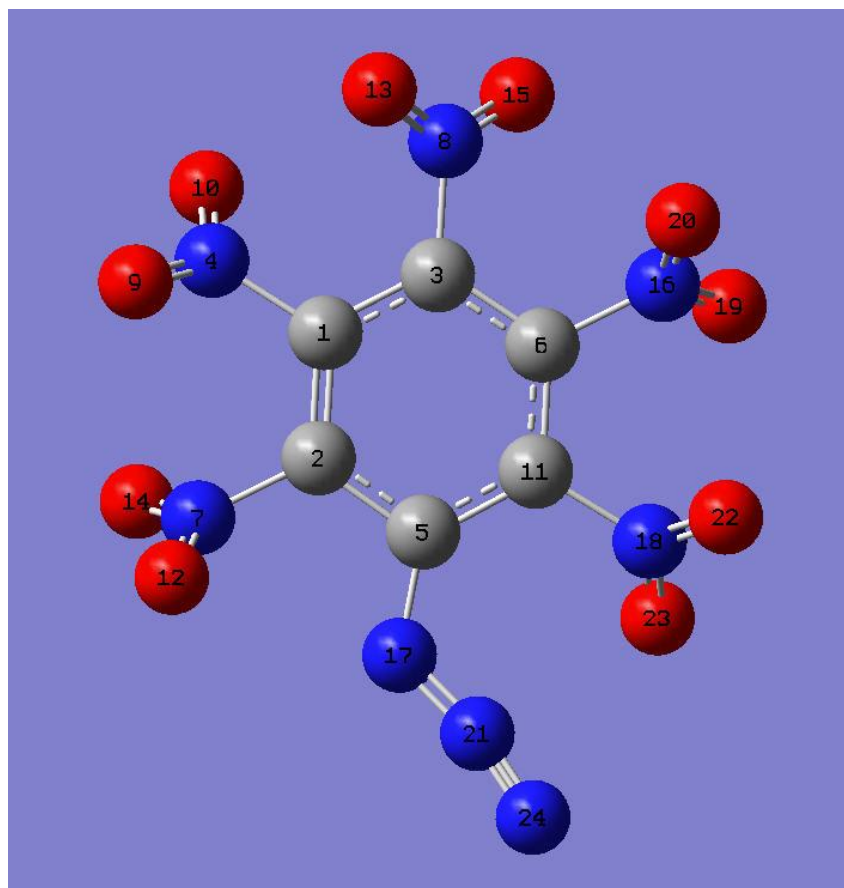


Figure A-17. CL16 with atoms labeled.

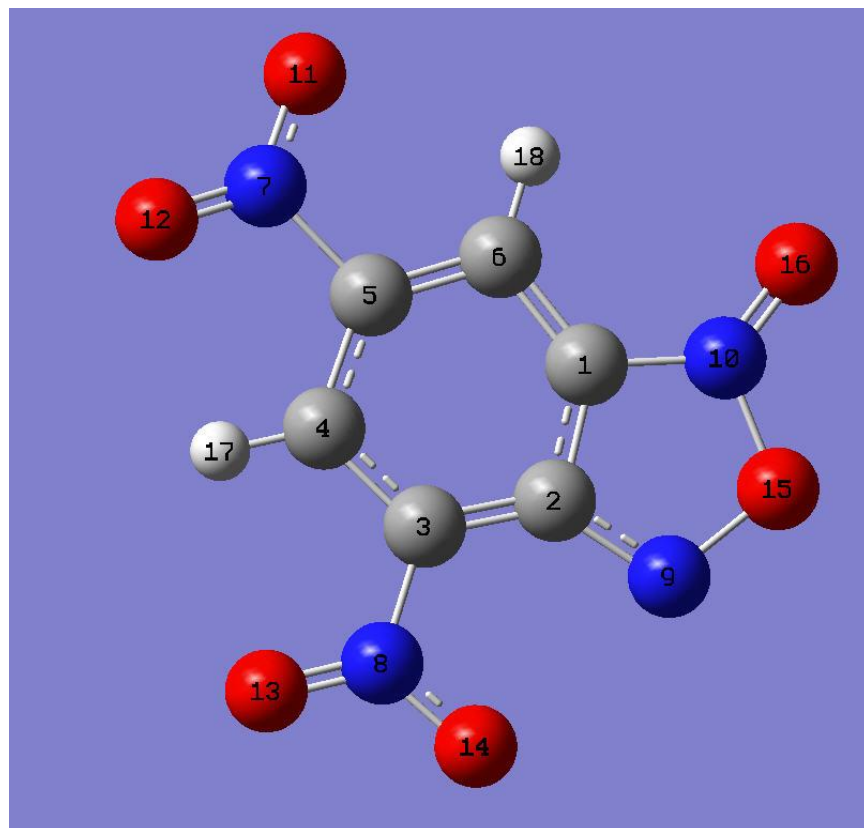


Figure A-18. DNBF with atoms labeled.

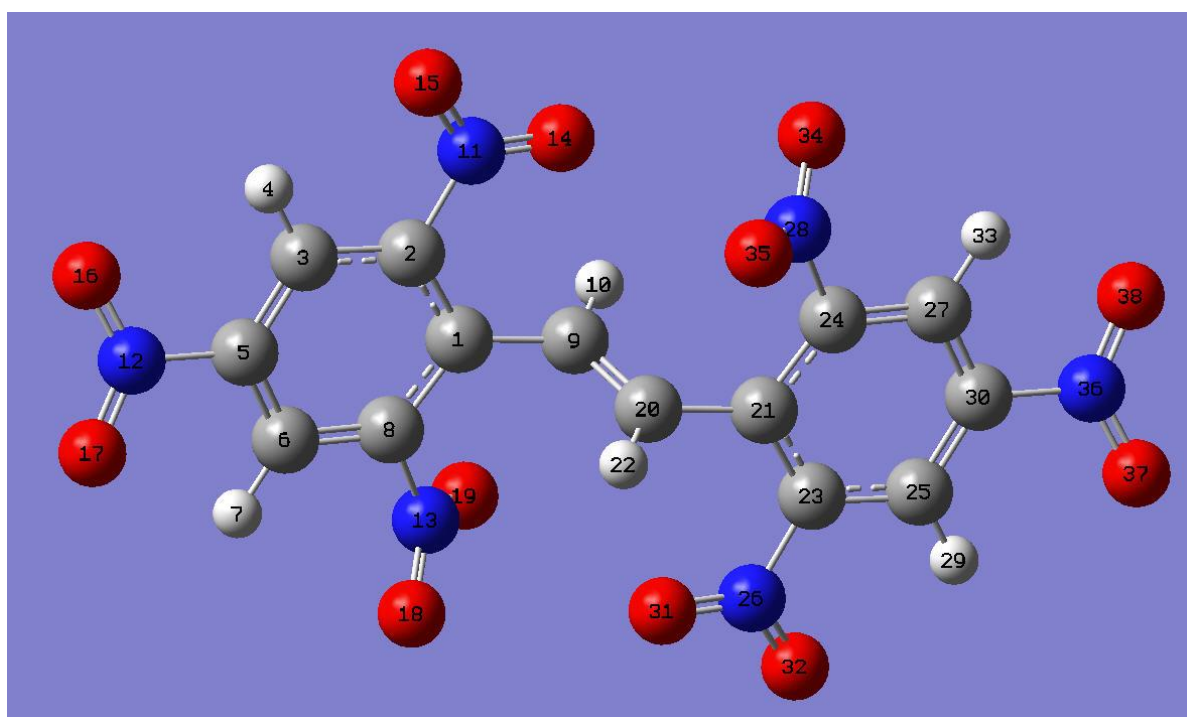


Figure A-19. HNS with atoms labeled.

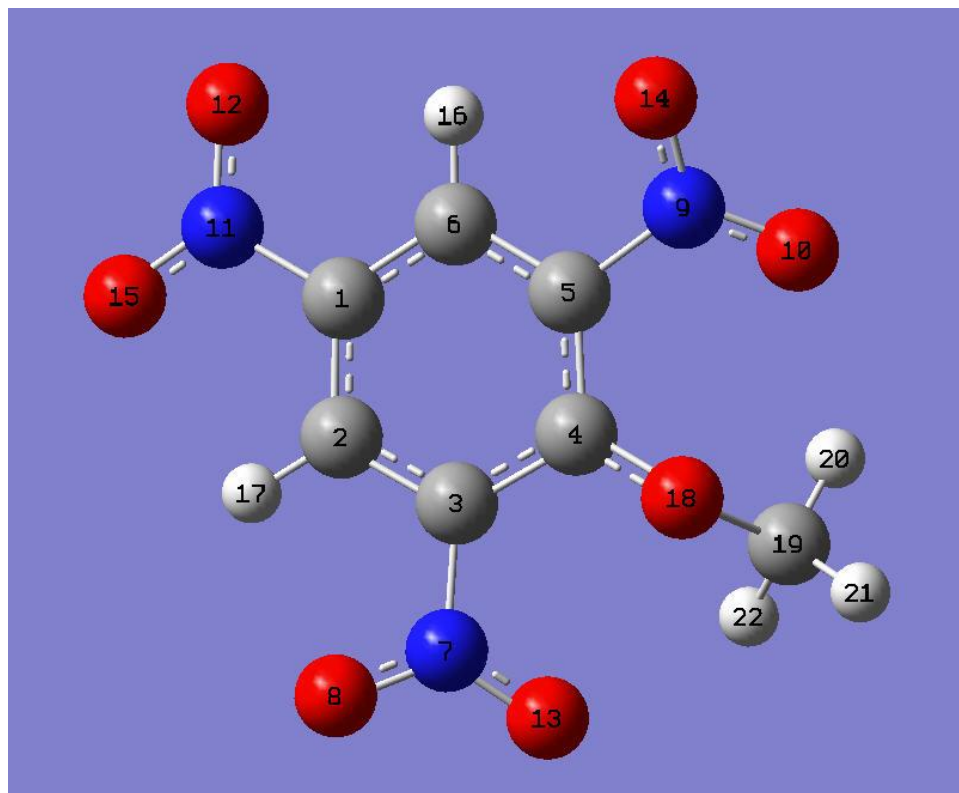


Figure A-20. Methyl picrate with atoms labeled.

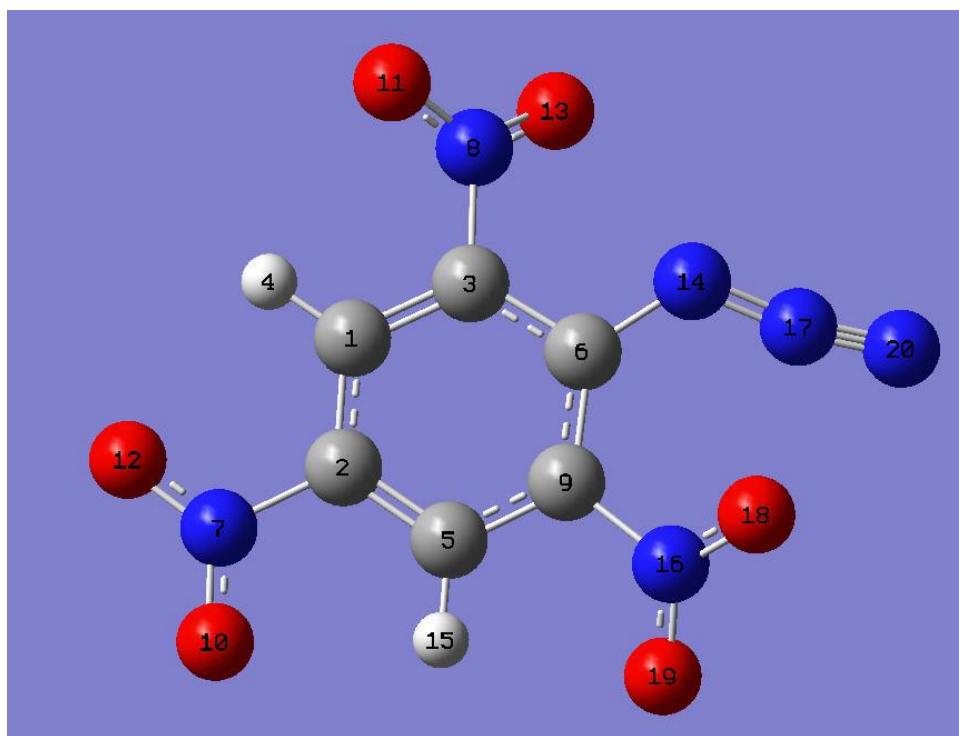


Figure A-21. Picryl azide with atoms labeled.

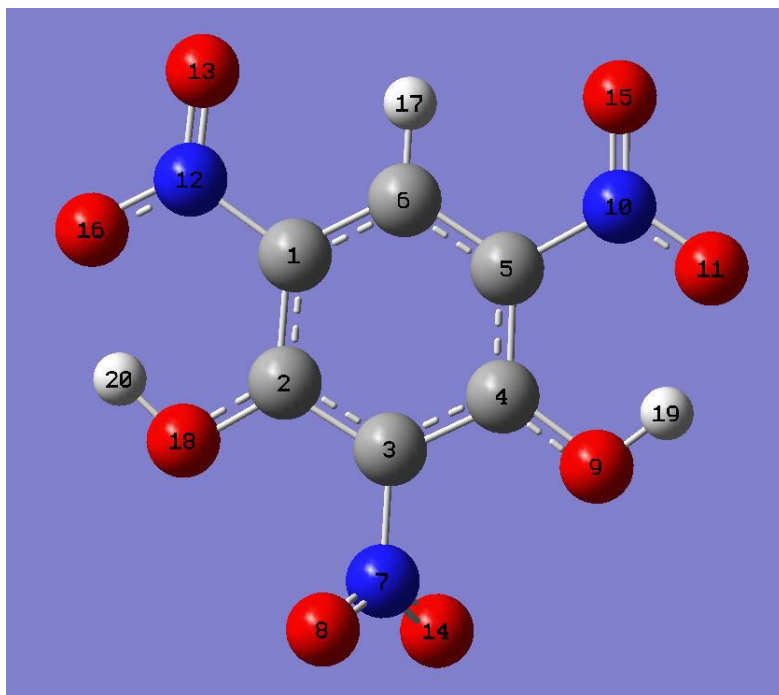


Figure A-22. Styphnic acid with atoms labeled.

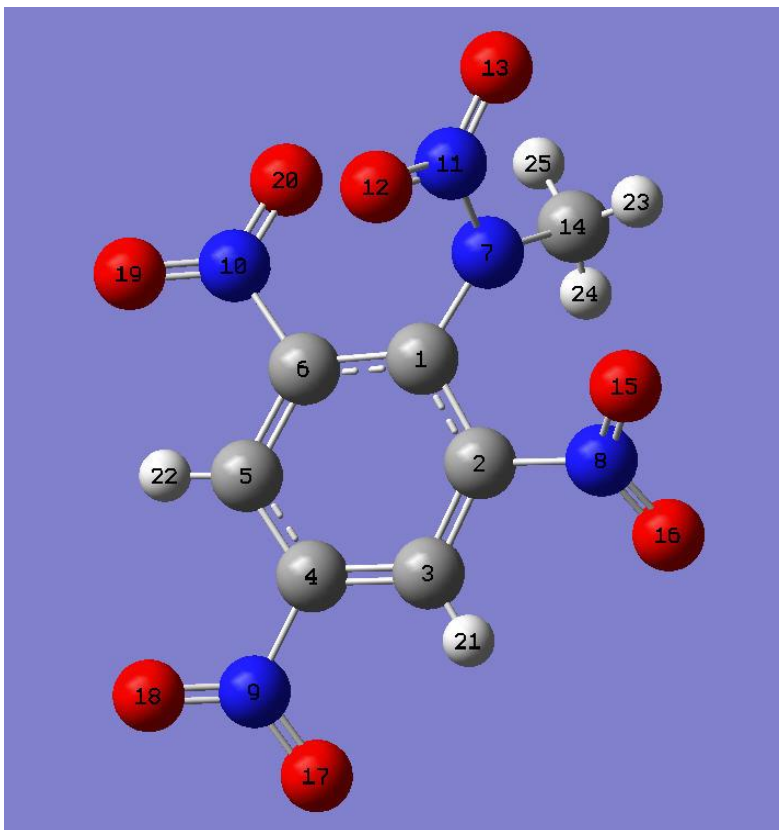


Figure A-23. Tetryl with atoms labeled.

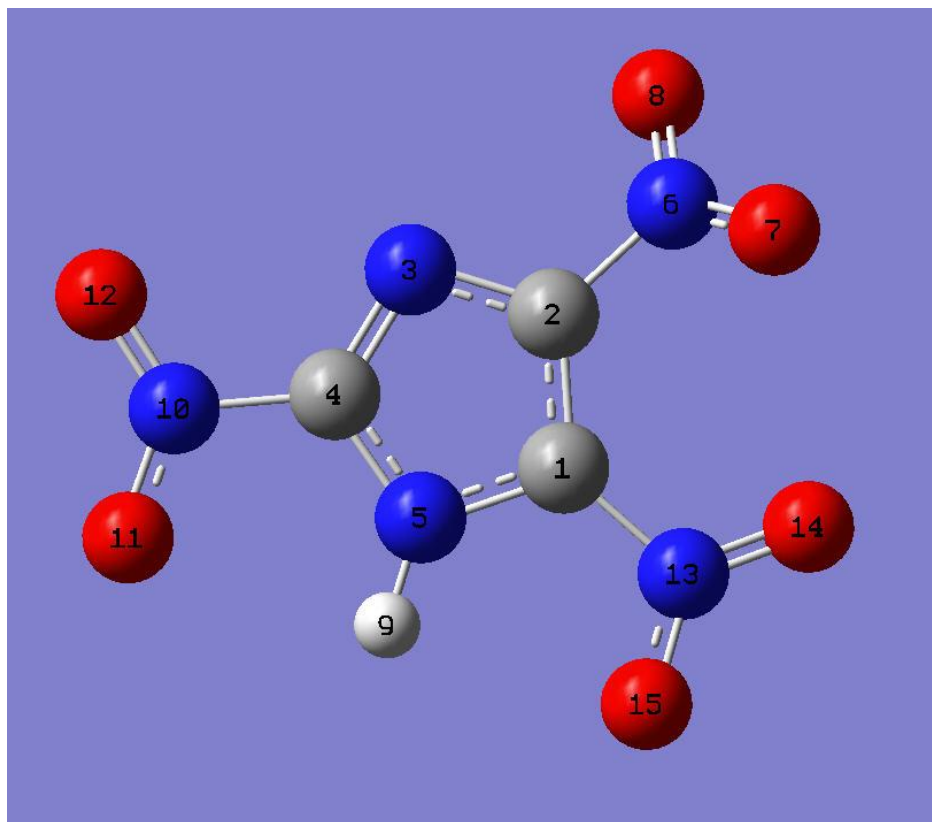


Figure A-24. Tri245 with atoms labeled.

A.3 Training and Fitting Set Graphs

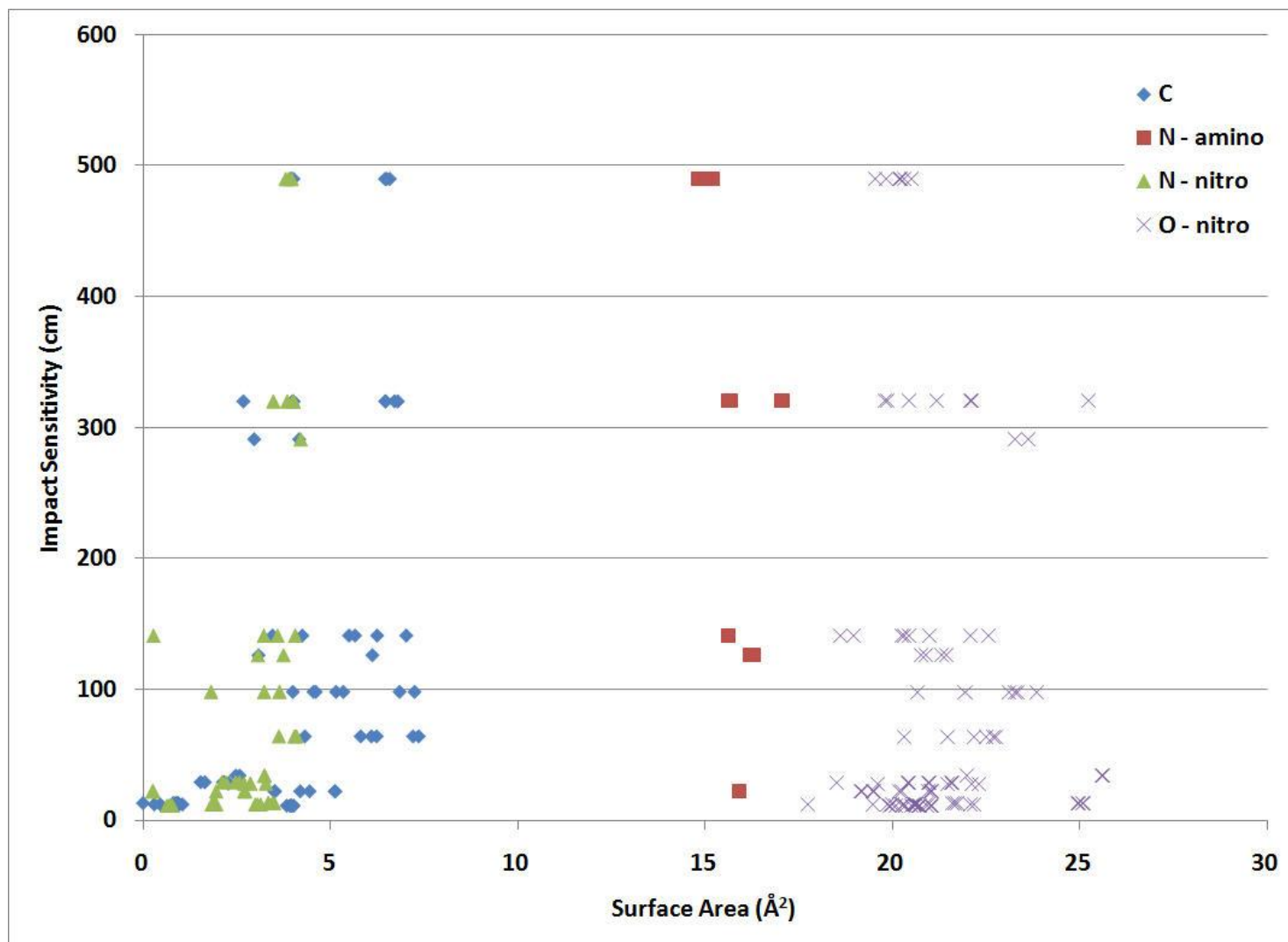


Figure A-25. Impact sensitivity (cm) vs. atomic surface area ($\text{\AA}^2$) for PBE/6-31G**.

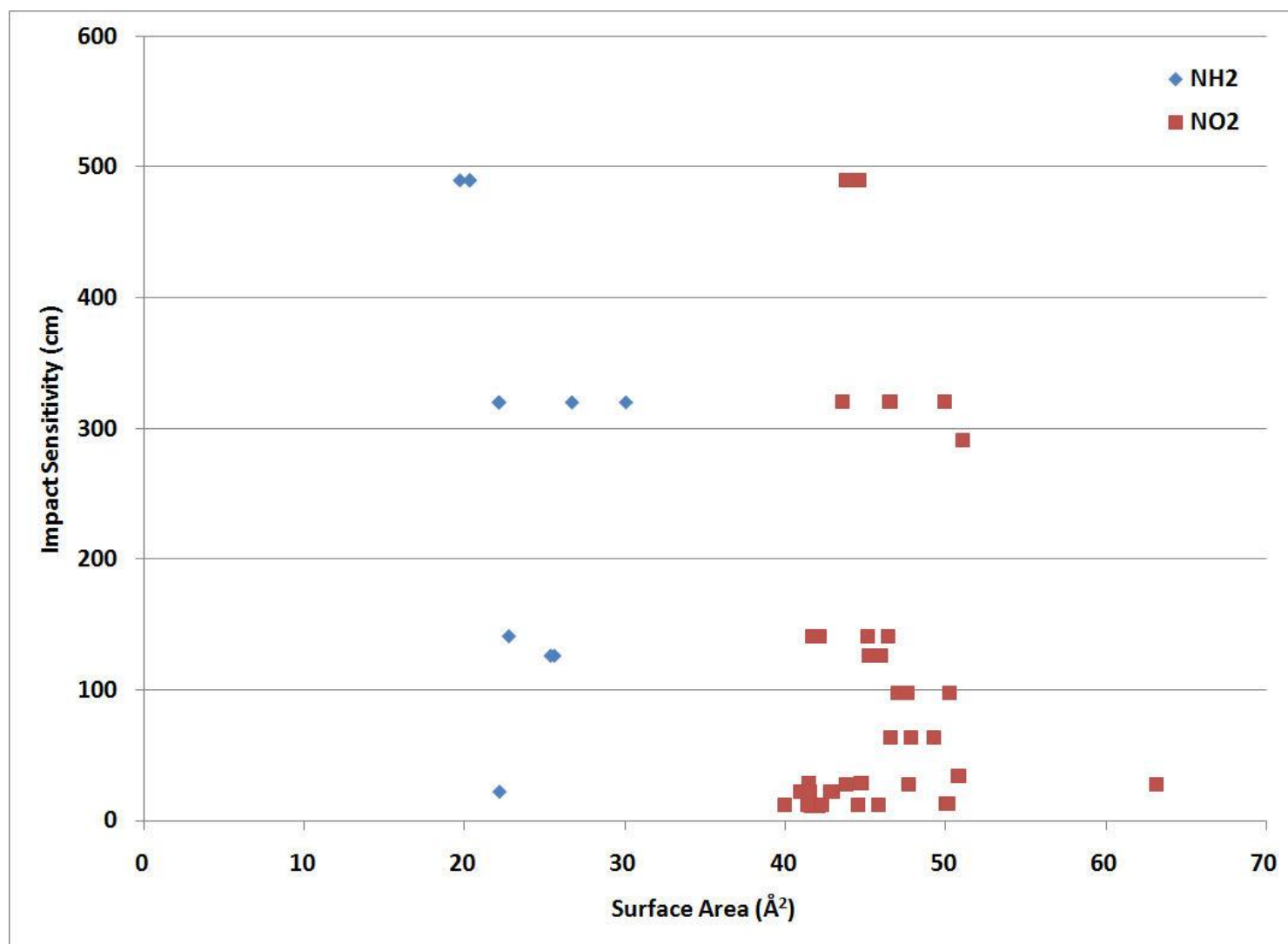


Figure A-26. Impact sensitivity (cm) vs. nitro or animo group surface area (Å²) for PBE/6-31G**.

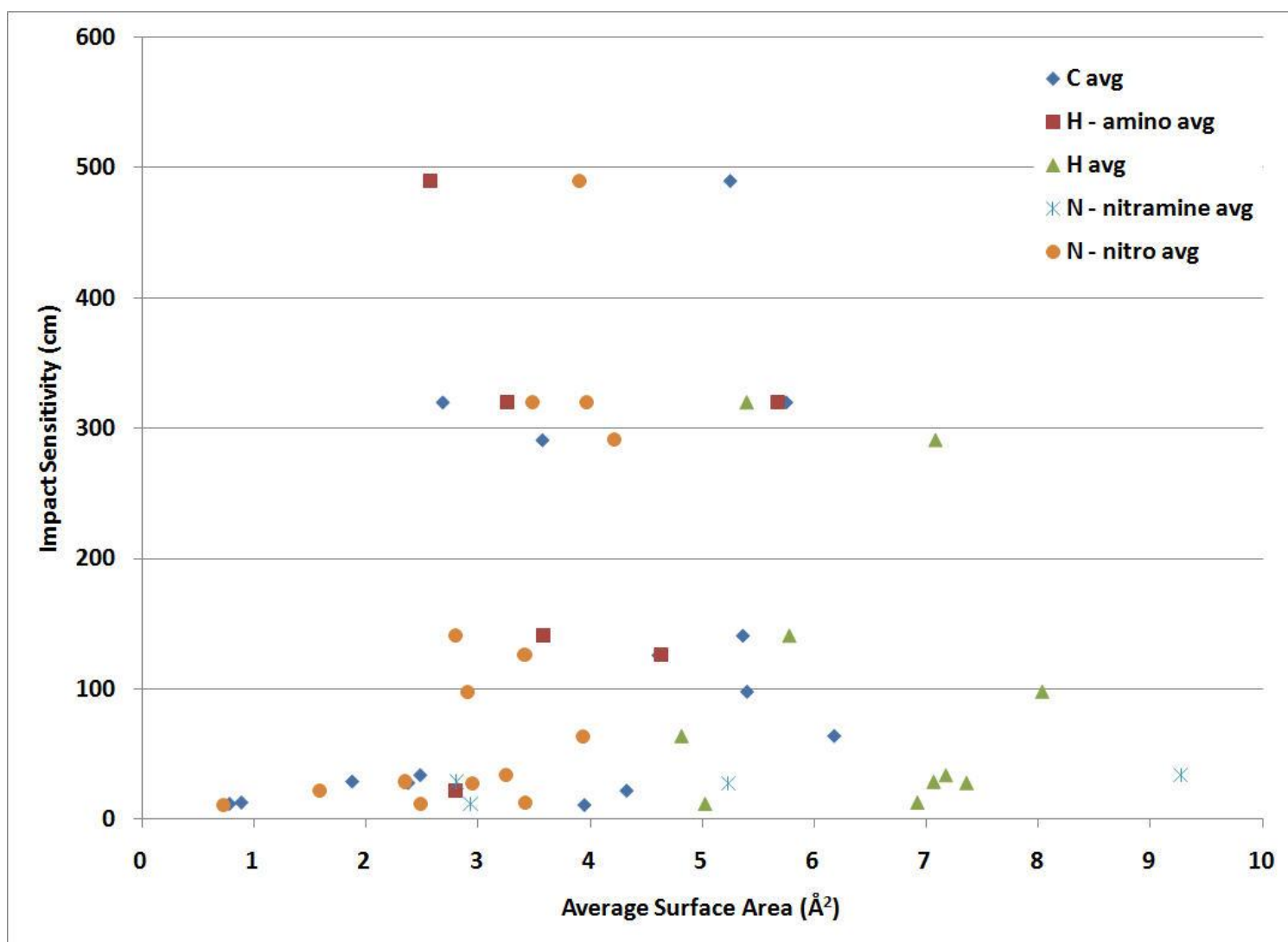


Figure A-27. Impact sensitivity (cm) vs. atomic average surface area ($\text{\AA}^2$) for carbon, hydrogen, amino hydrogens, nitro nitrogens and nitramine nitrogens for PBE/6-31G**.

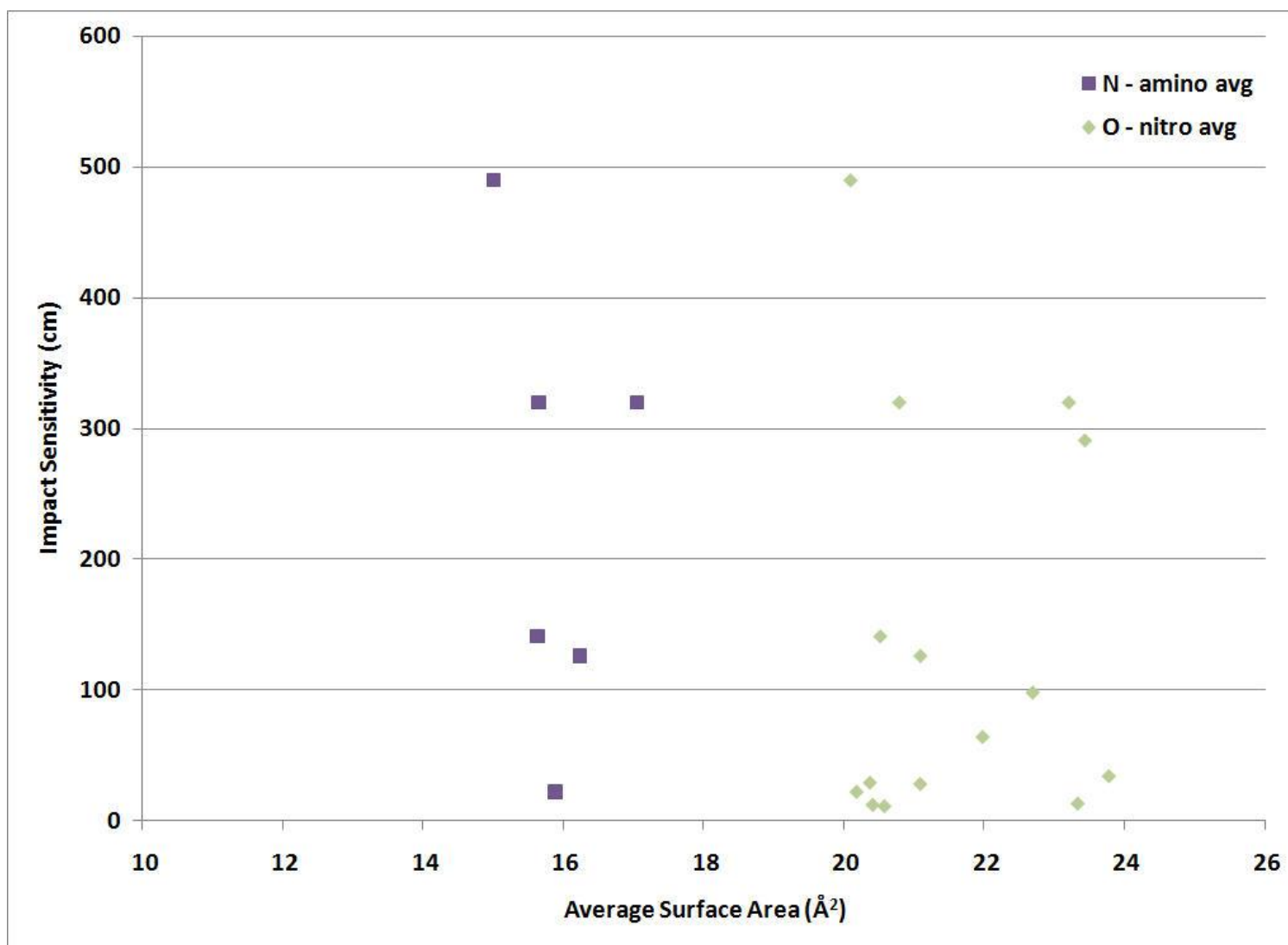


Figure A-28. Impact sensitivity (cm) vs. atomic average surface area (Å²) for amino nitrogen and nitro oxygen for PBE/6-31G**.

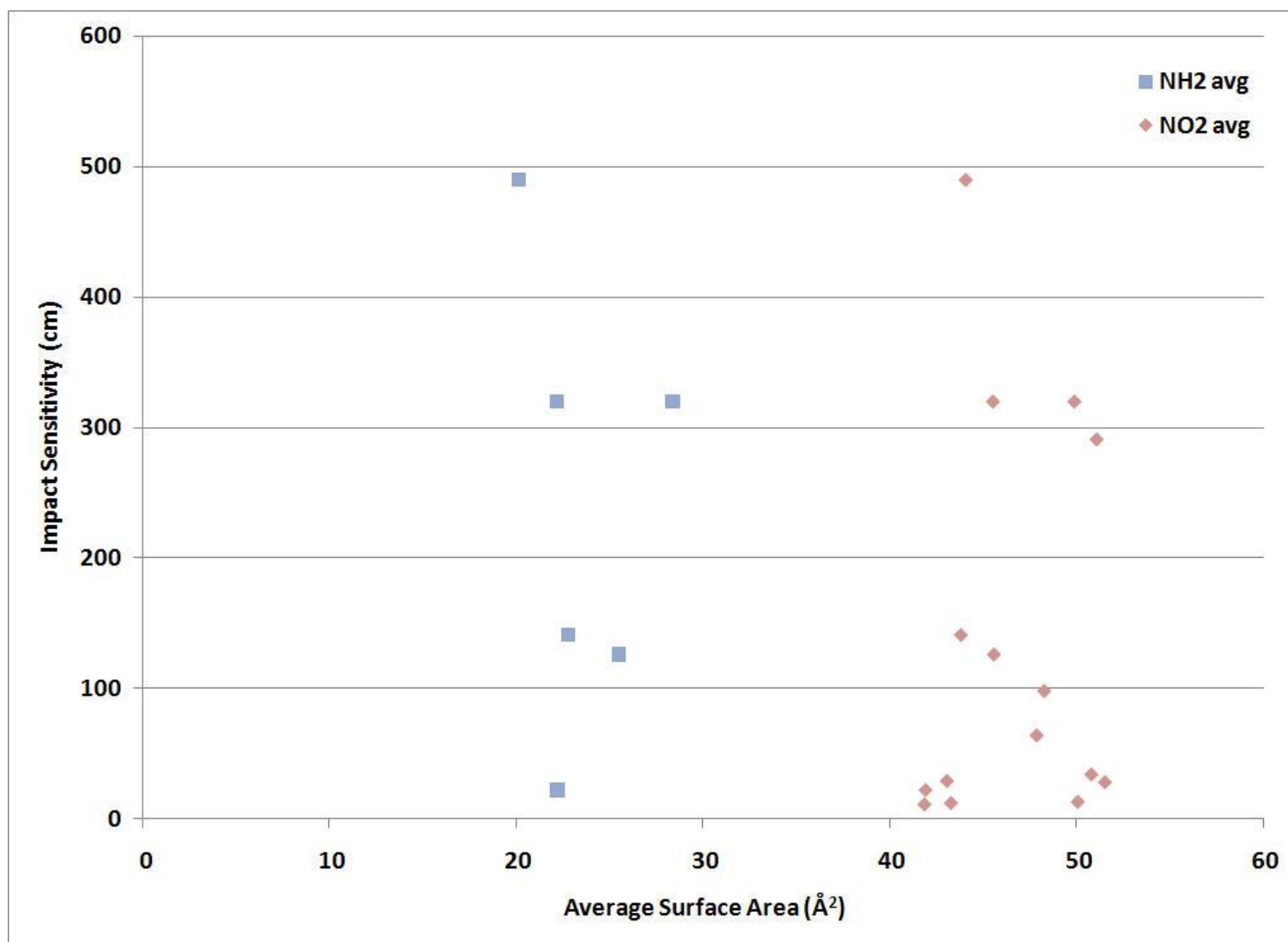


Figure A-29. Impact sensitivity (cm) vs. group average surface area ($\text{\AA}^2$) for PBE/6-31G**.

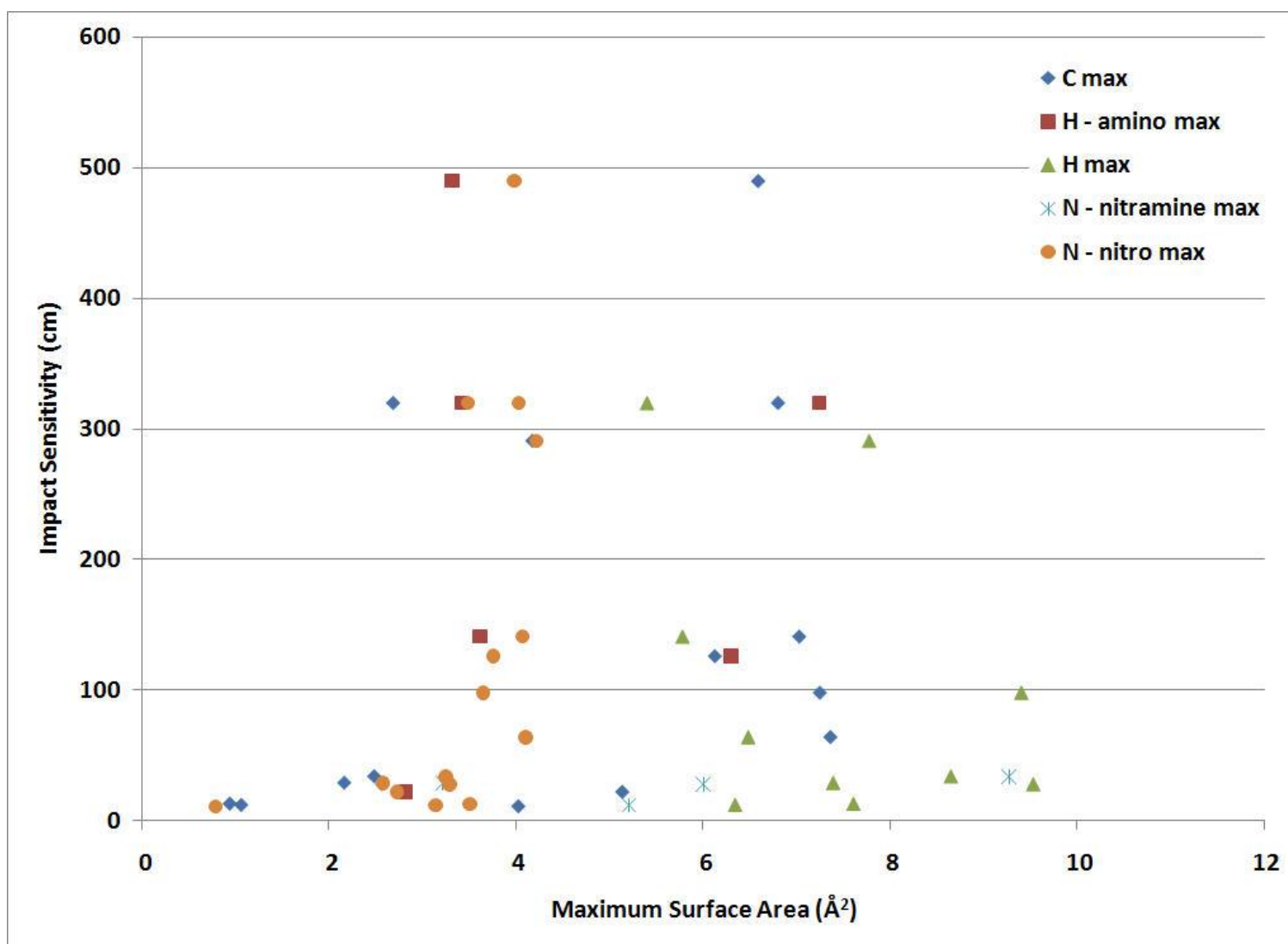


Figure A-30. Impact sensitivity (cm) vs. atomic maximum surface area (Å²) for carbon, hydrogen, amino hydrogens, nitro nitrogens and nitramine nitrogens for PBE/6-31G**.

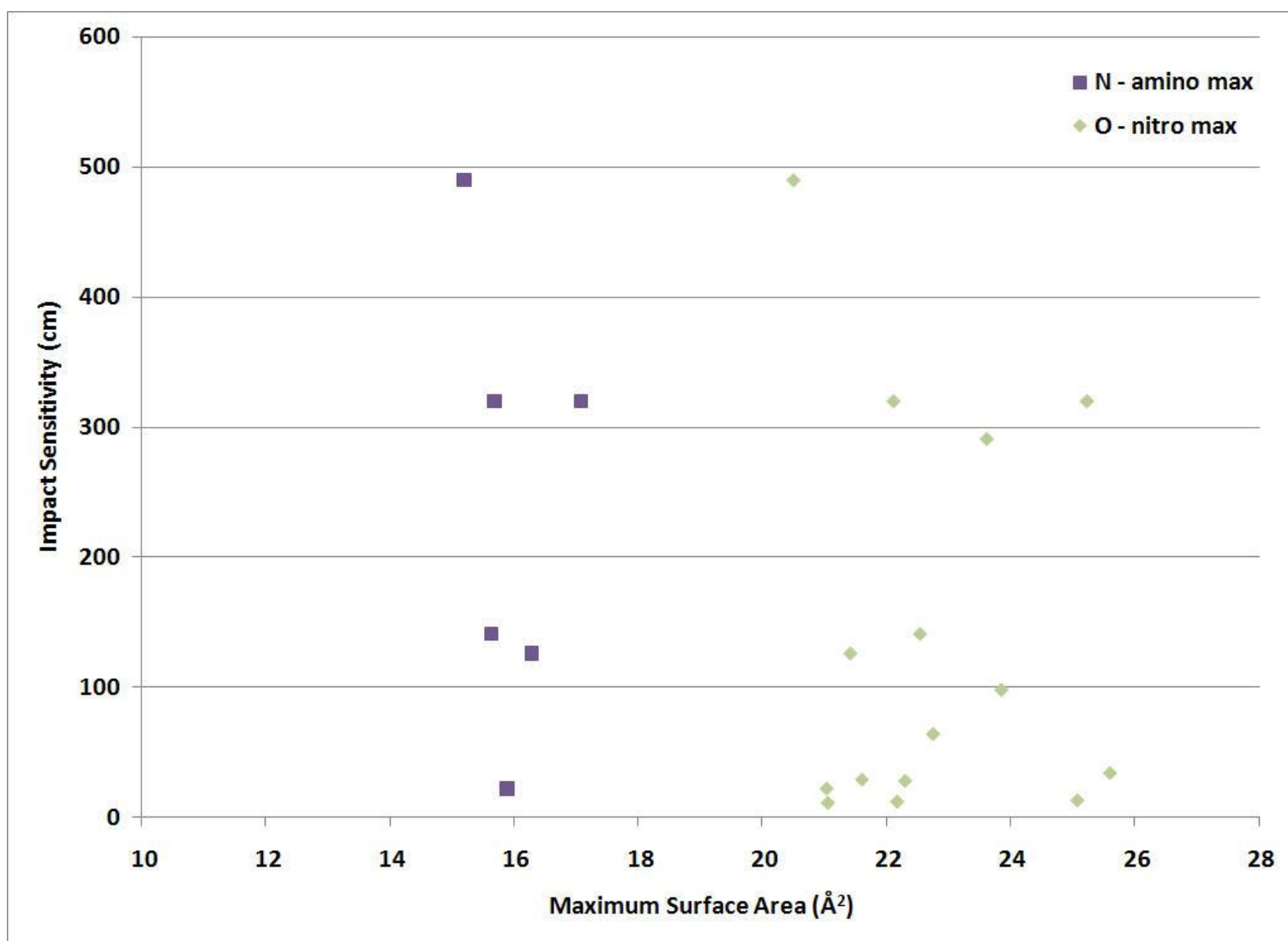


Figure A-31. Impact sensitivity (cm) vs. atomic maximum surface area (Å²) for amino nitrogen and nitro oxygen for PBE/6-31G**.

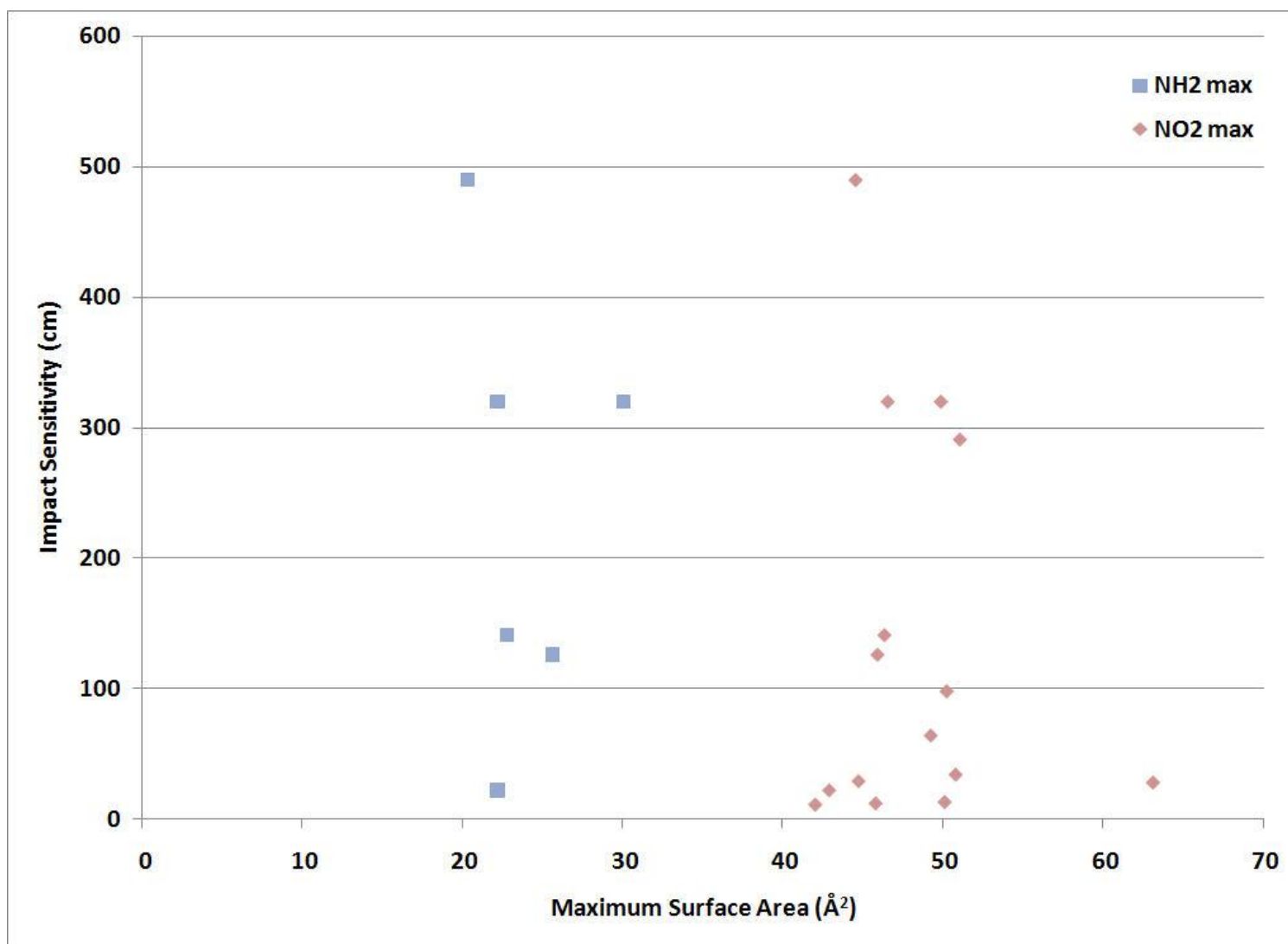


Figure A-32. Impact sensitivity (cm) vs. group maximum surface area ($\text{\AA}^2$) for PBE/6-31G**.

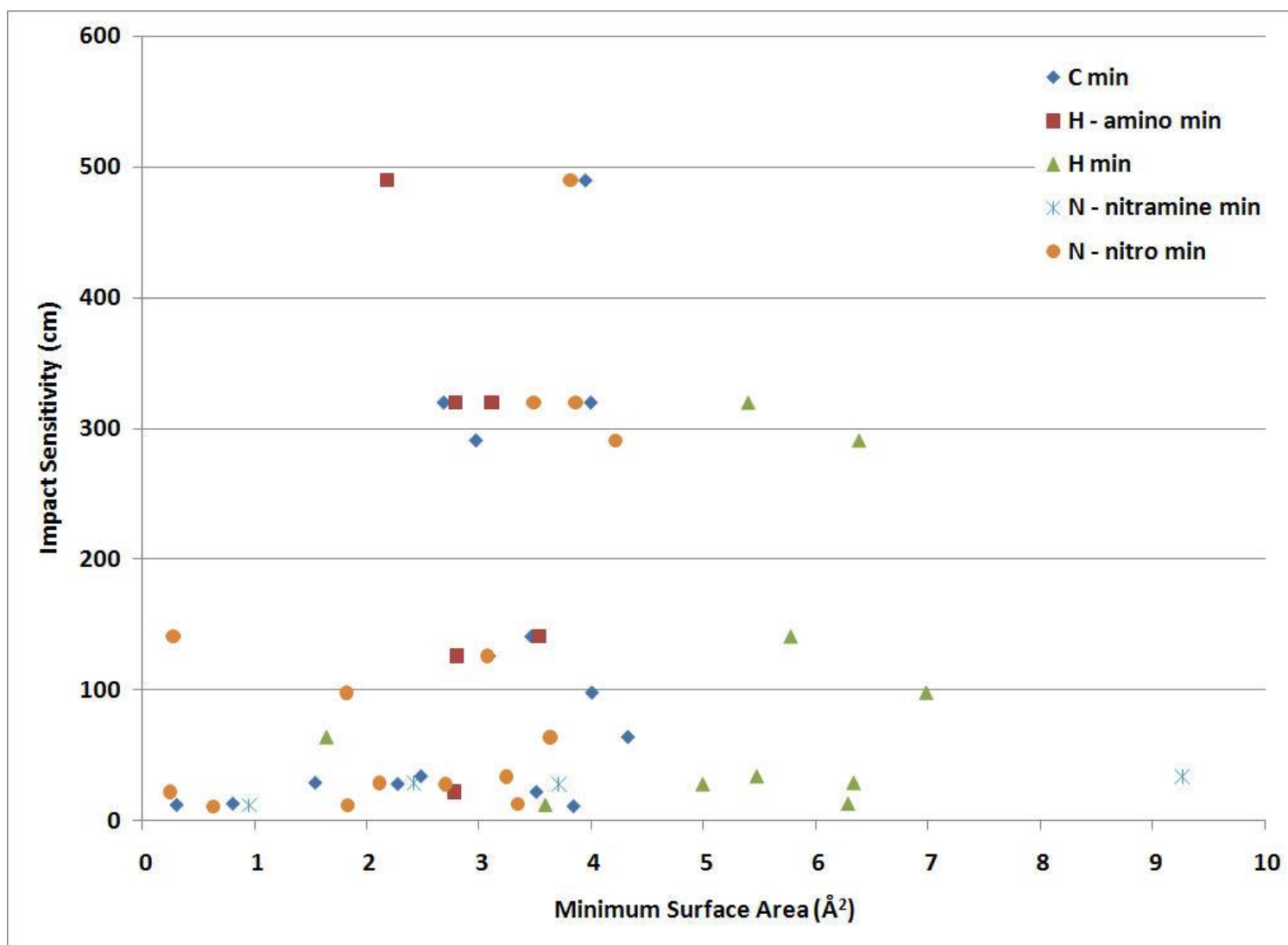


Figure A-33. Impact sensitivity (cm) vs. atomic minimum surface area ($\text{\AA}^2$) for carbon, hydrogen, amino hydrogens, nitro nitrogens and nitramine nitrogens for PBE/6-31G**.

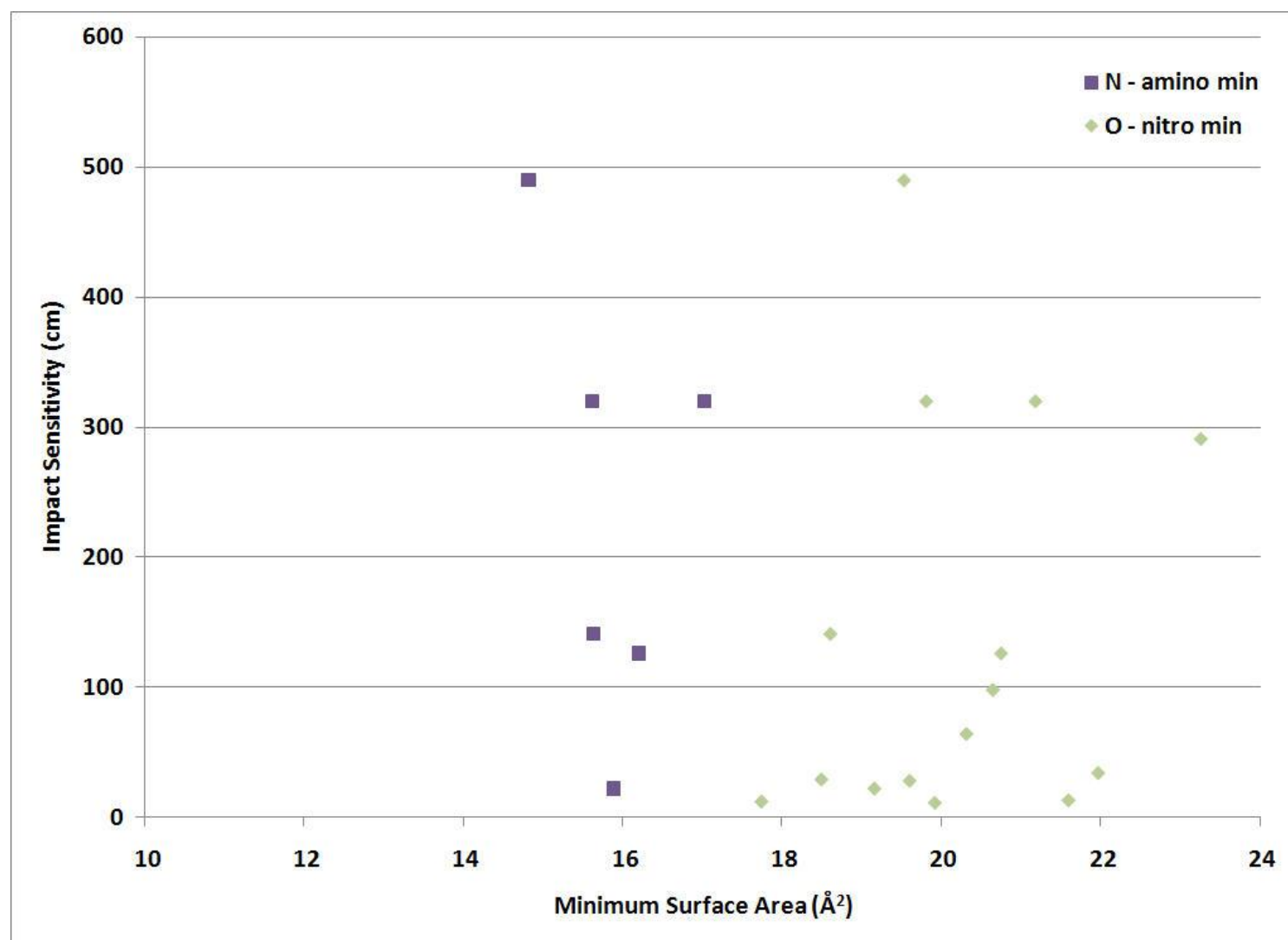


Figure A-34. Impact sensitivity (cm) vs. atomic minimum surface area ($\text{\AA}^2$) for amino nitrogen and nitro oxygen for PBE/6-31G**.

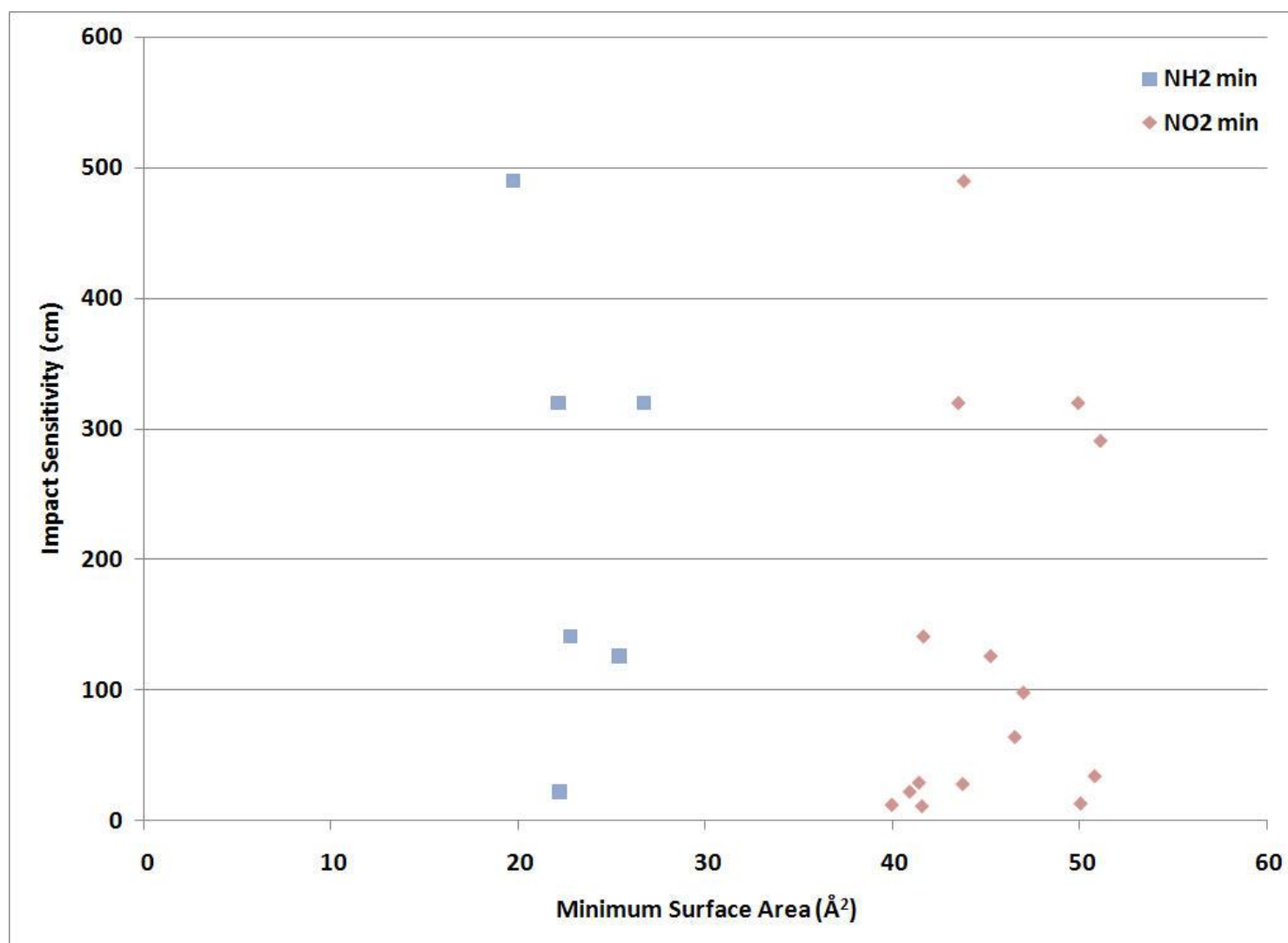


Figure A-35. Impact sensitivity (cm) vs. group minimum surface area ($\text{\AA}^2$) for PBE/6-31G**.

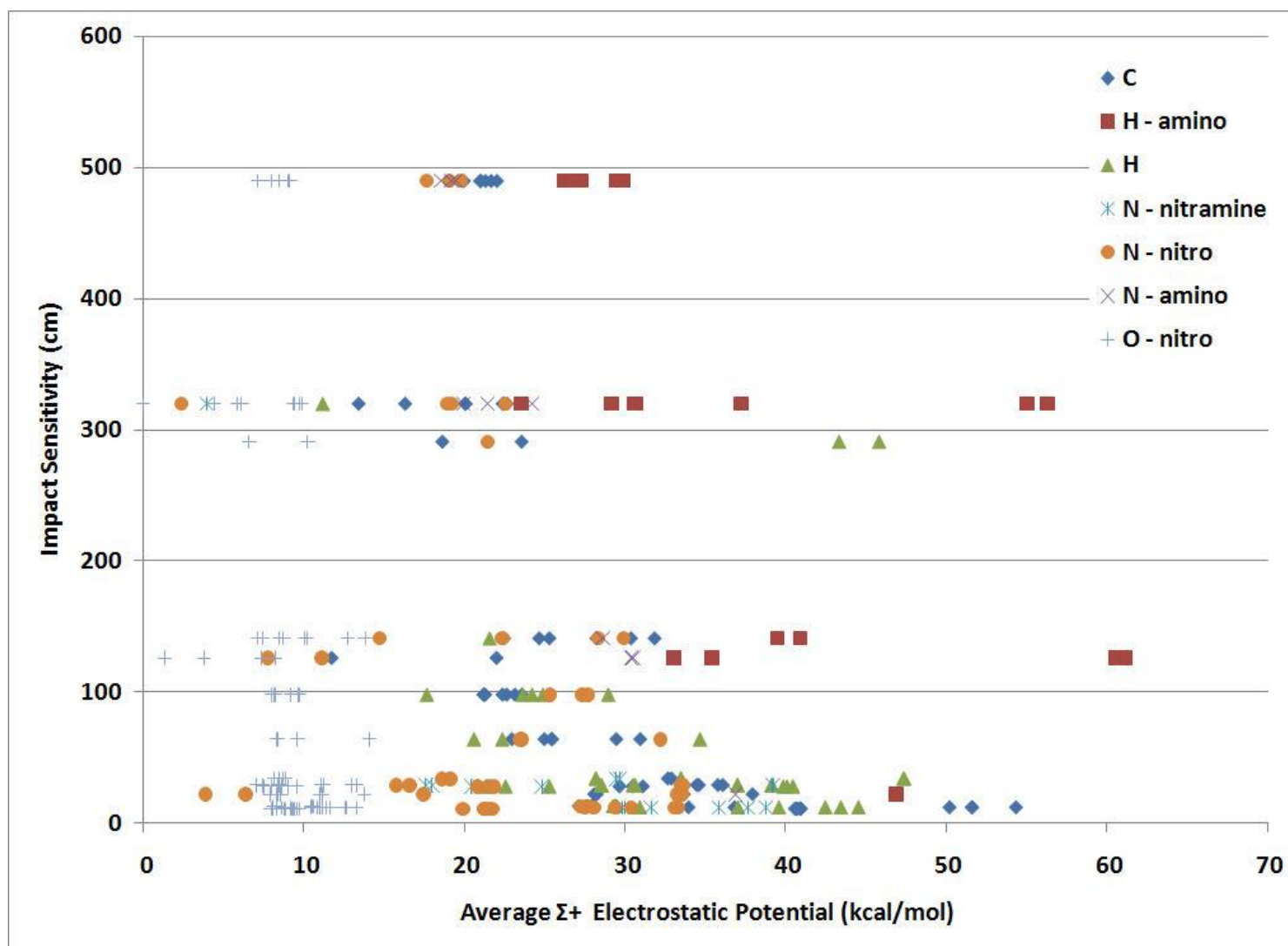


Figure A-36. Impact sensitivity (cm) vs. atomic average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

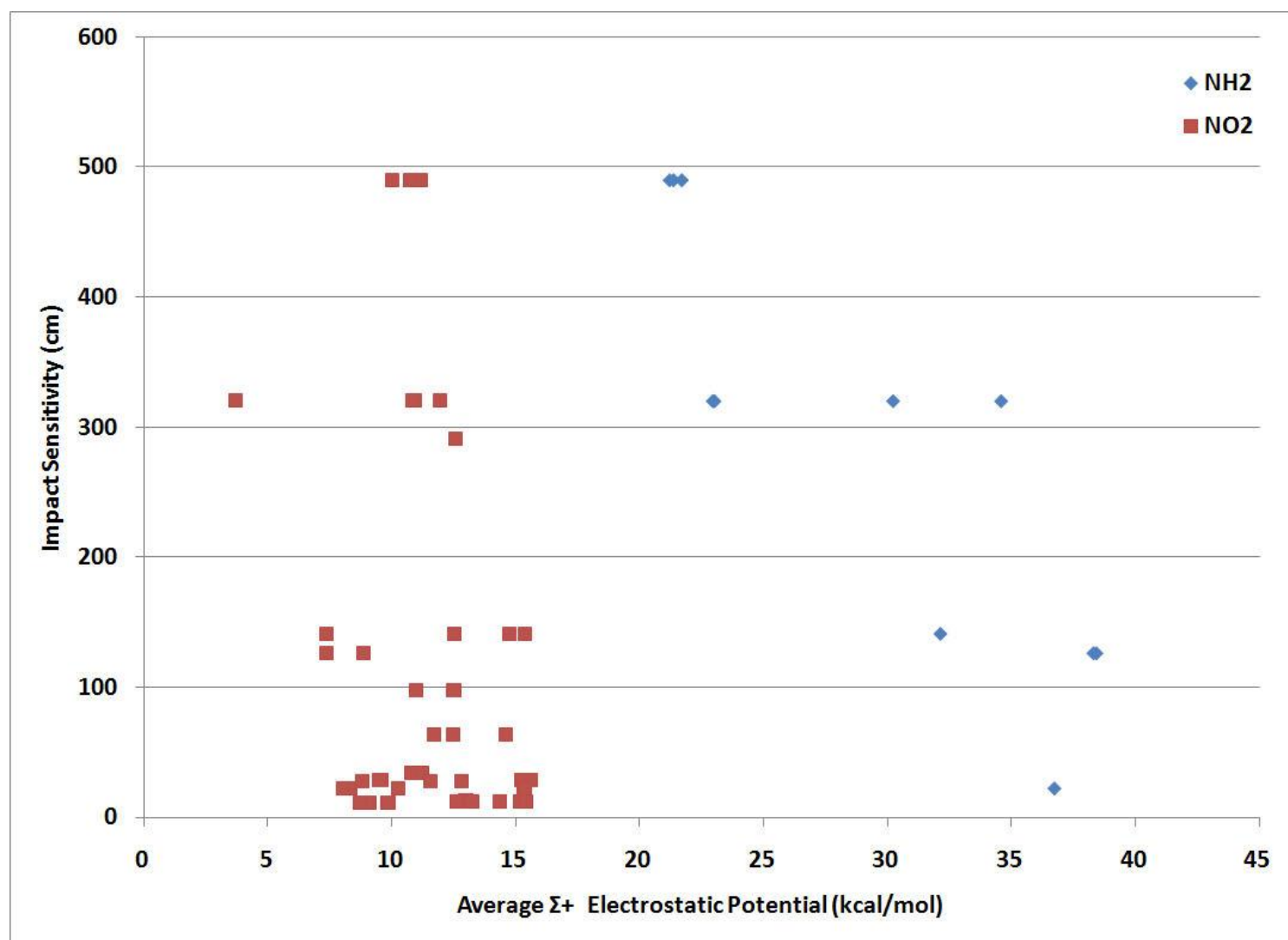


Figure A-37. Impact sensitivity (cm) vs. group average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

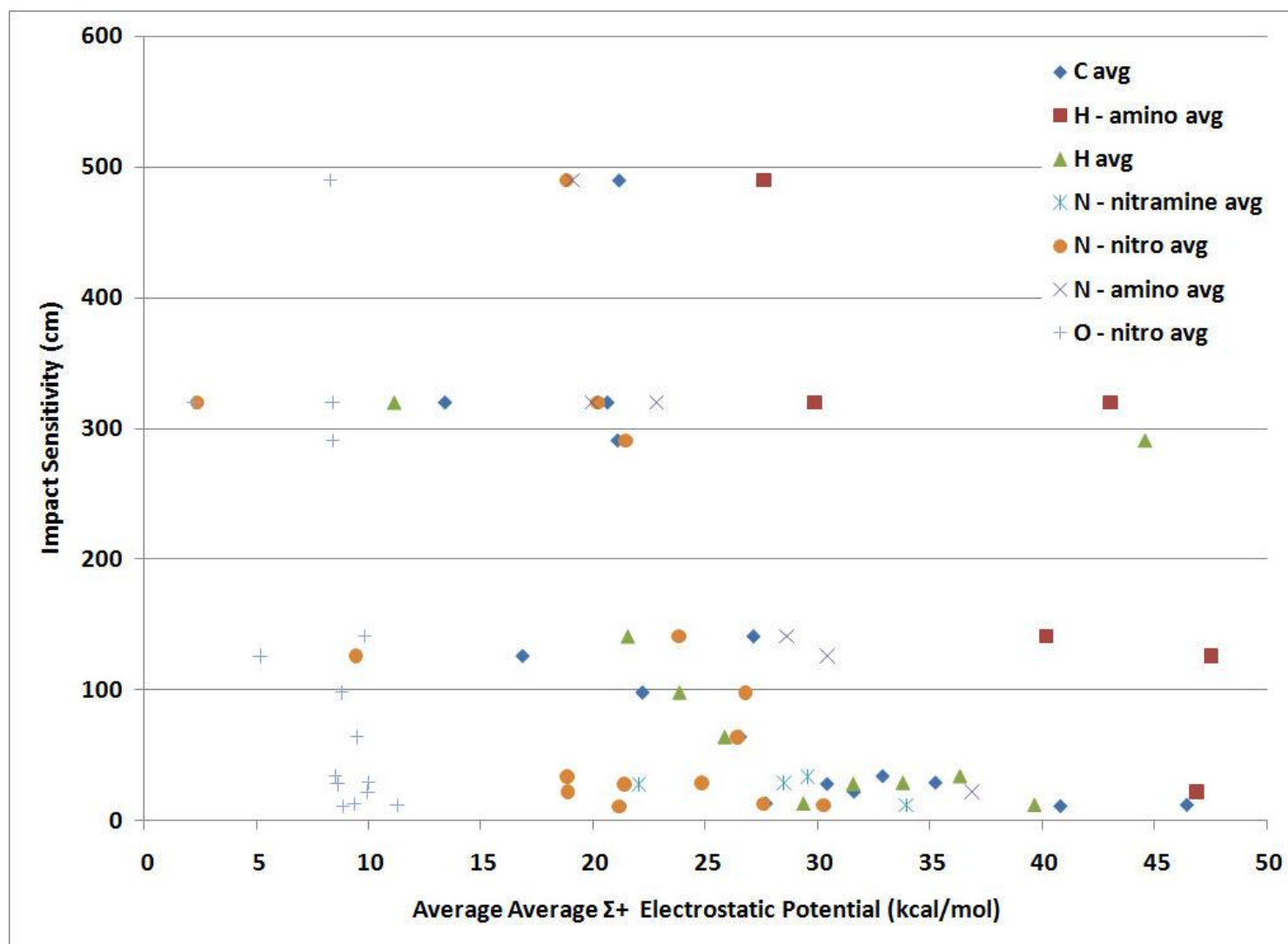


Figure A-38. Impact sensitivity (cm) vs. atomic average average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

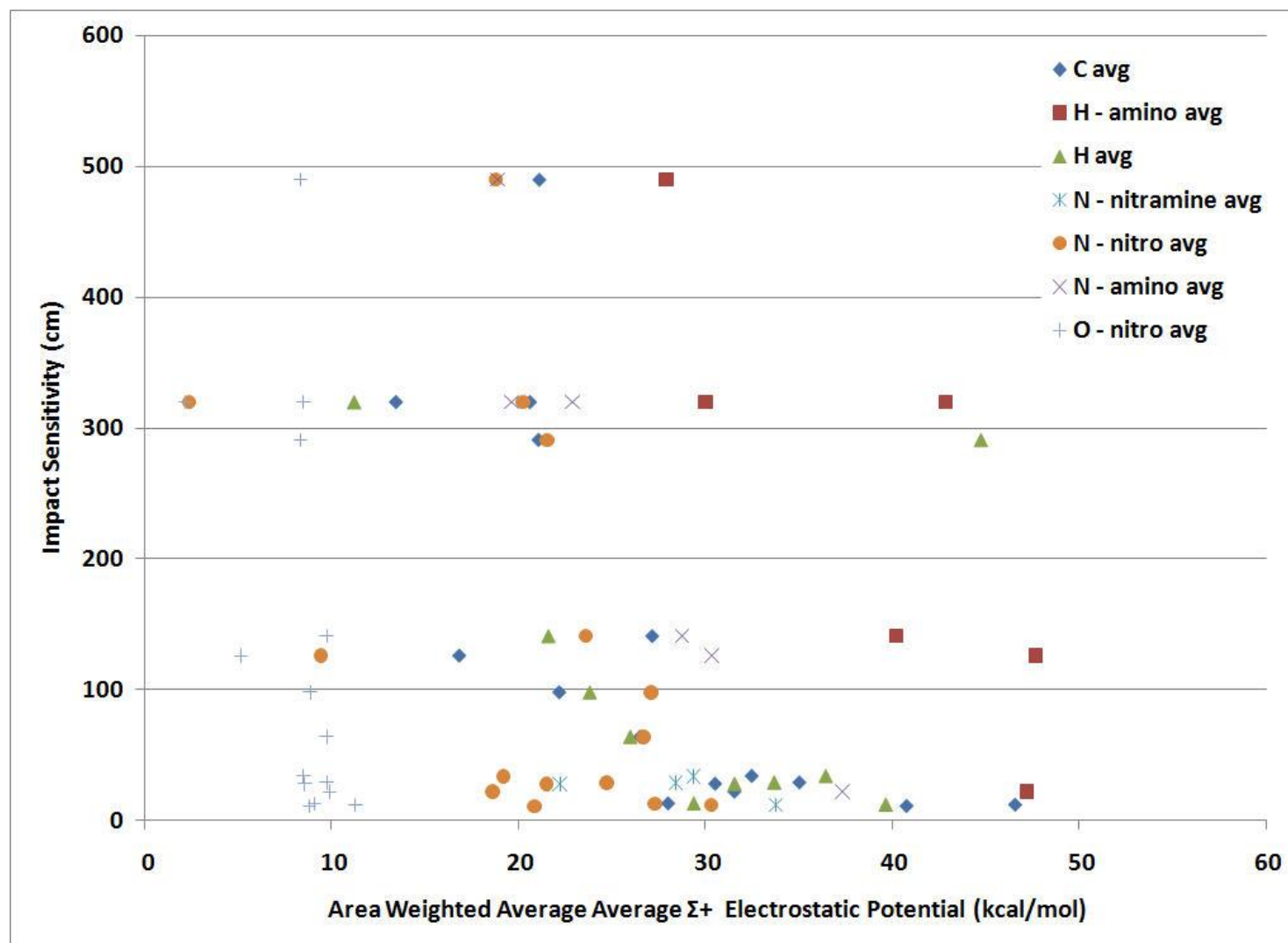


Figure A-39. Impact sensitivity (cm) vs. area weighted atomic average average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

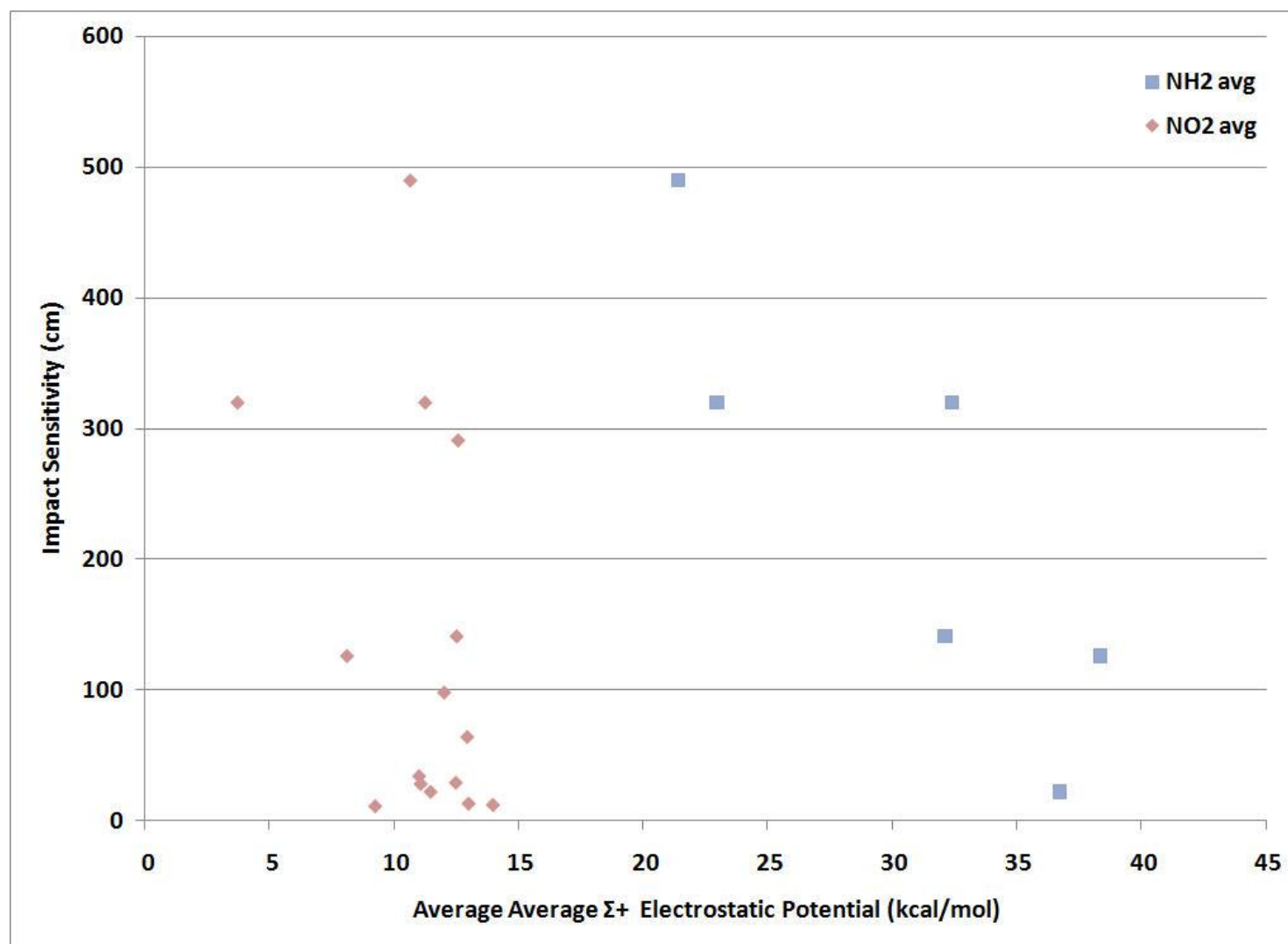


Figure A-40. Impact sensitivity (cm) vs. group average average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

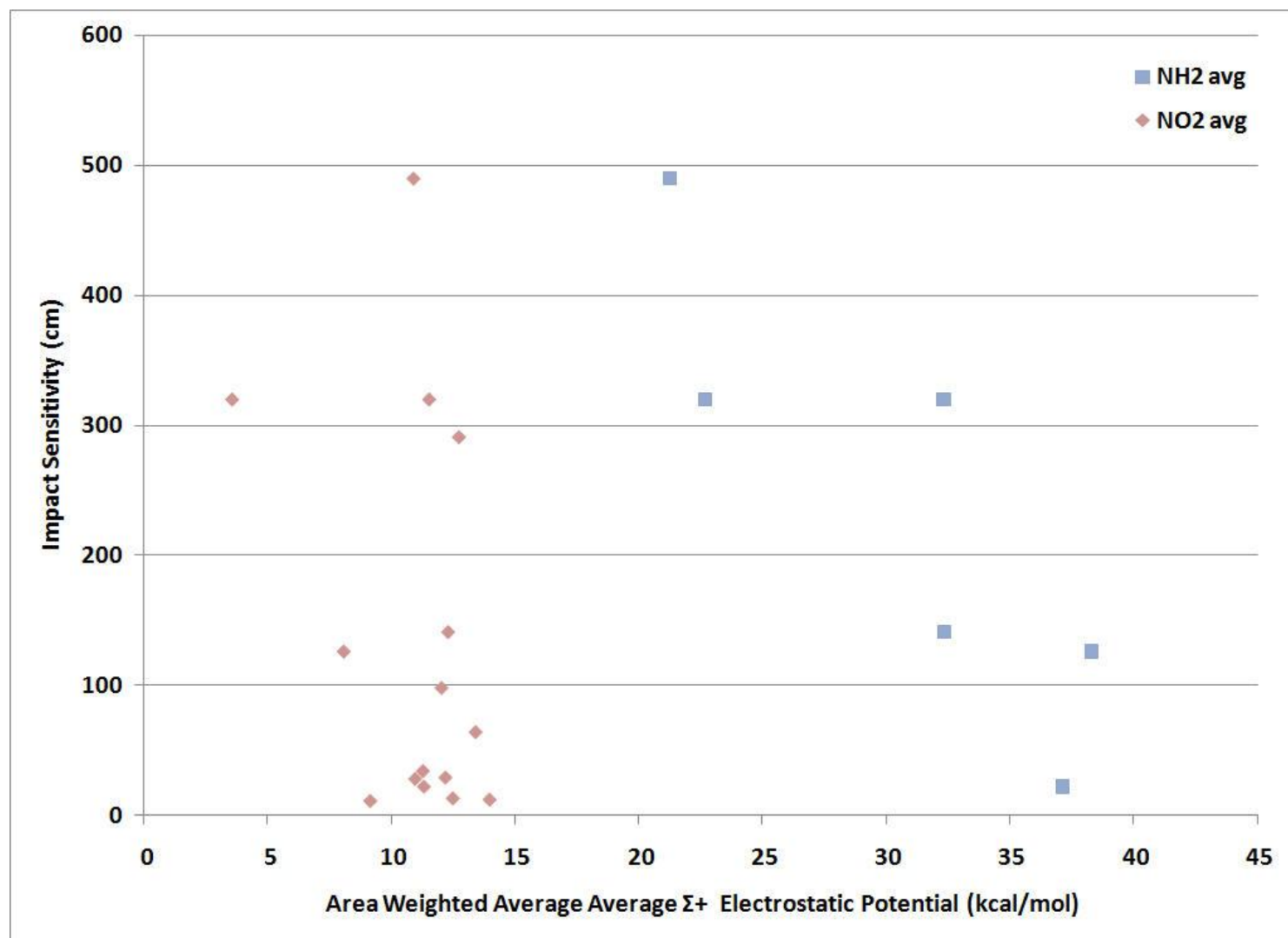


Figure A-41. Impact sensitivity (cm) vs. area weighted group average average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

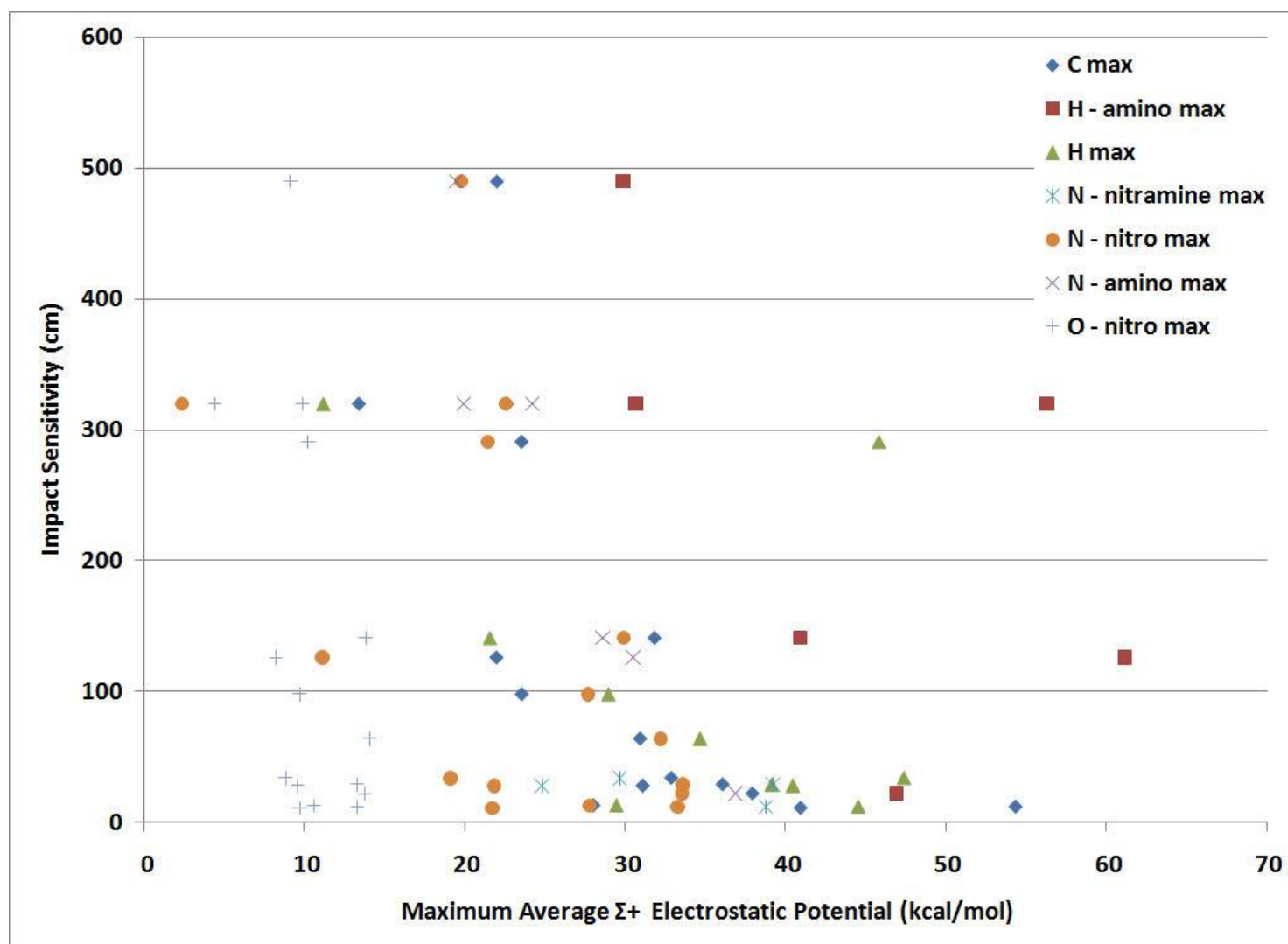


Figure A-42. Impact sensitivity (cm) vs. atomic maximum average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

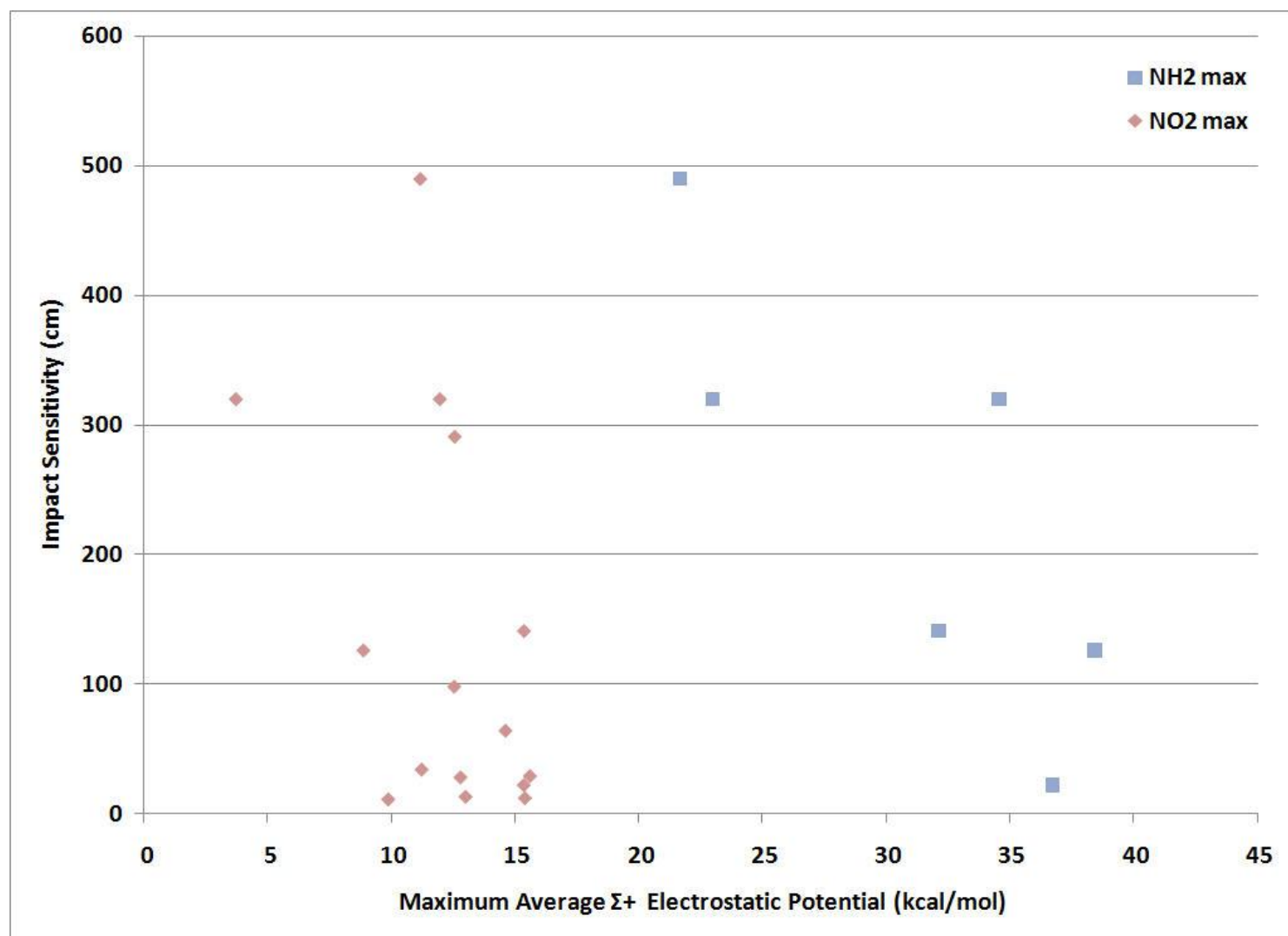


Figure A-43. Impact sensitivity (cm) vs. group maximum average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

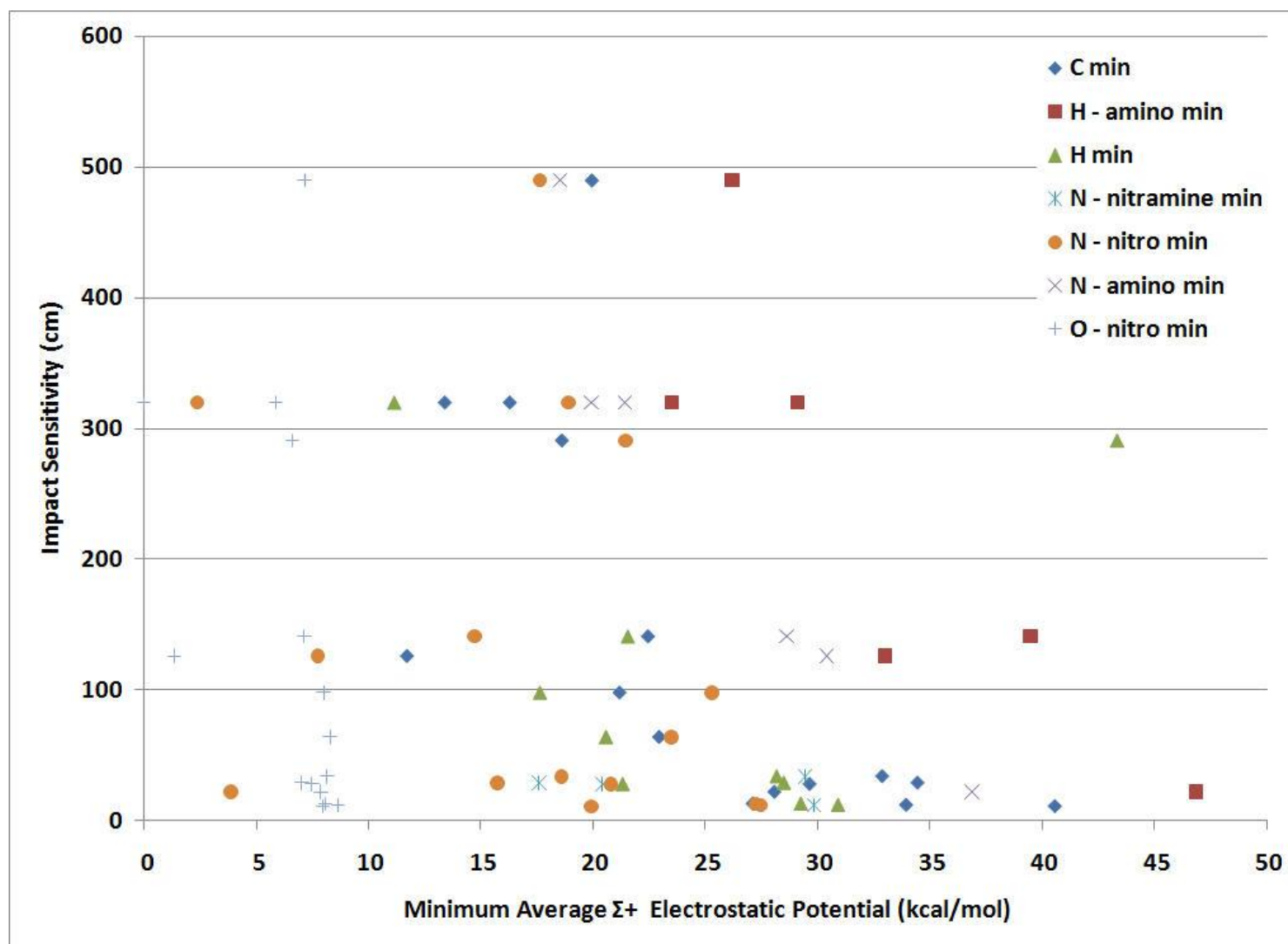


Figure A-44. Impact sensitivity (cm) vs. atomic minimum average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

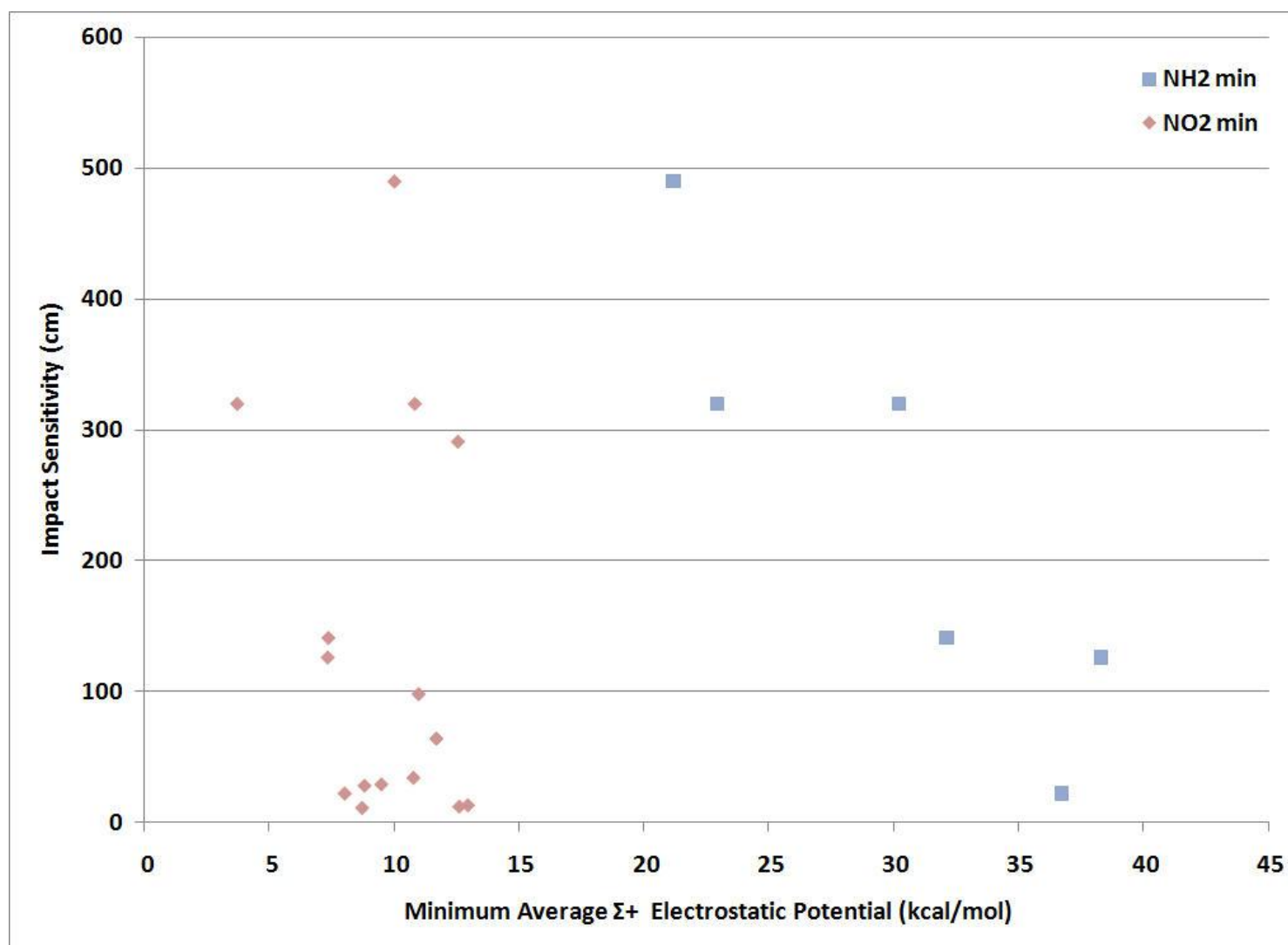


Figure A-45. Impact sensitivity (cm) vs. group minimum average Σ^+ electrostatic potential (kcal/mol) for PBE/6-31G**.

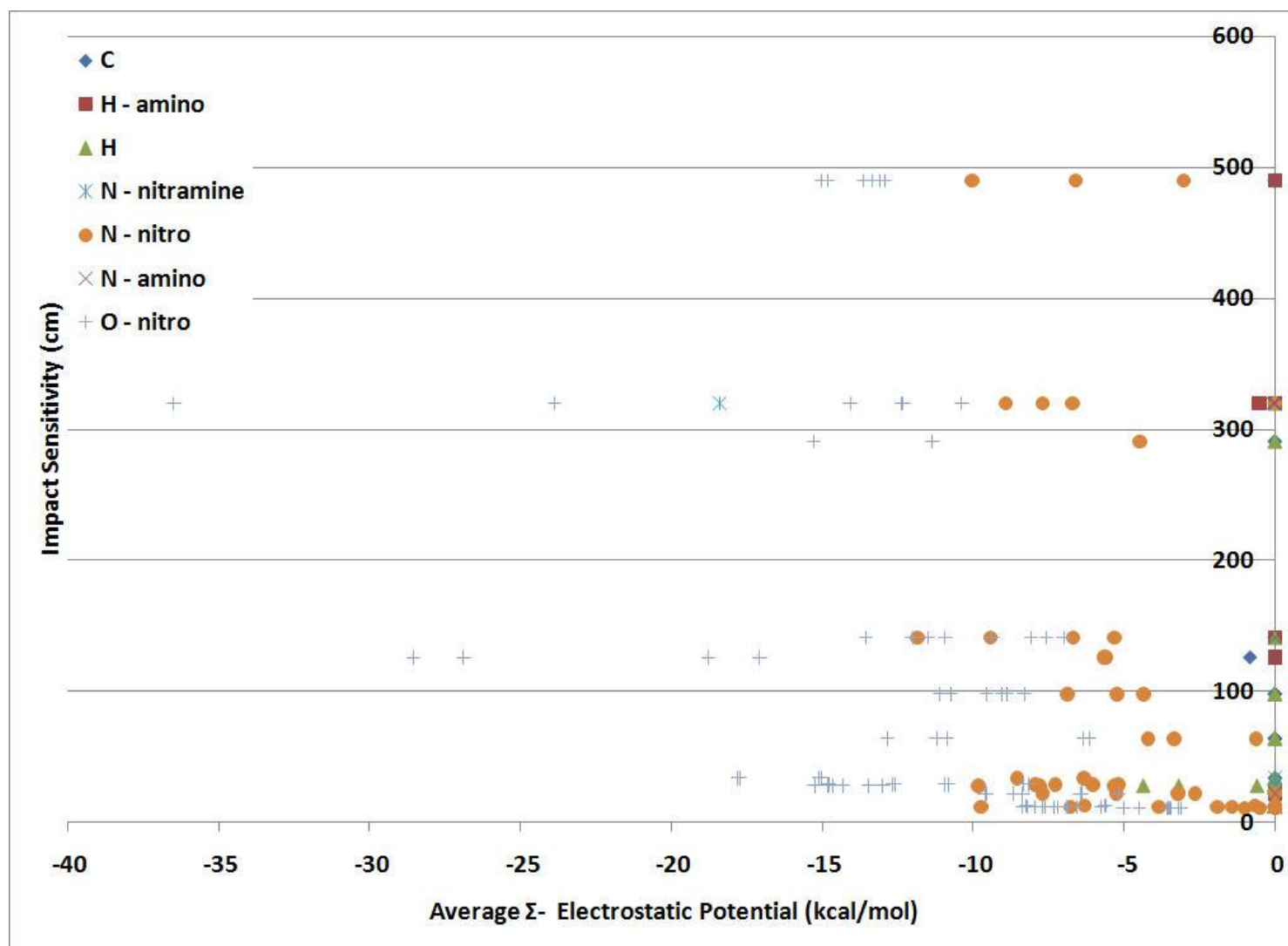


Figure A-46. Impact sensitivity (cm) vs. atomic average Σ - electrostatic potential (kcal/mol) for PBE/6-31G**.

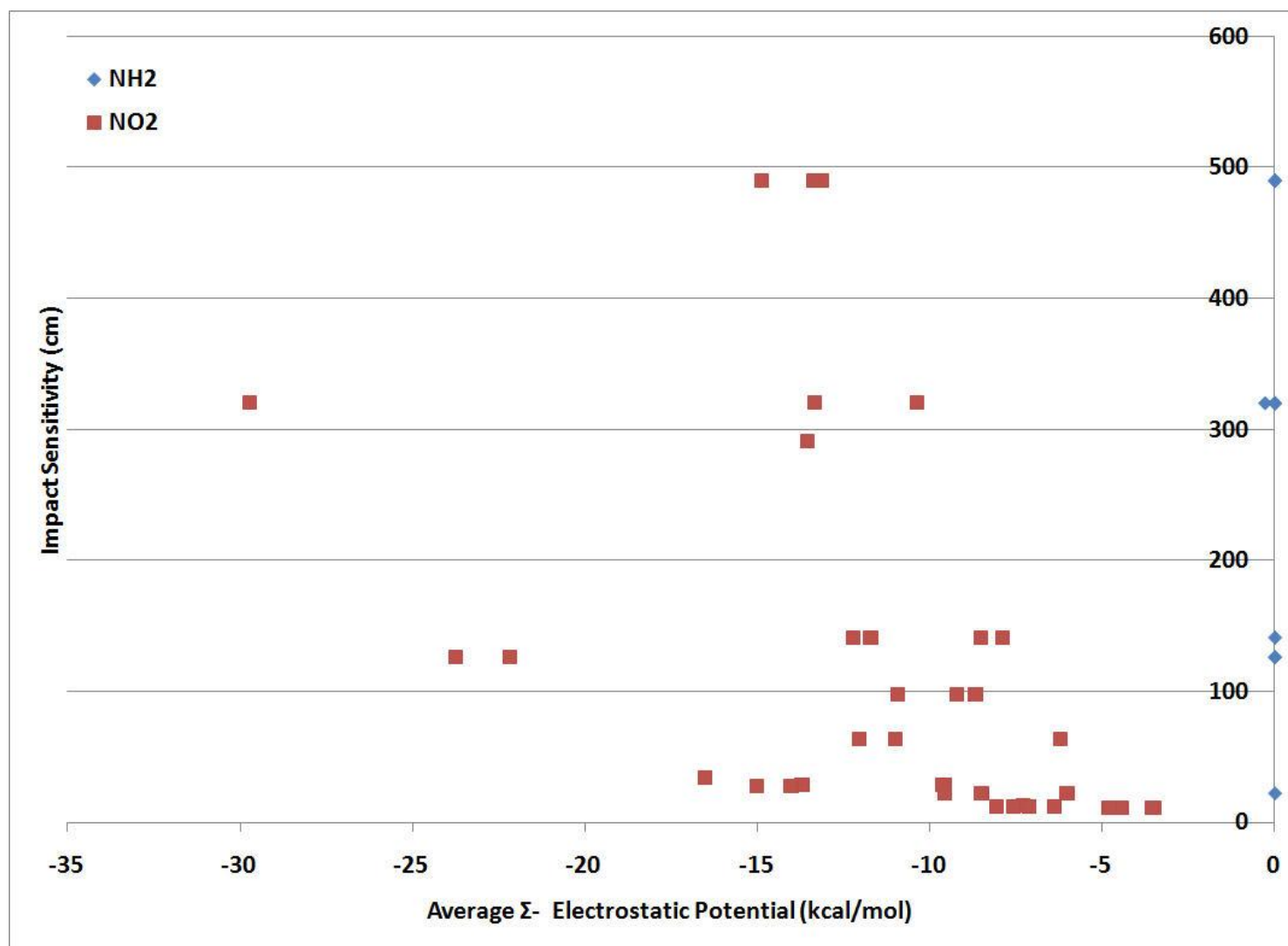


Figure A-47. Impact sensitivity (cm) vs. group average Σ^- electrostatic potential (kcal/mol) for PBE/6-31G**.

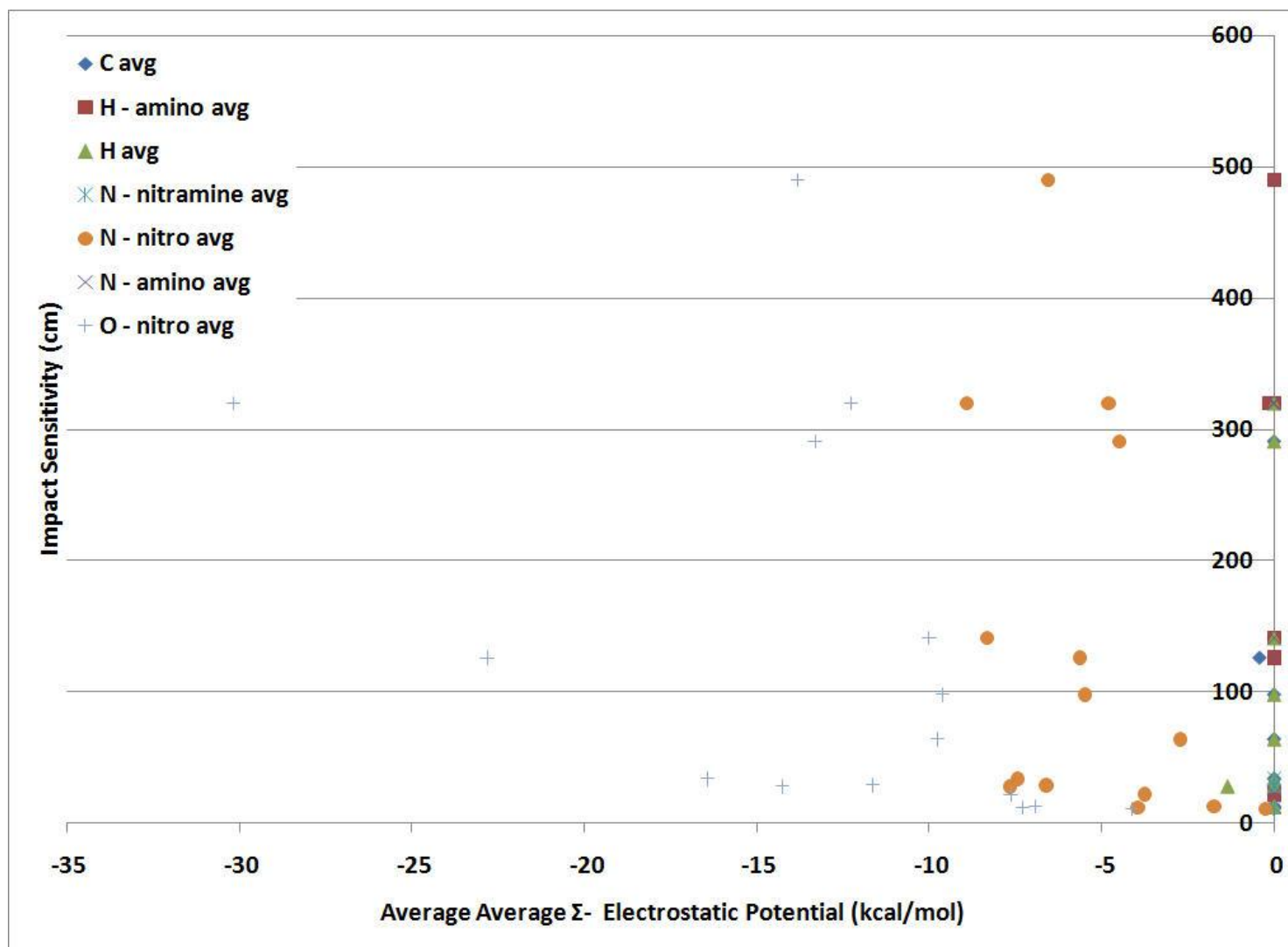


Figure A-48. Impact sensitivity (cm) vs. atomic average average Σ - electrostatic potential (kcal/mol) for PBE/6-31G**.

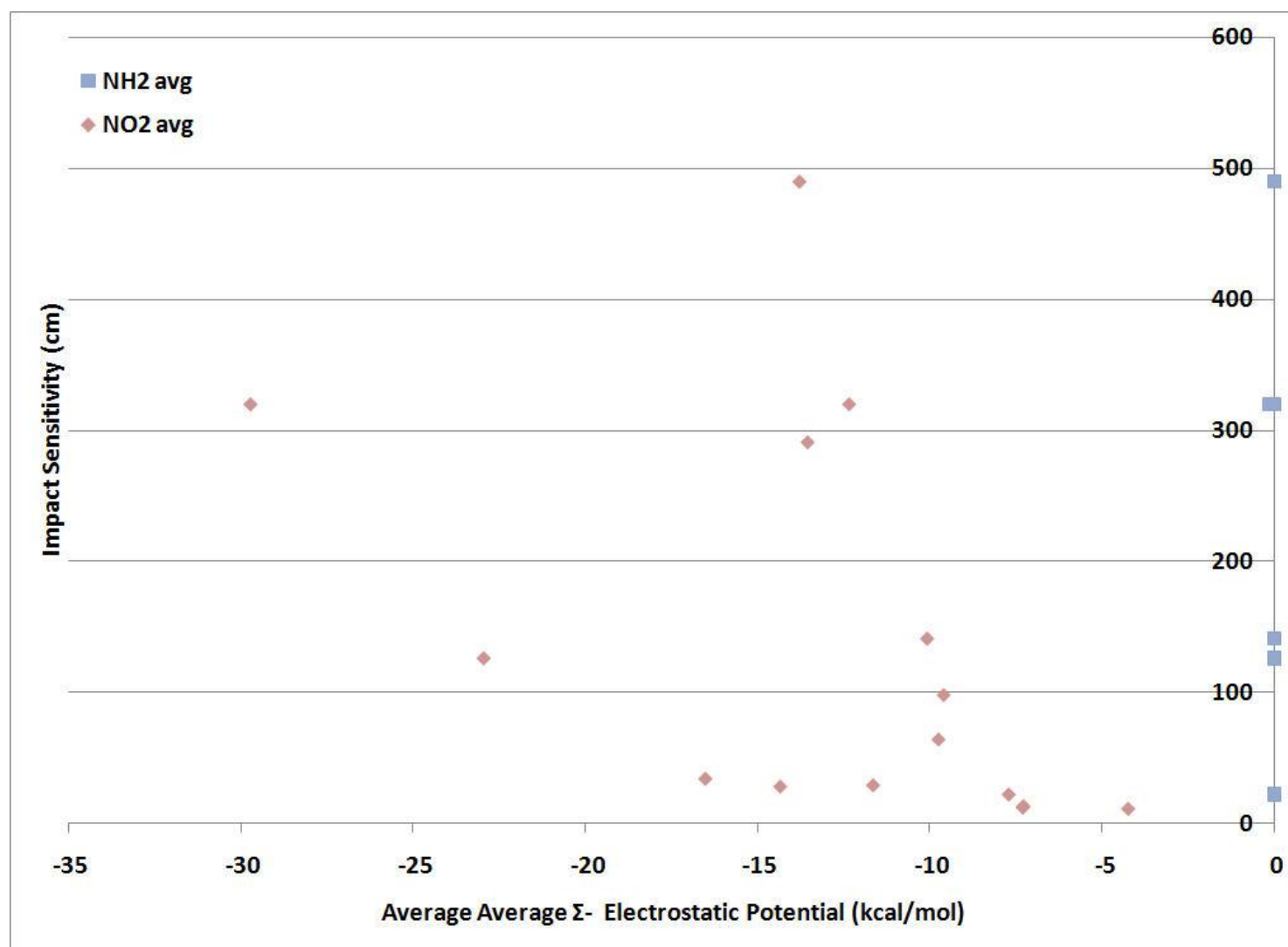


Figure A-49. Impact sensitivity (cm) vs. group average average Σ - electrostatic potential (kcal/mol) for PBE/6-31G**.

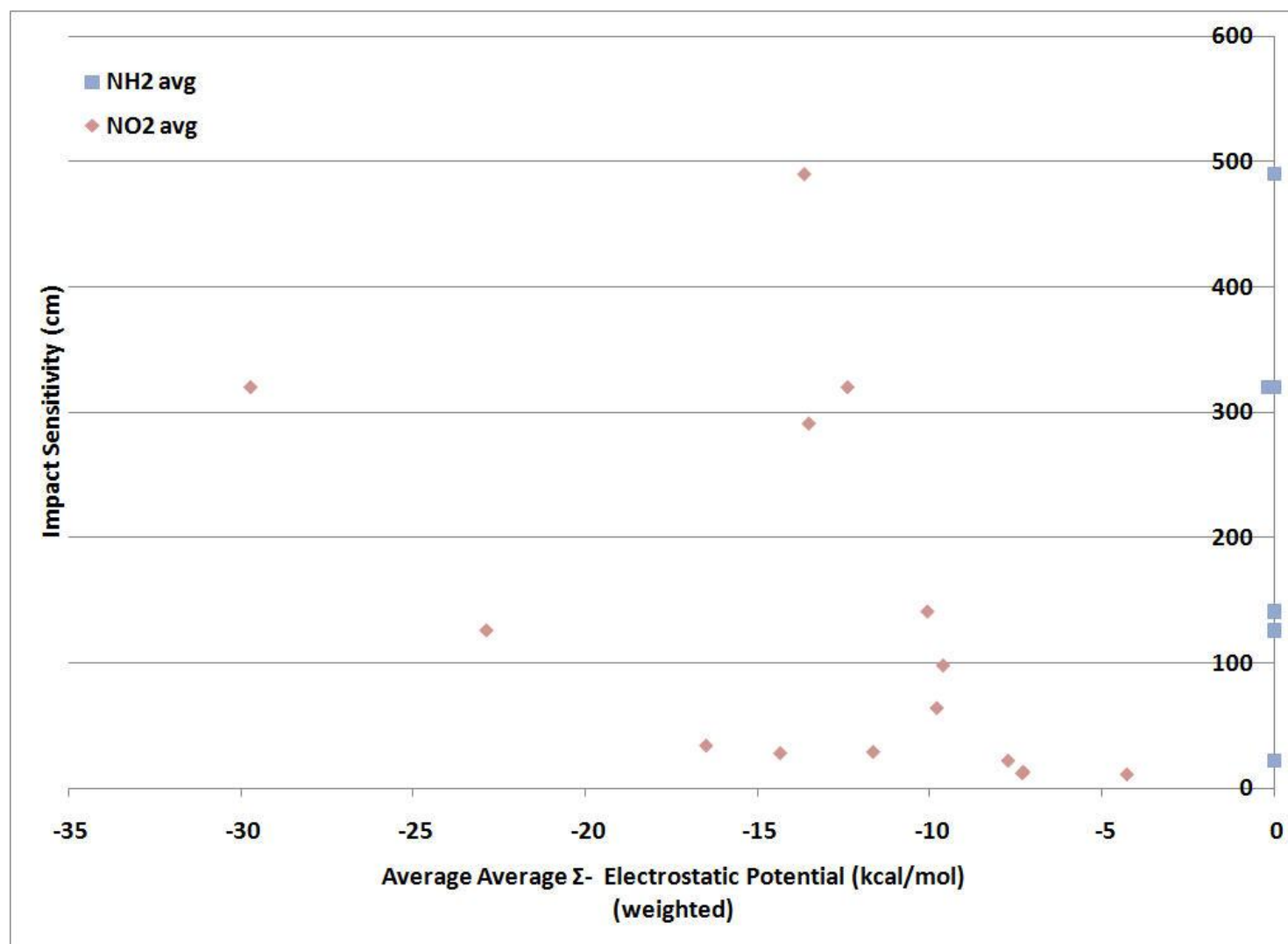


Figure A-50. Impact sensitivity (cm) vs. area weighted group average average Σ^- electrostatic potential (kcal/mol) for PBE/6-31G**.

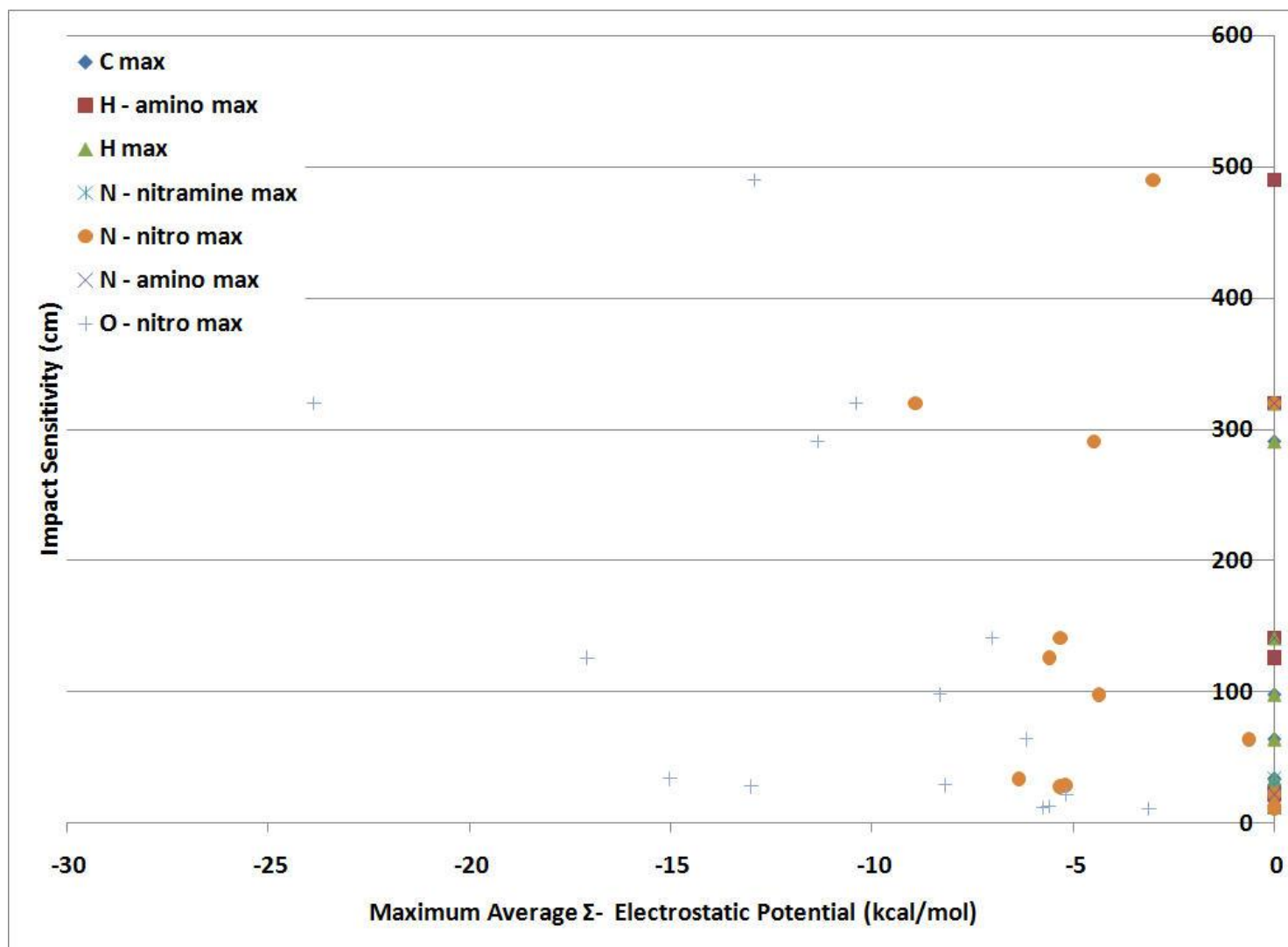


Figure A-51. Impact sensitivity (cm) vs. atomic maximum average Σ^- electrostatic potential (kcal/mol) for PBE/6-31G**.

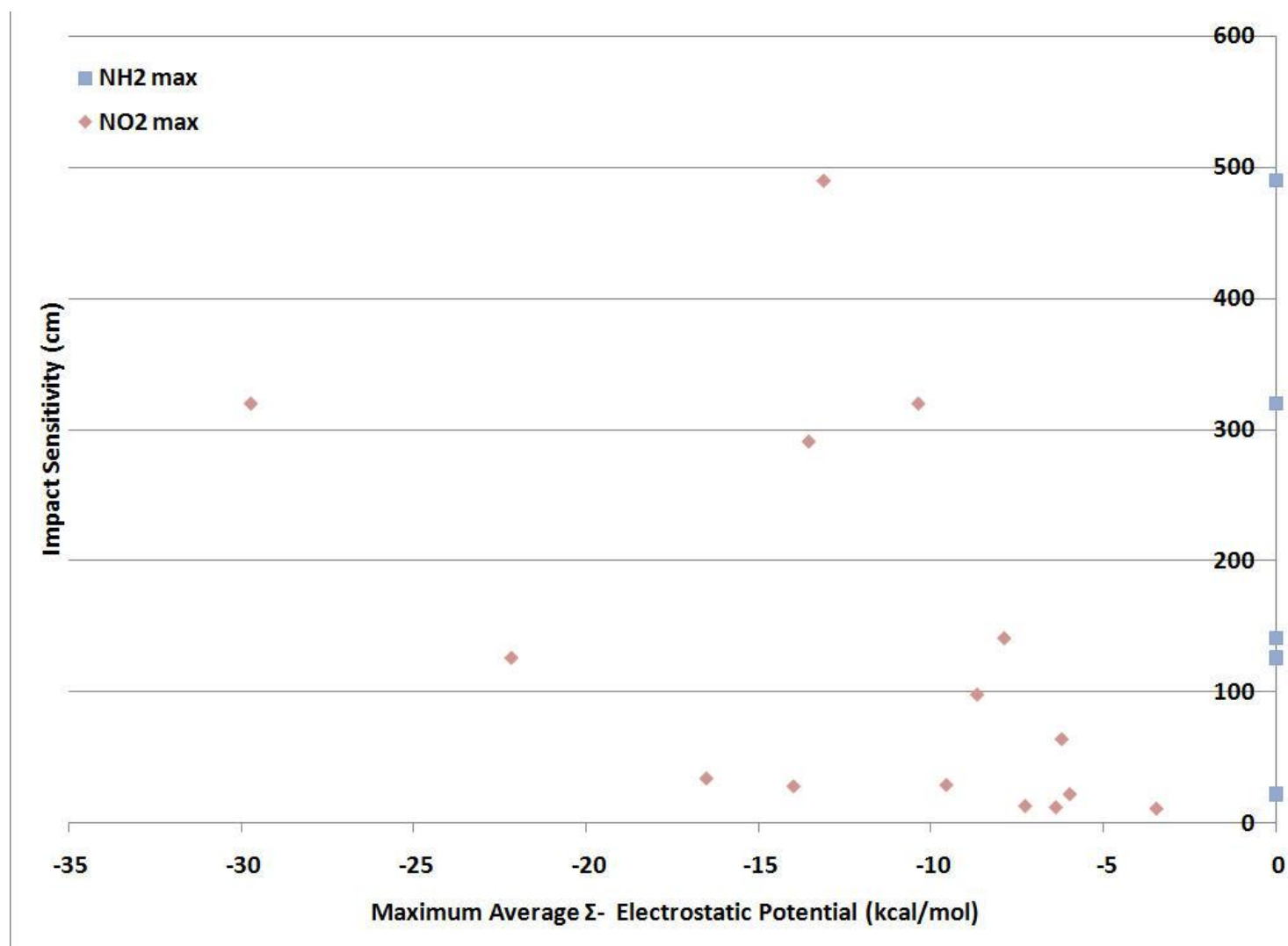


Figure A-52. Impact sensitivity (cm) vs. group maximum average Σ^- electrostatic potential (kcal/mol) for PBE/6-31G**.

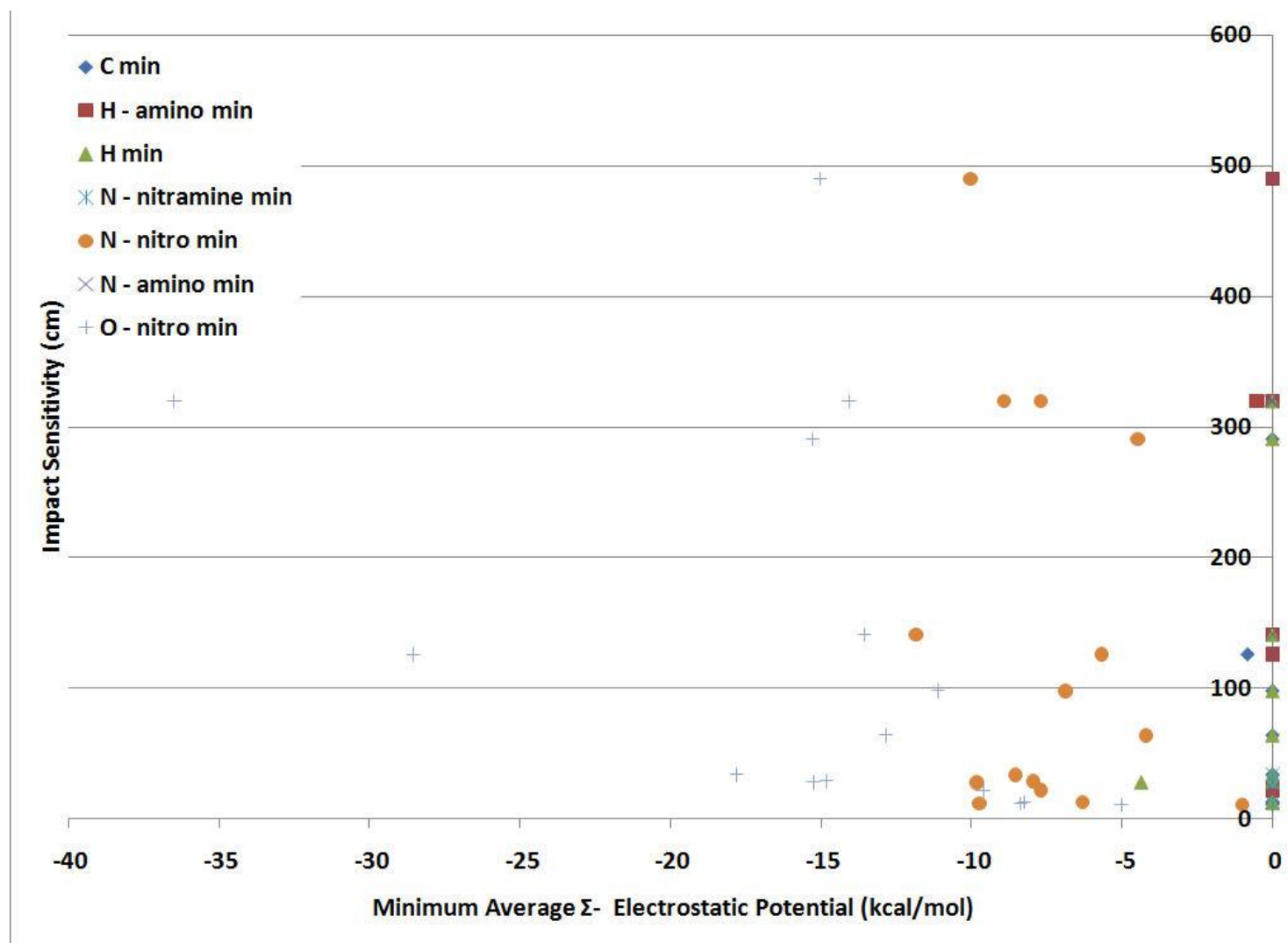


Figure A-53. Impact sensitivity (cm) vs. atomic minimum average Σ - electrostatic potential (kcal/mol) for PBE/6-31G**.

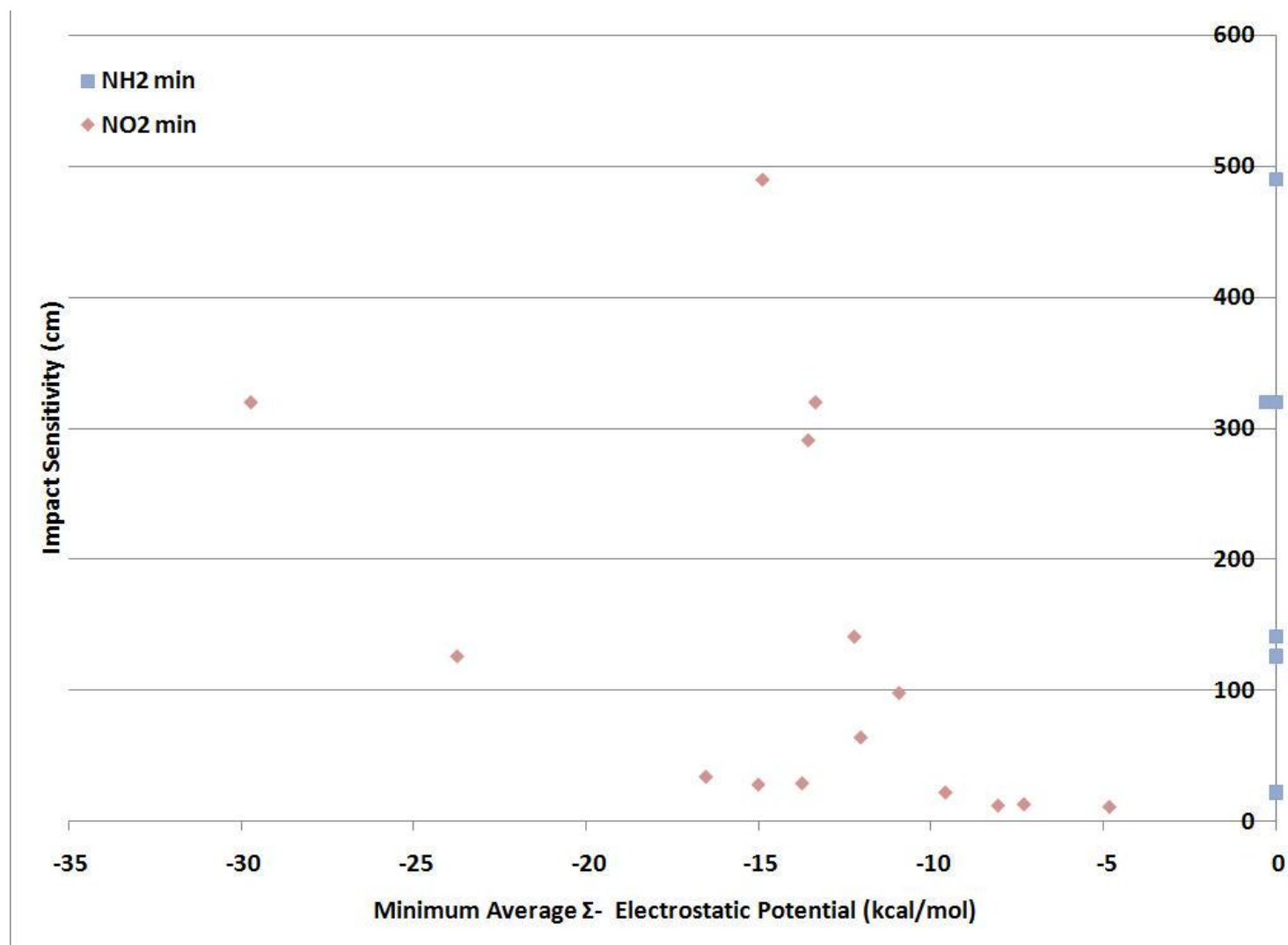


Figure A-54. Impact sensitivity (cm) vs. group minimum average Σ^- electrostatic potential (kcal/mol) for PBE/6-31G**.

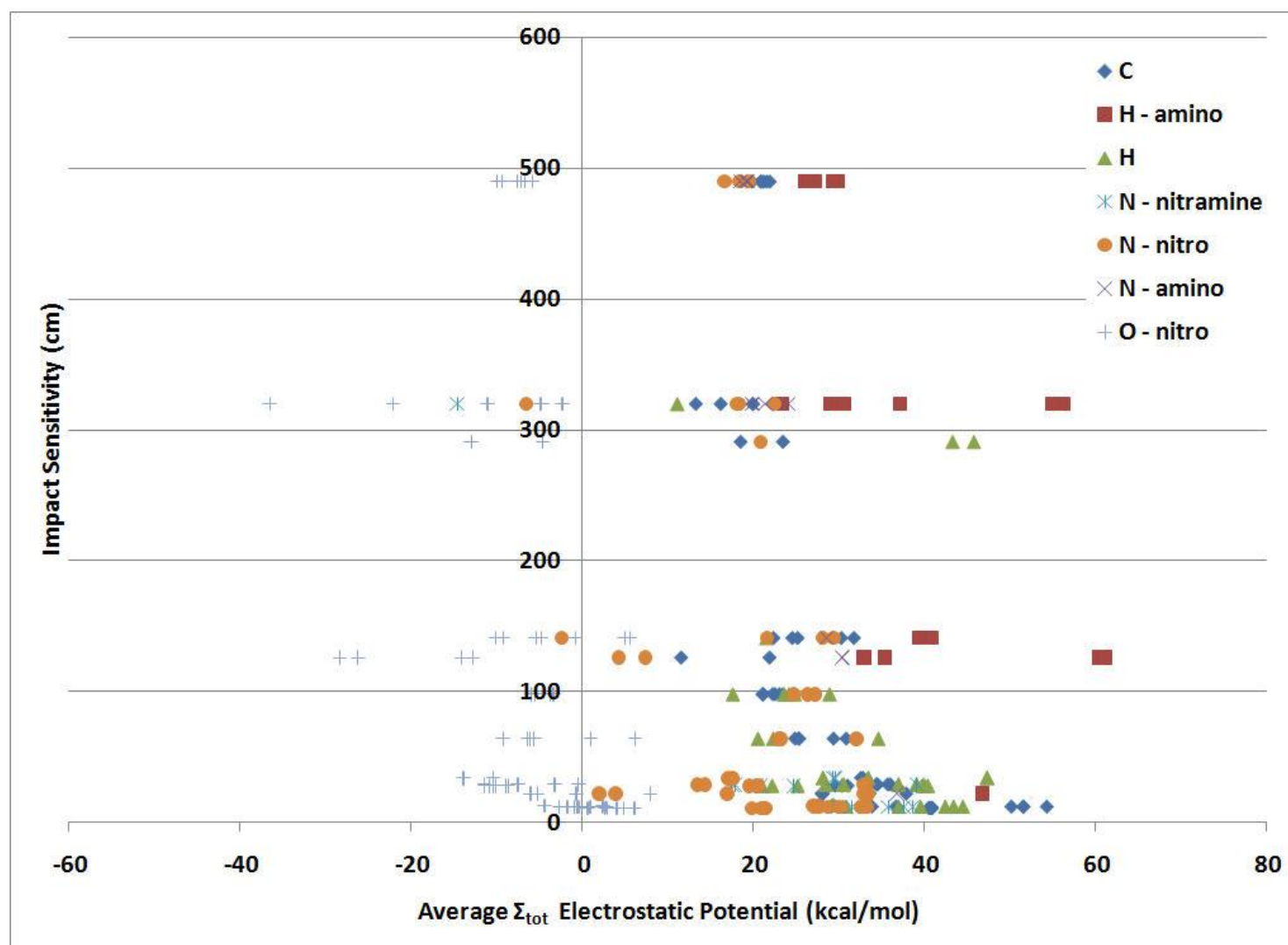


Figure A-55. Impact sensitivity (cm) vs. atomic average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

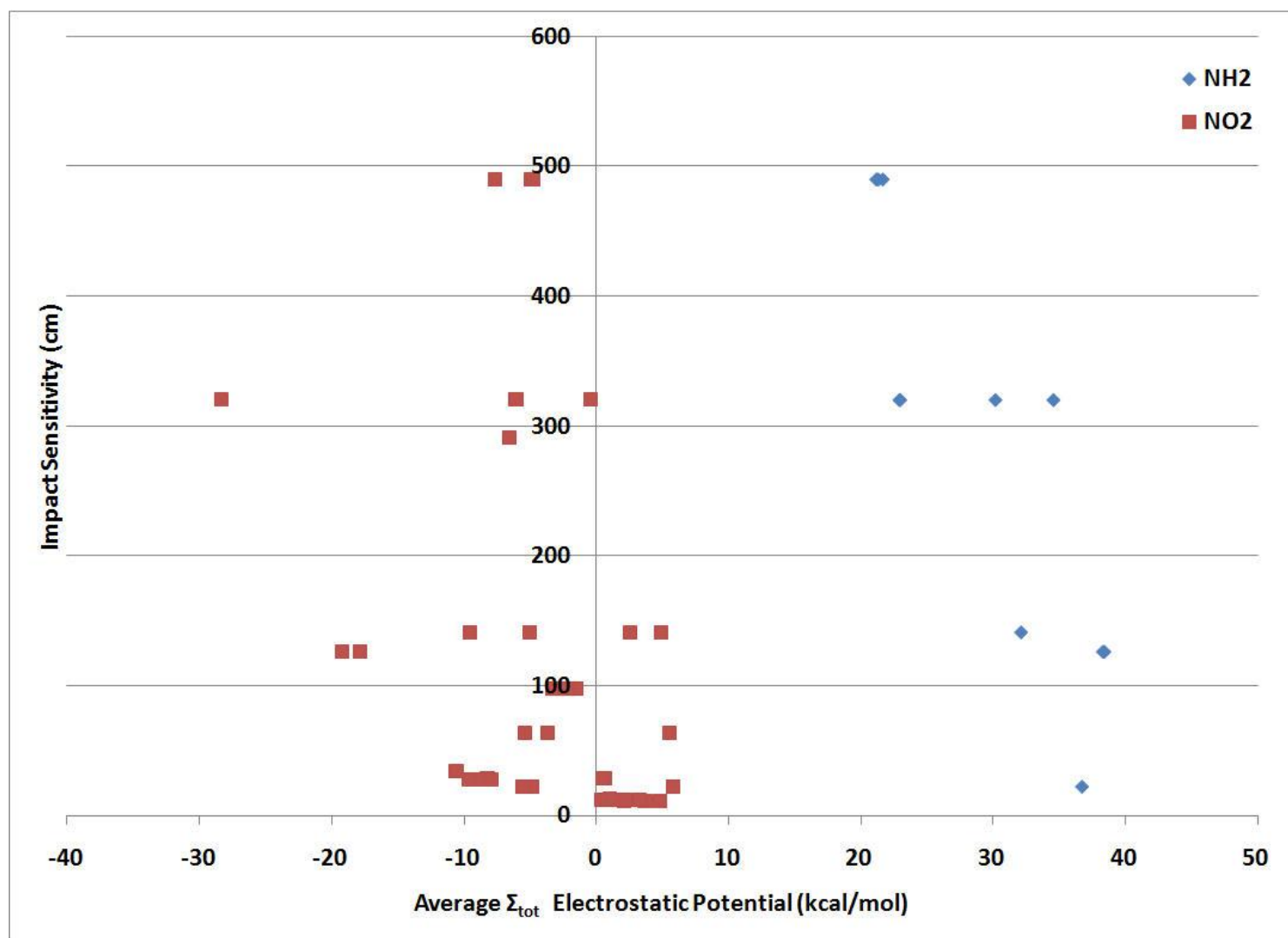


Figure A-56. Impact sensitivity (cm) vs. group average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

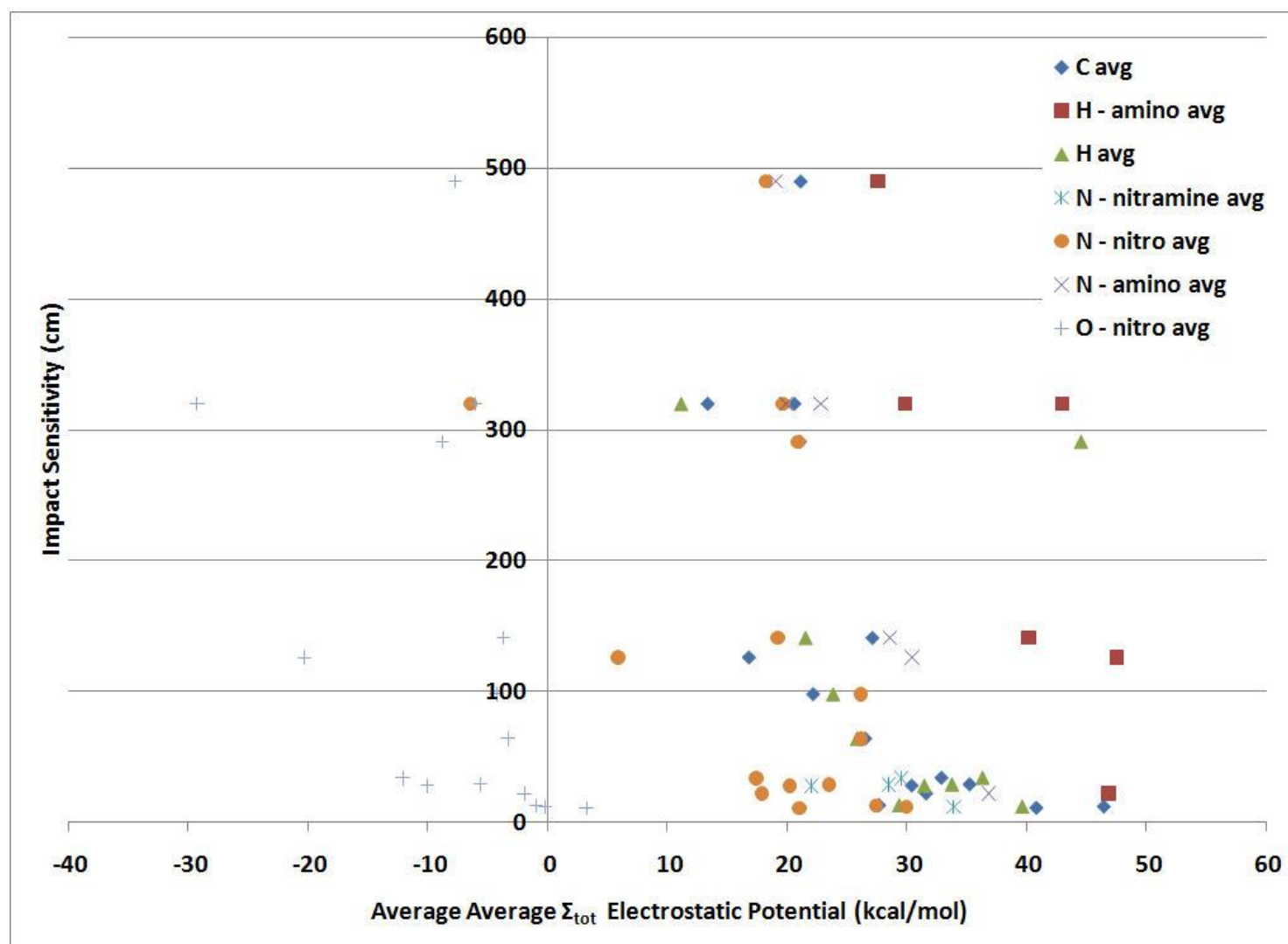


Figure A-57. Impact sensitivity (cm) vs. atomic average average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

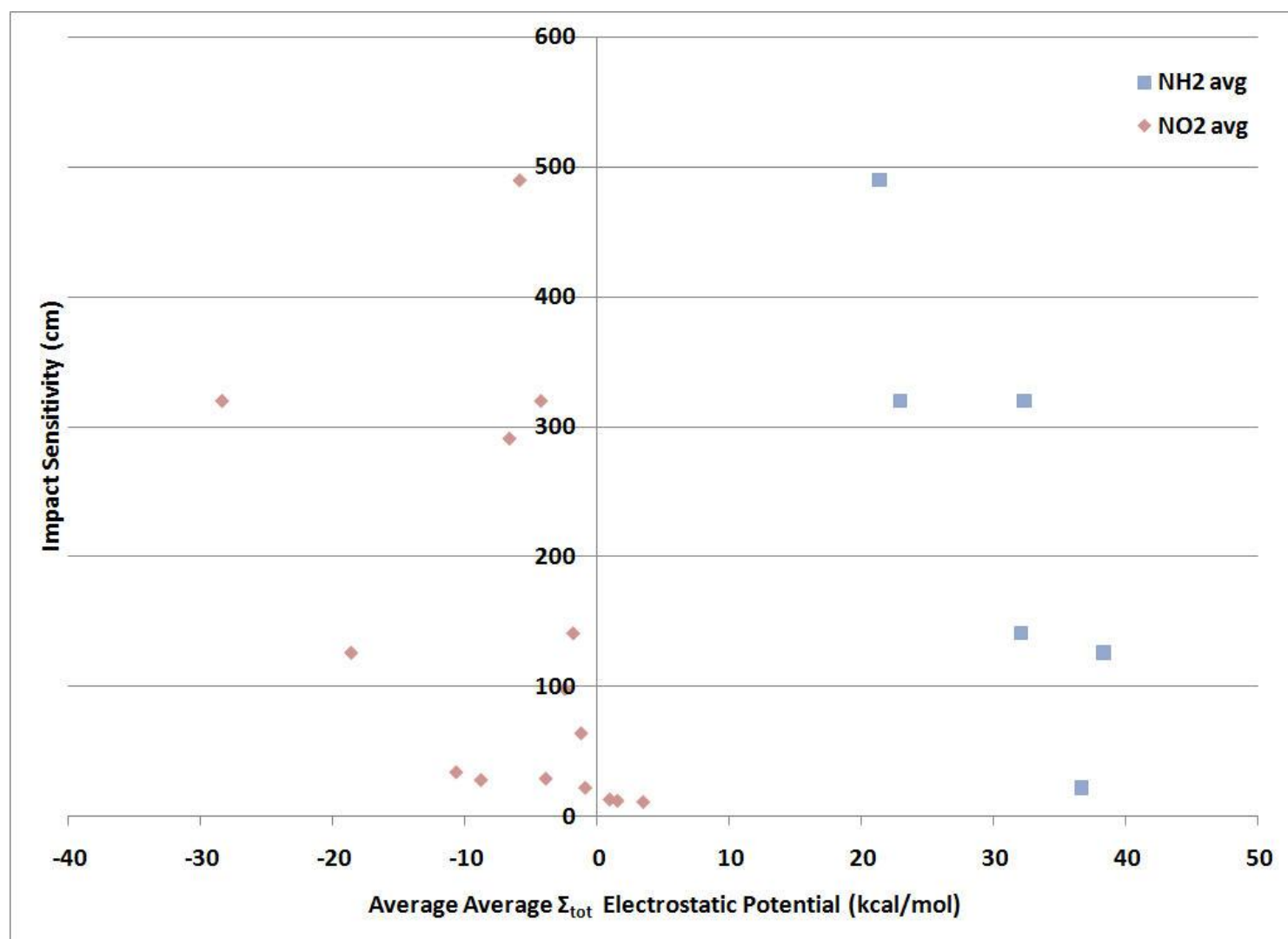


Figure A-58. Impact sensitivity (cm) vs. group average average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

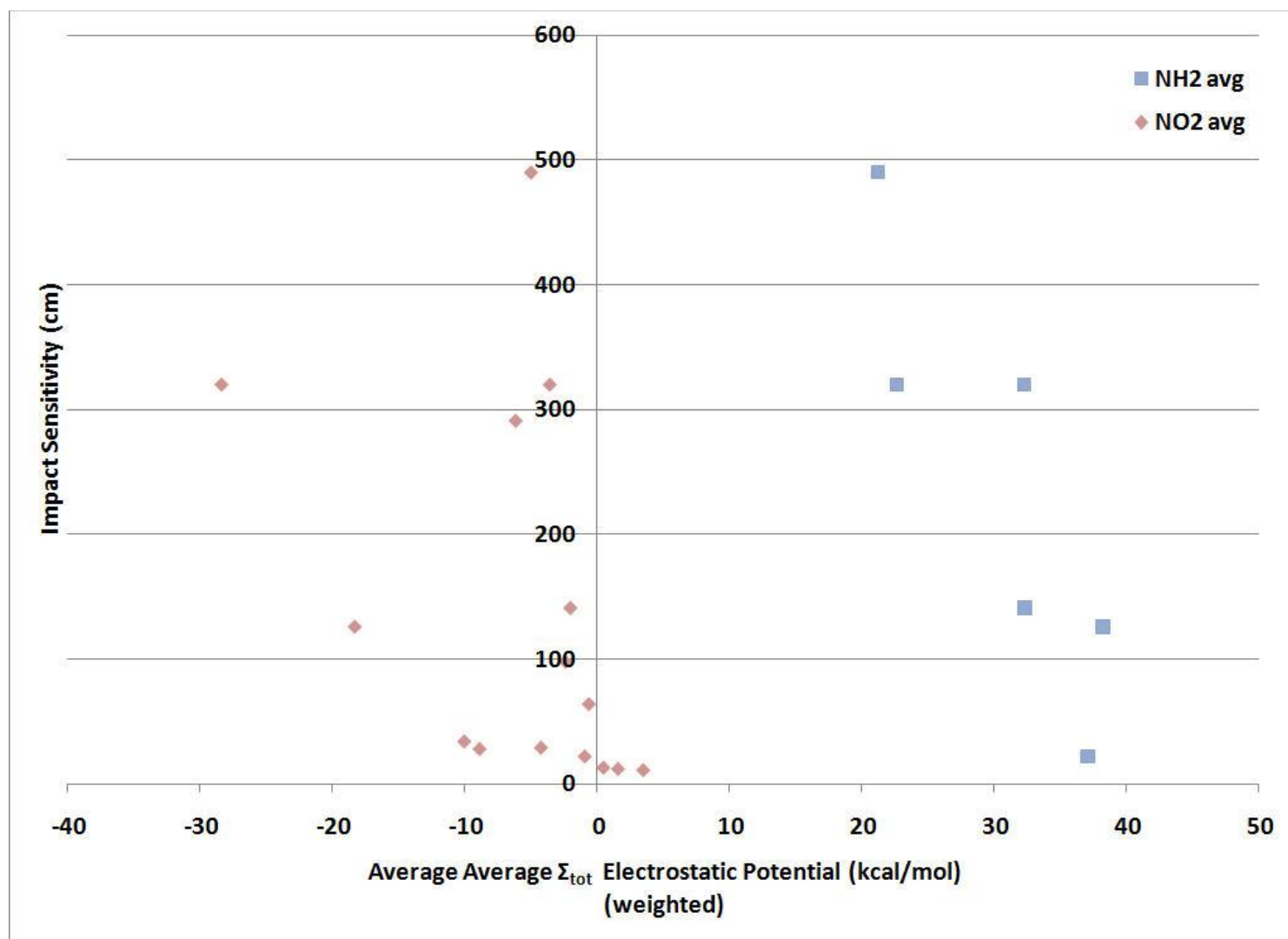


Figure A-59. Impact sensitivity (cm) vs. area weighted group average average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

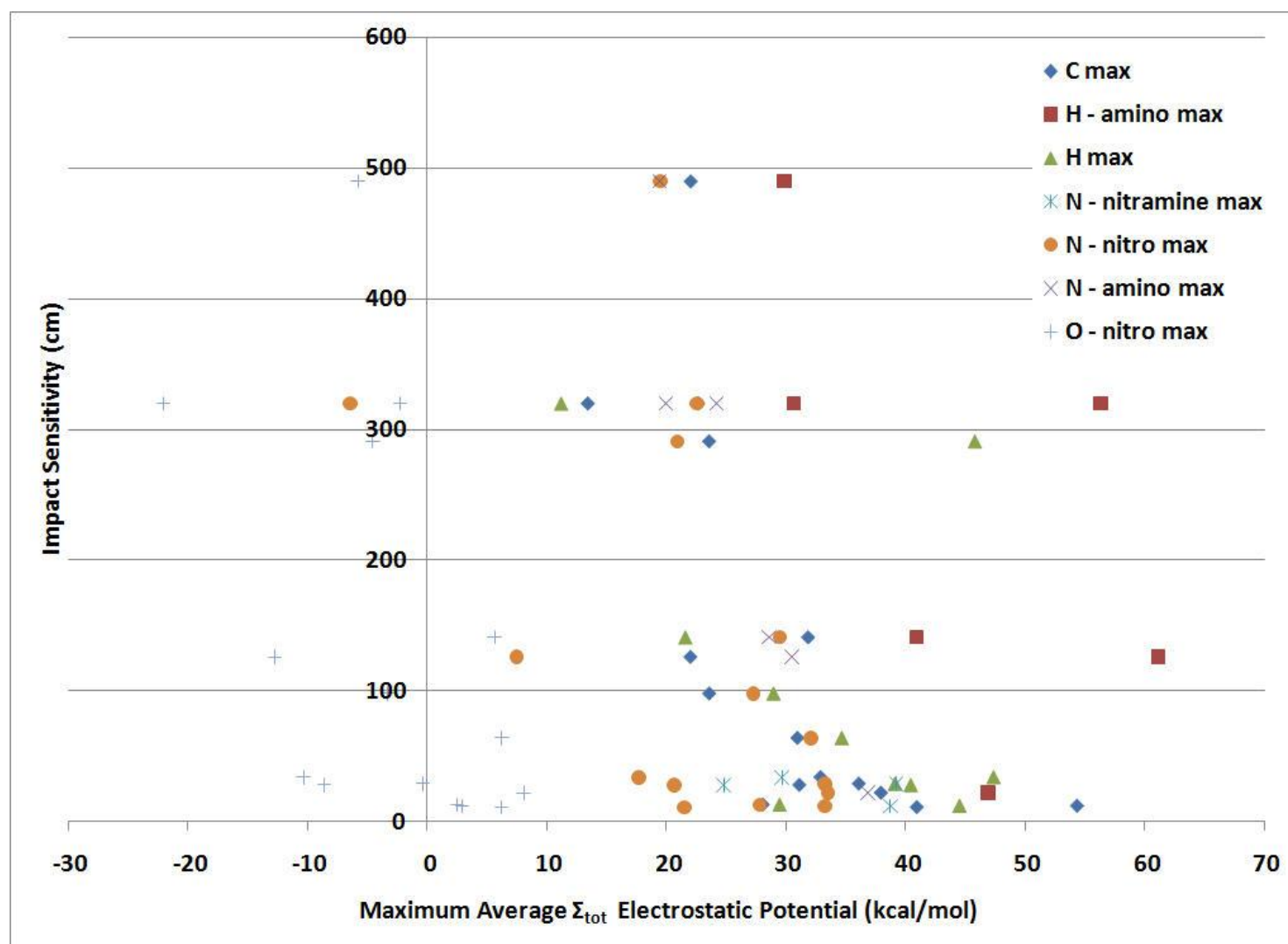


Figure A-60. Impact sensitivity (cm) vs. atomic maximum average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

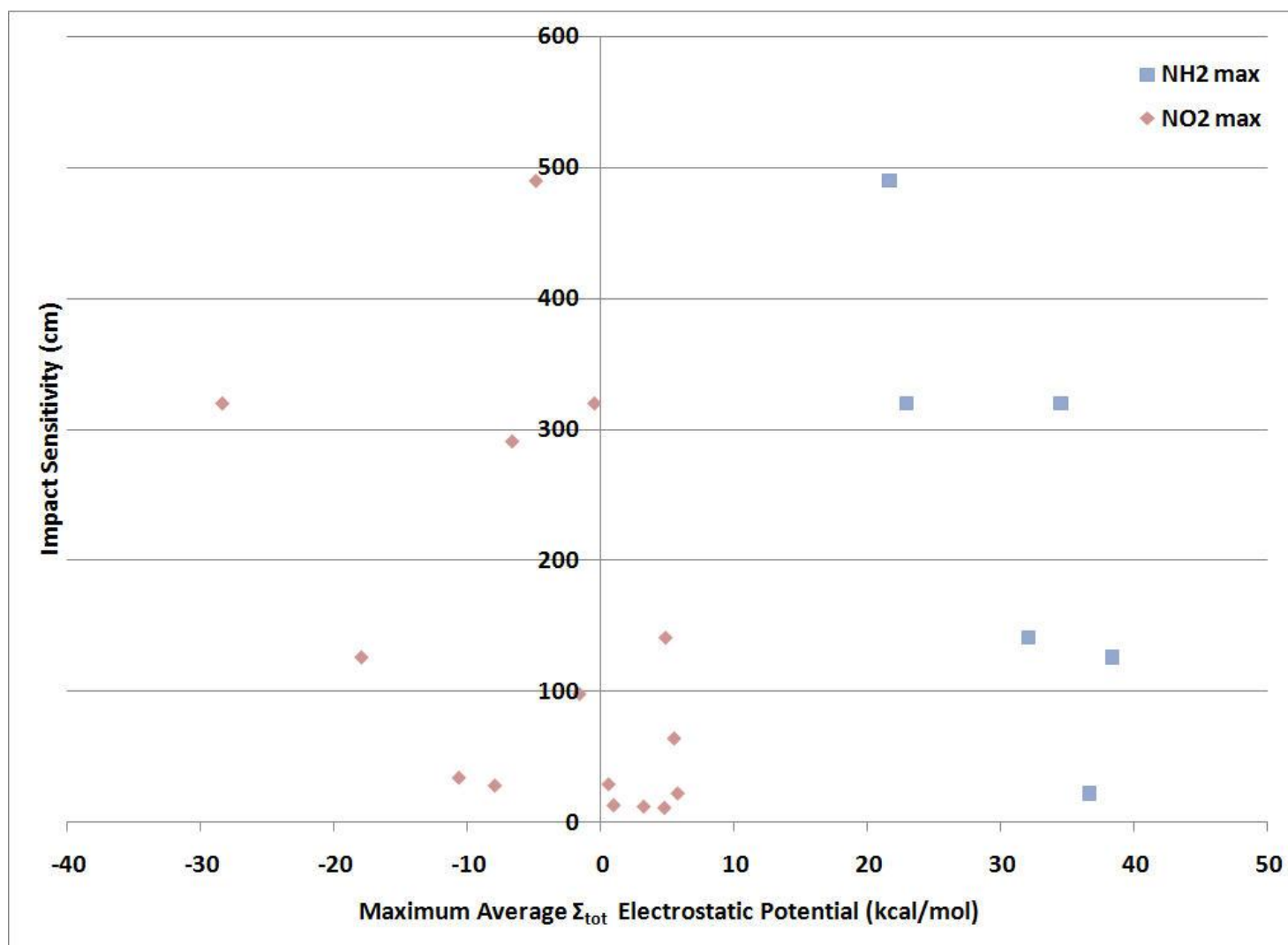


Figure A-61. Impact sensitivity (cm) vs. group maximum average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

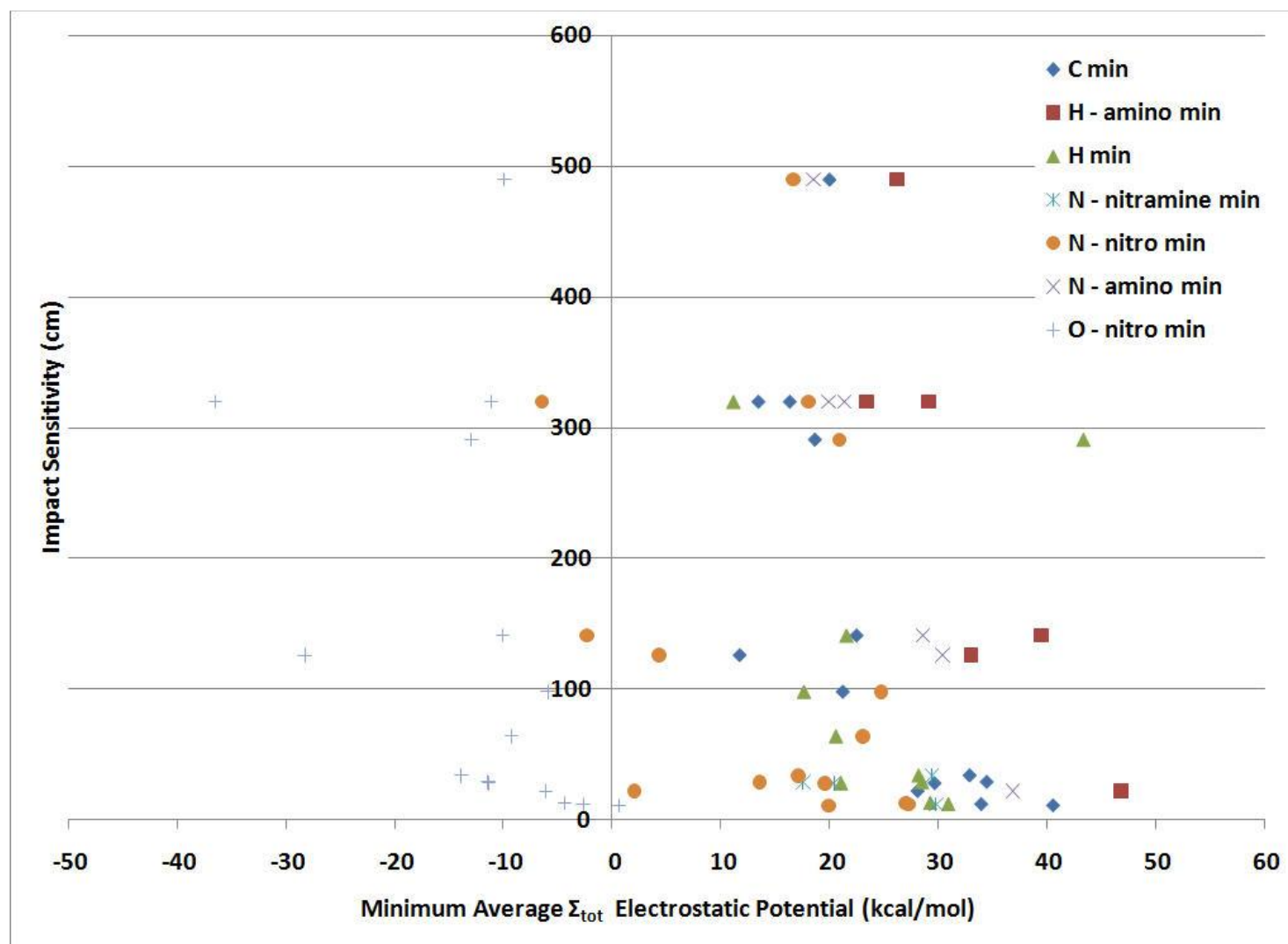


Figure A-62. Impact sensitivity (cm) vs. atomic minimum average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

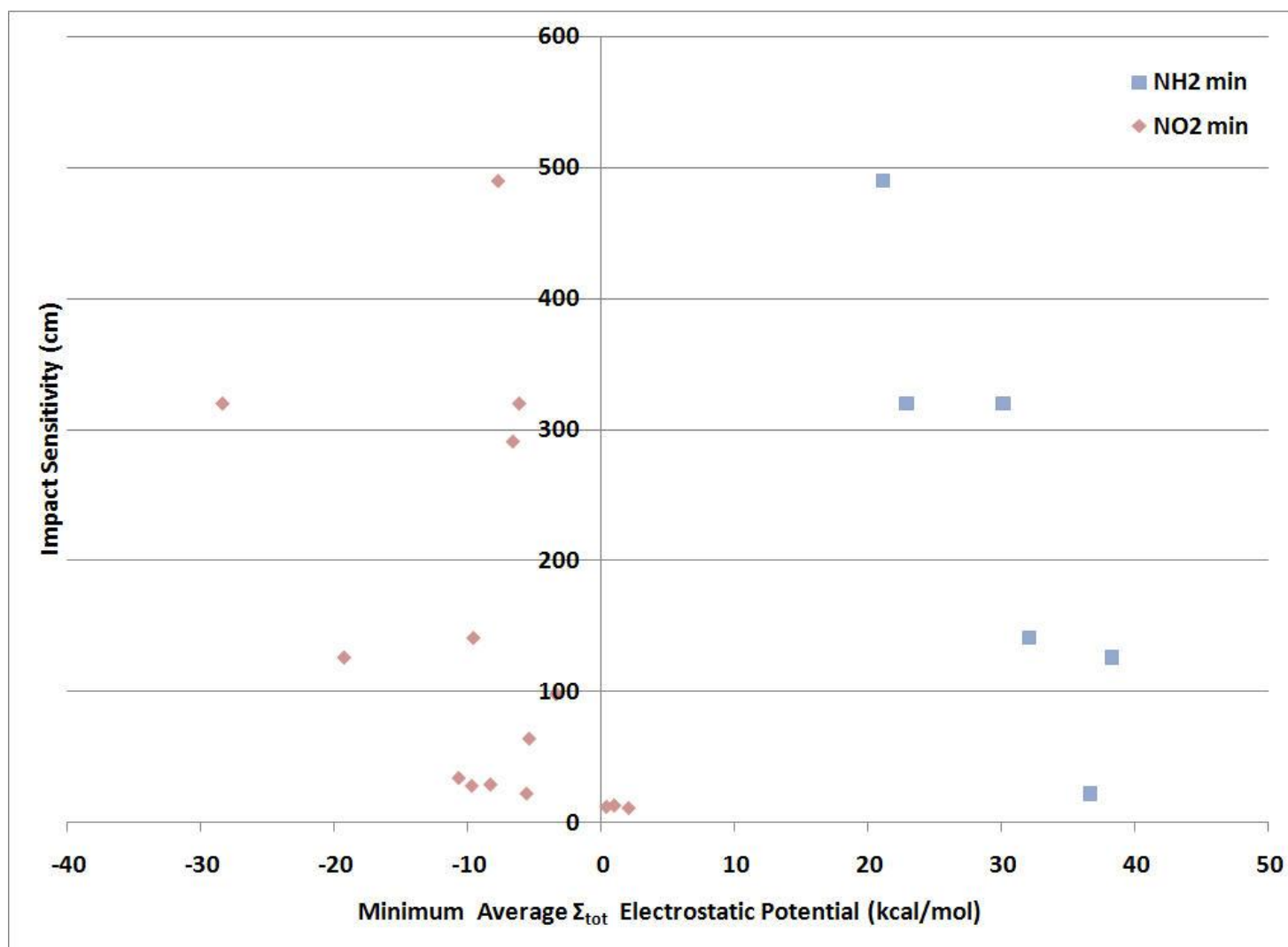


Figure A-63. Impact sensitivity (cm) vs. group minimum average Σ_{tot} electrostatic potential (kcal/mol) for PBE/6-31G**.

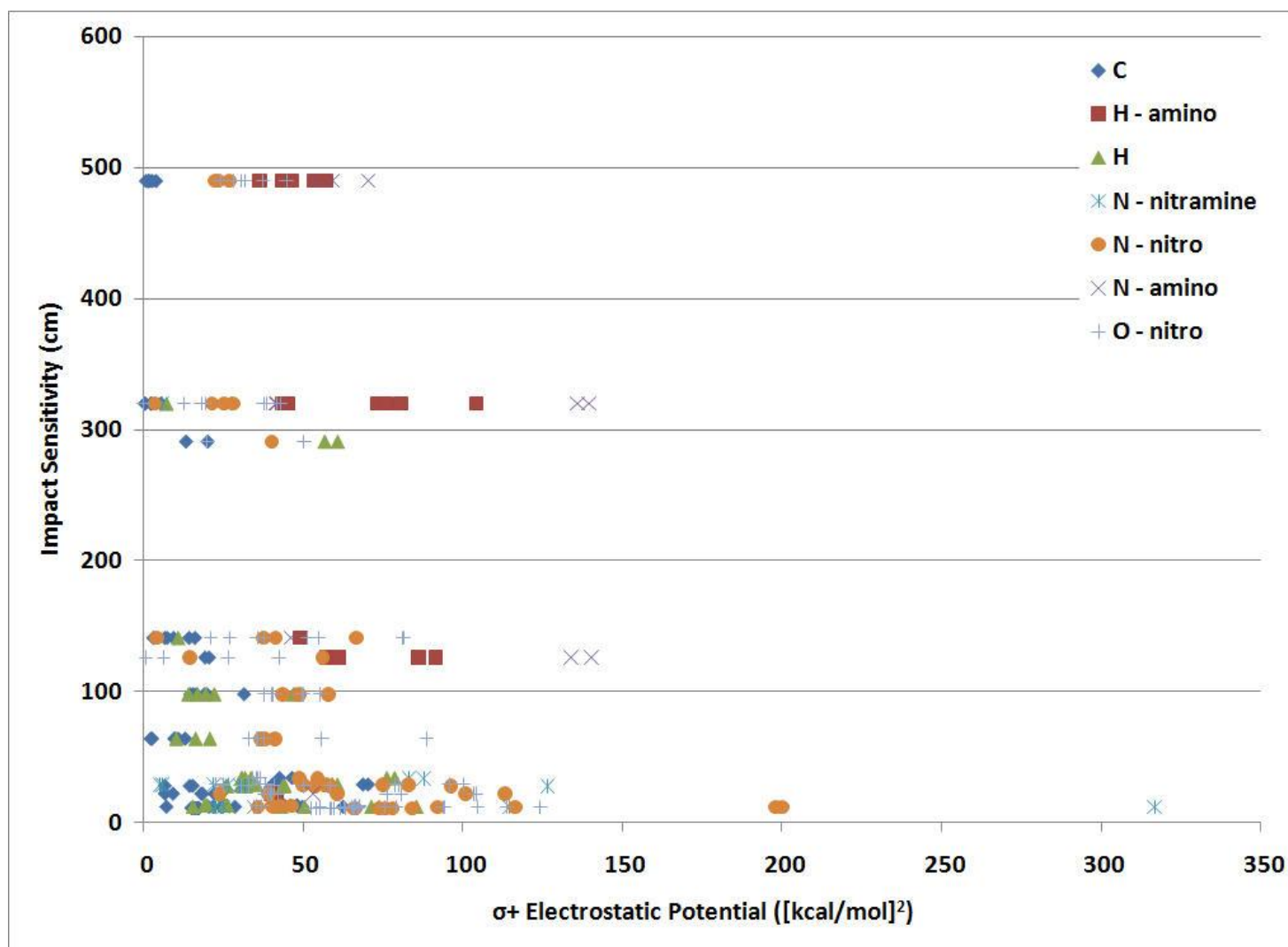


Figure A-64. Impact sensitivity (cm) vs. atomic σ^{22+} electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

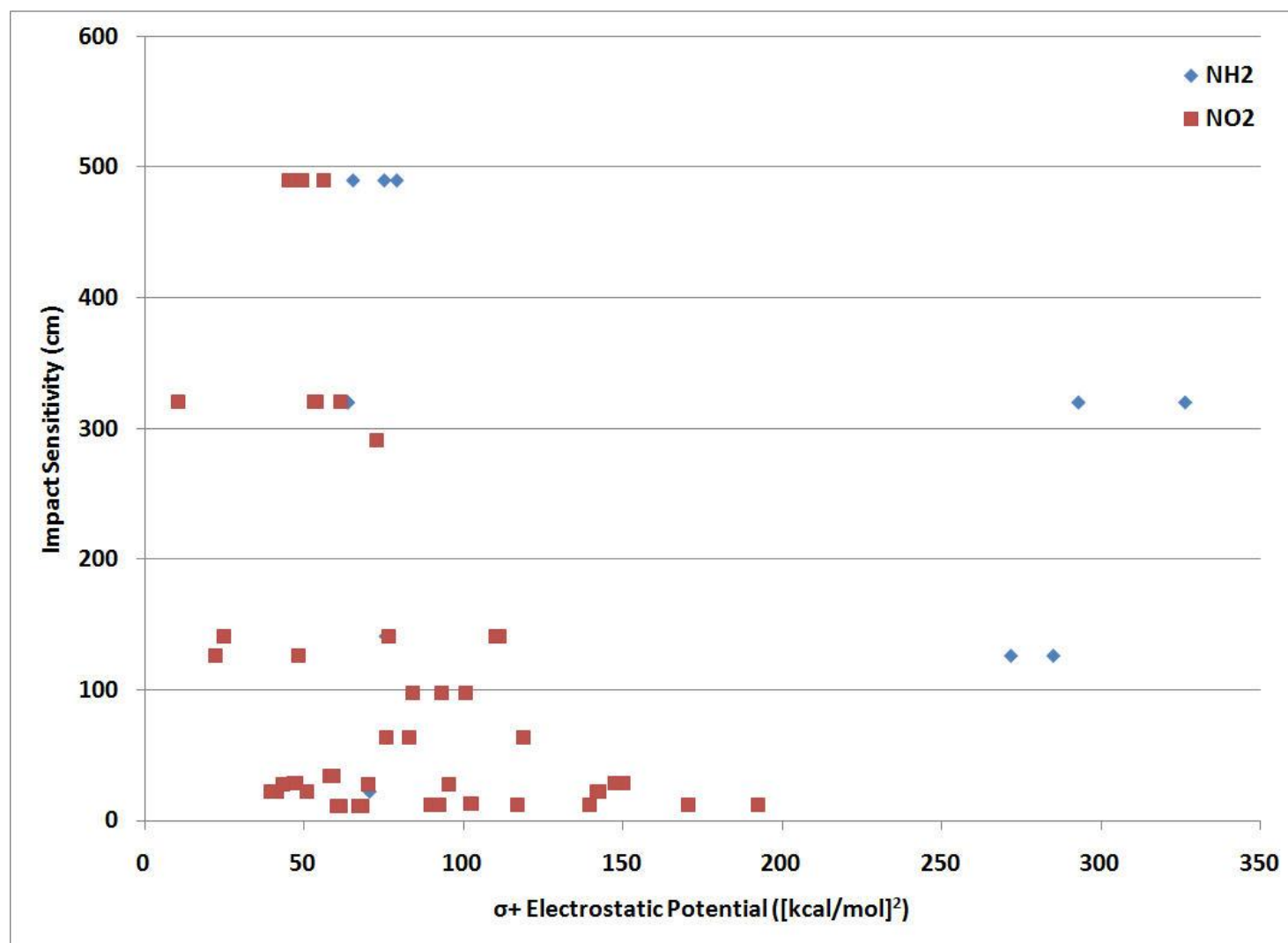


Figure A-65. Impact sensitivity (cm) vs. group σ^2+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

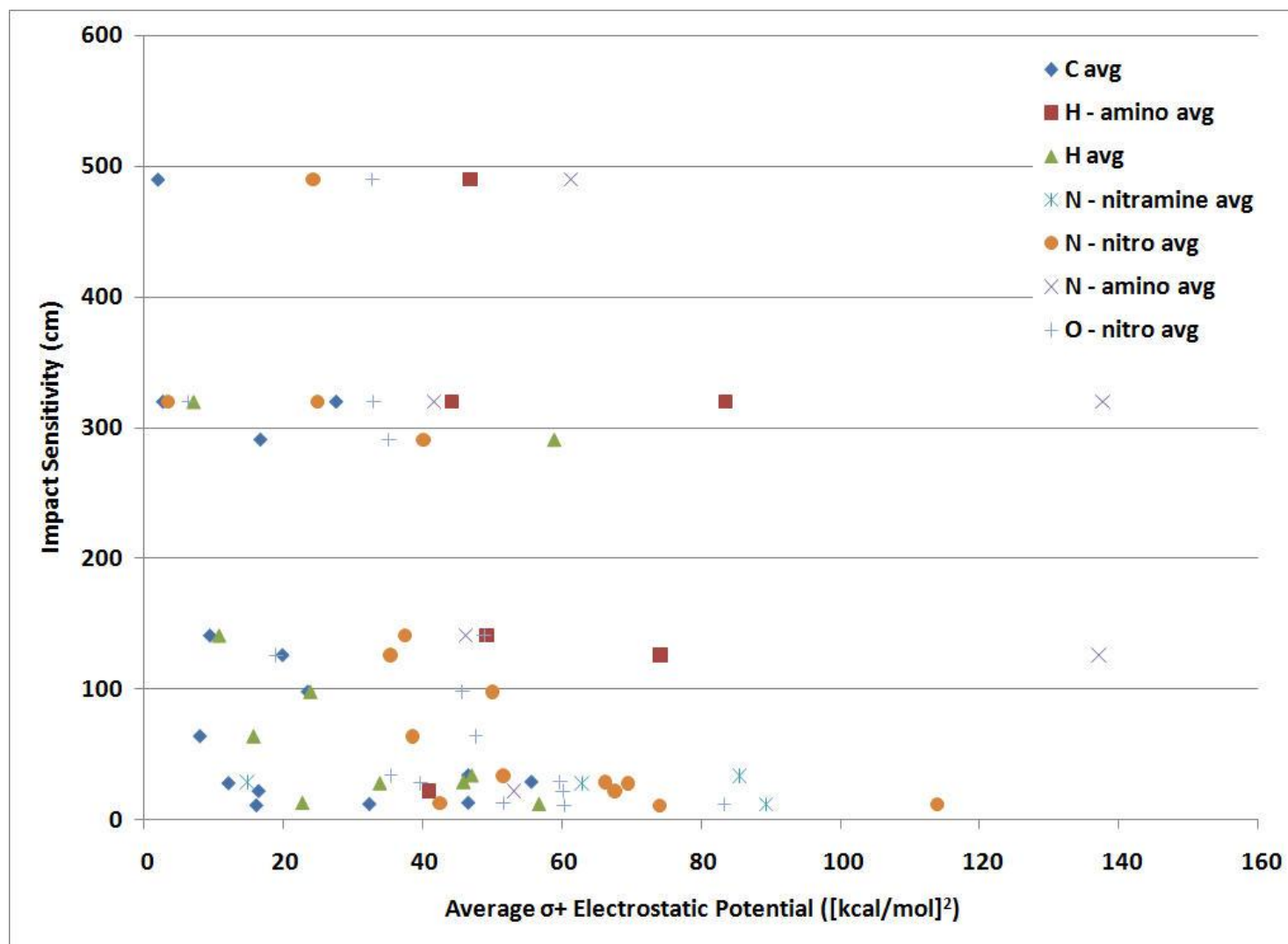


Figure A-66. Impact sensitivity (cm) vs. atomic average σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

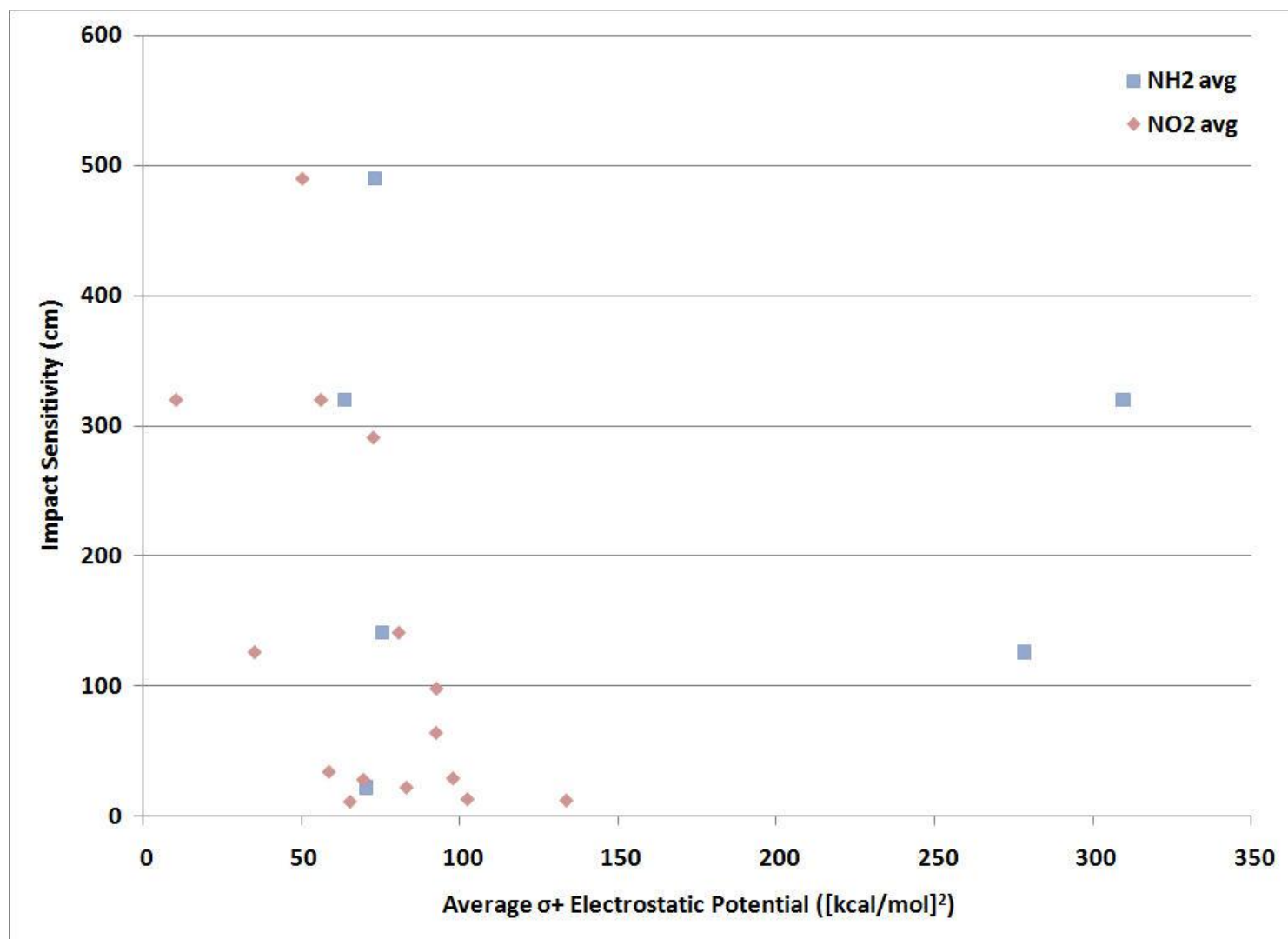


Figure A-67. Impact sensitivity (cm) vs. group average σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

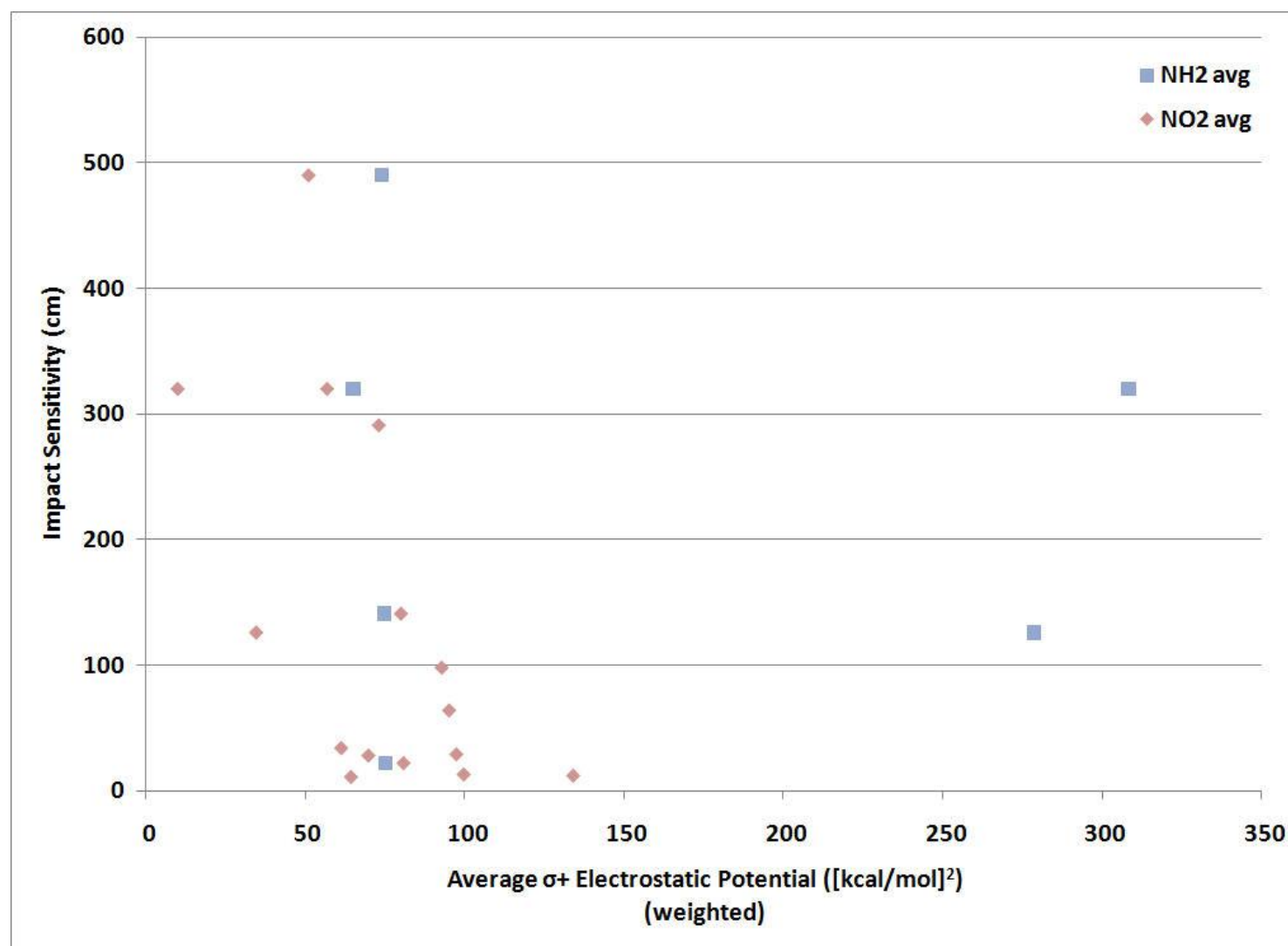


Figure A-68. Impact sensitivity (cm) vs. area weighted group average σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

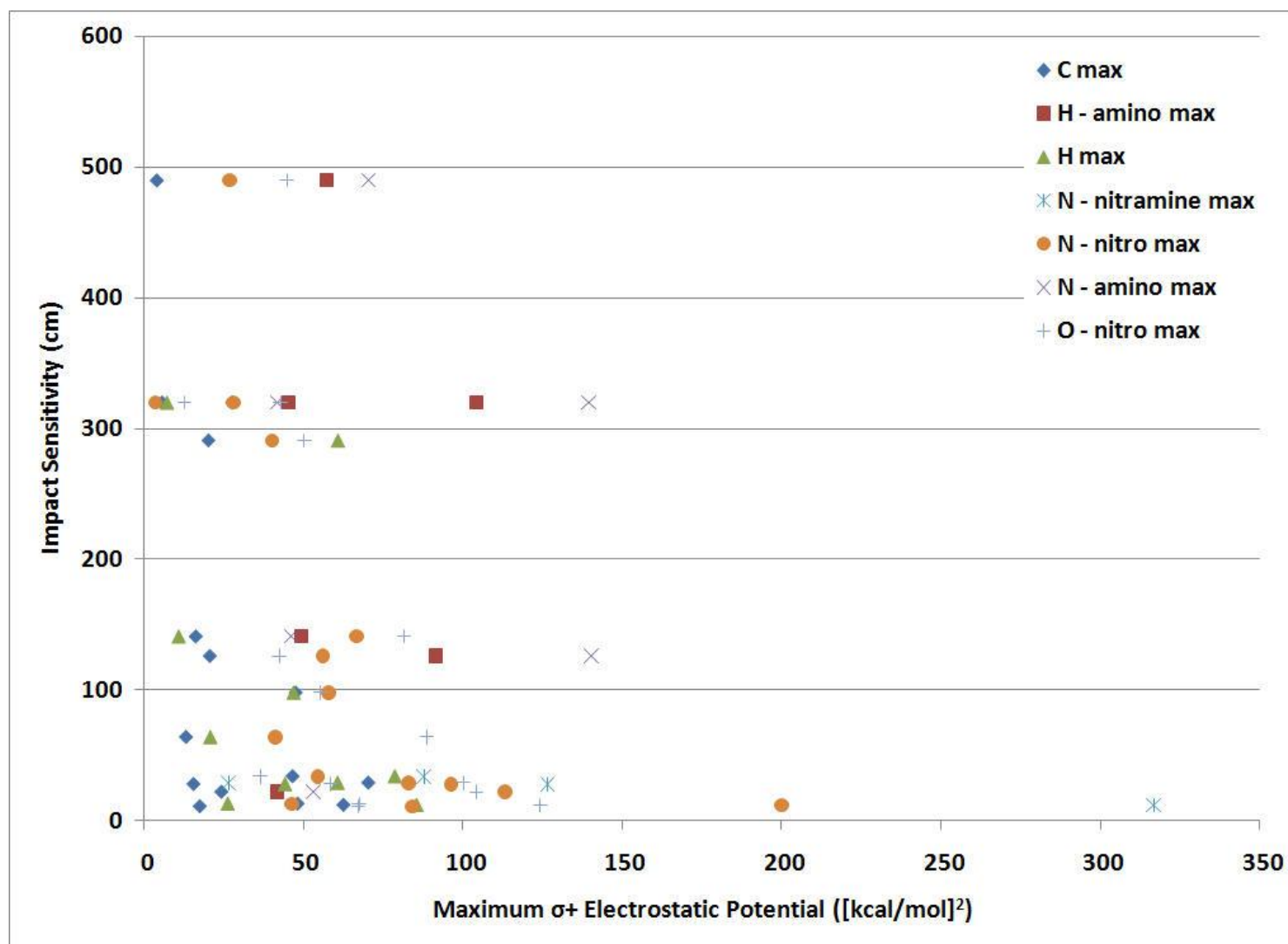


Figure A-69. Impact sensitivity (cm) vs. atomic maximum σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

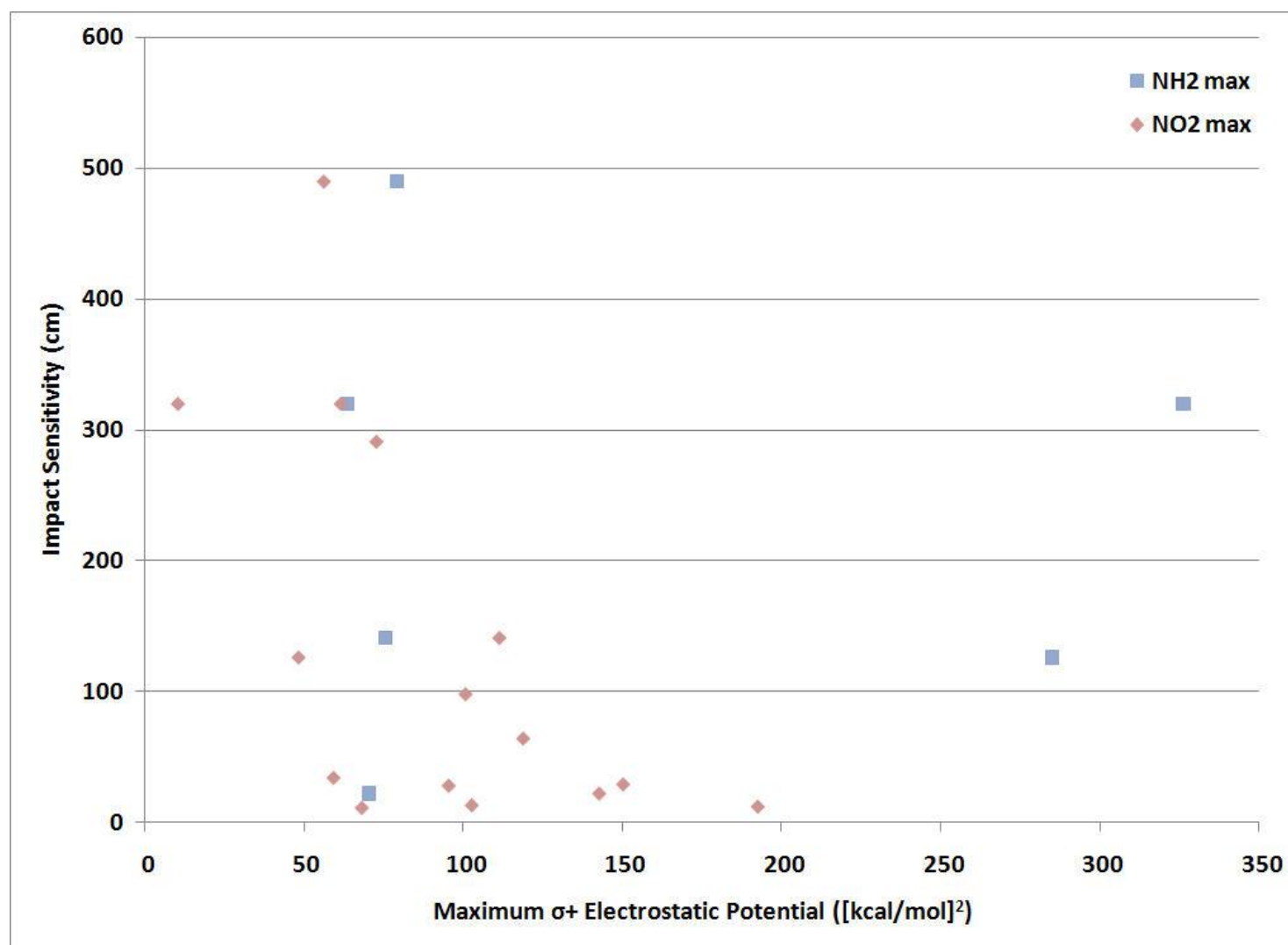


Figure A-70. Impact sensitivity (cm) vs. group maximum σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

Figure A-71. Impact sensitivity (cm) vs. atomic minimum σ^{2+} electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

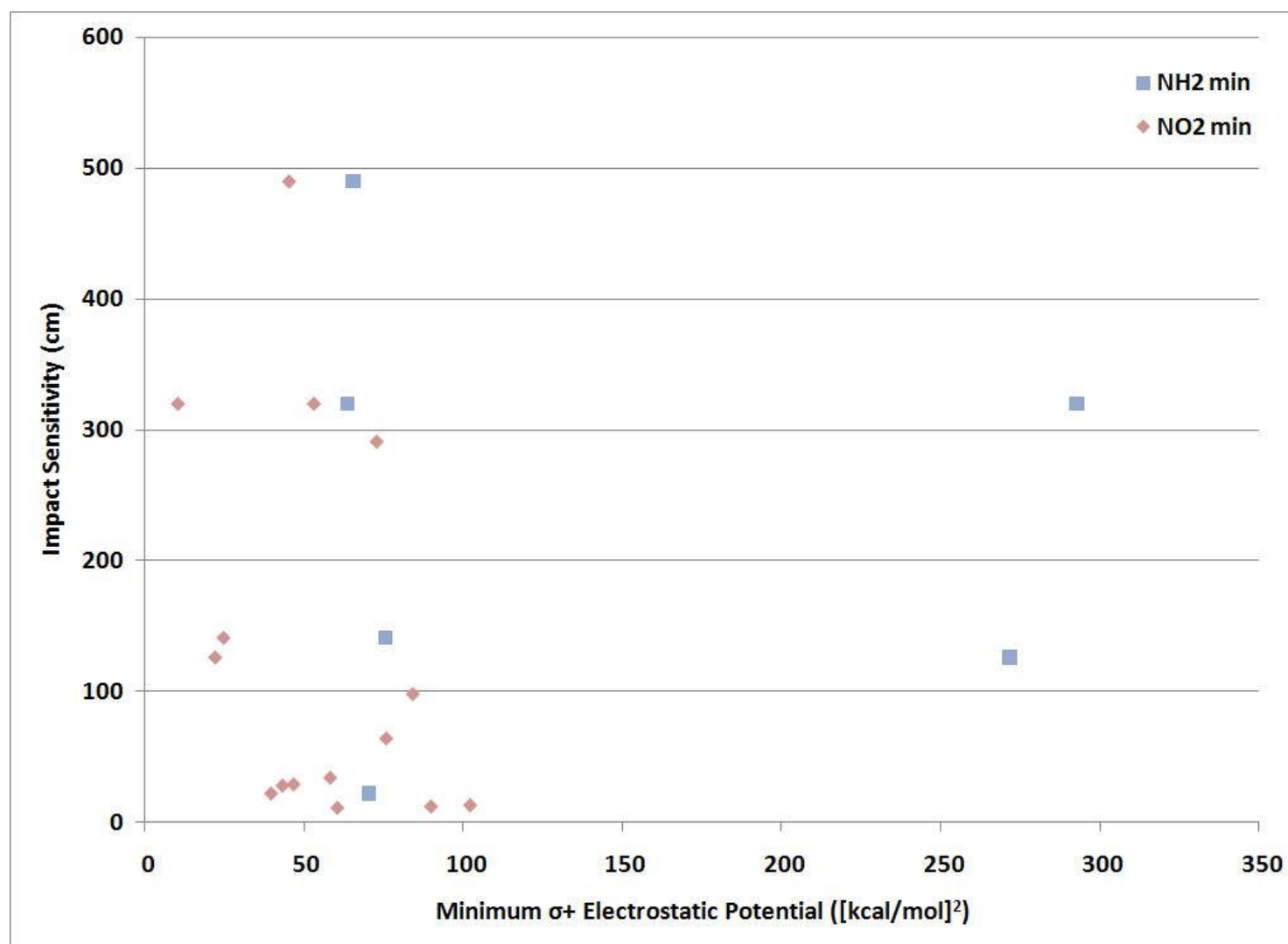


Figure A-72. Impact sensitivity (cm) vs. group minimum σ^+ electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

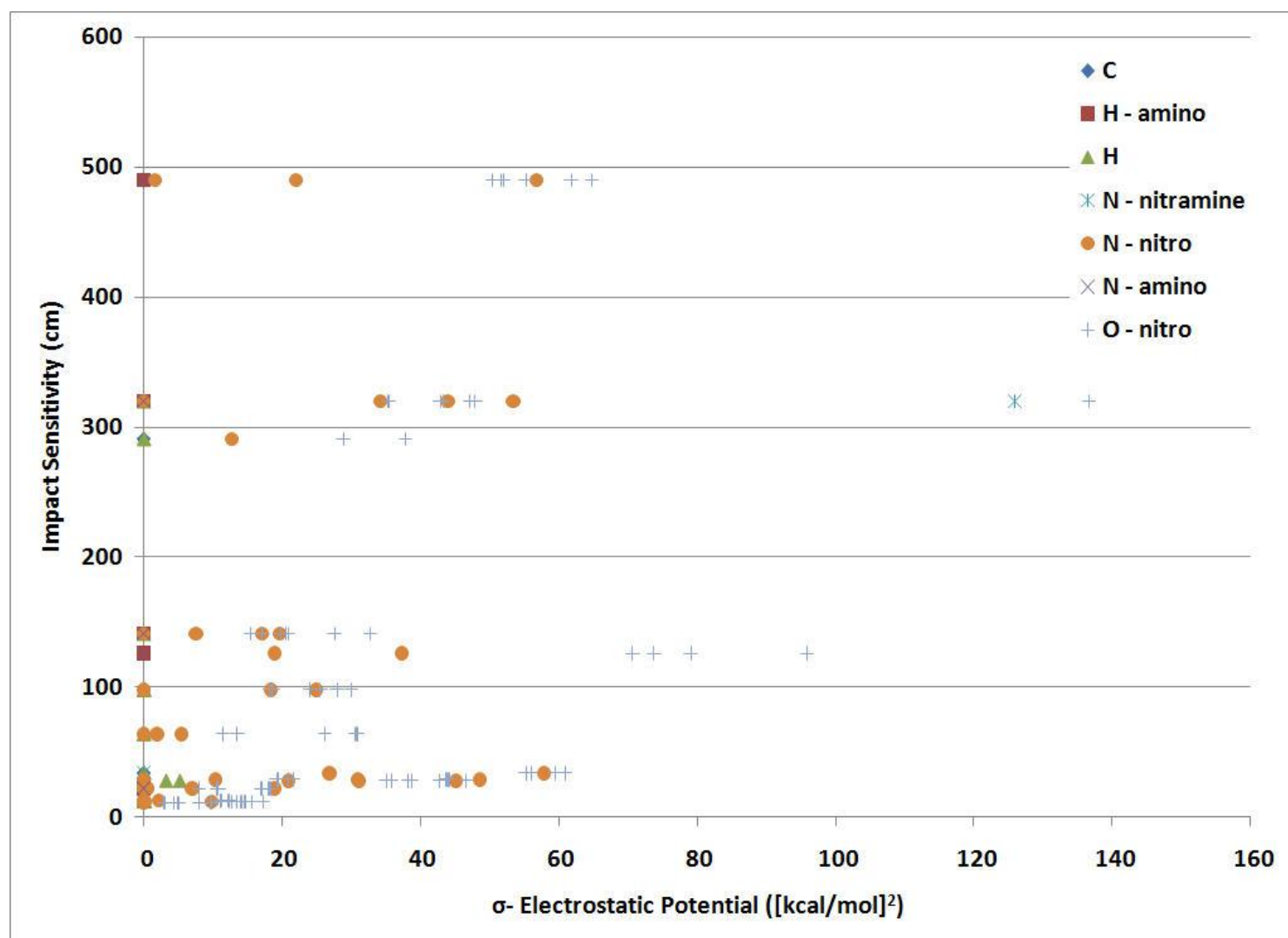


Figure A-73. Impact sensitivity (cm) vs. atomic σ^2 -electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

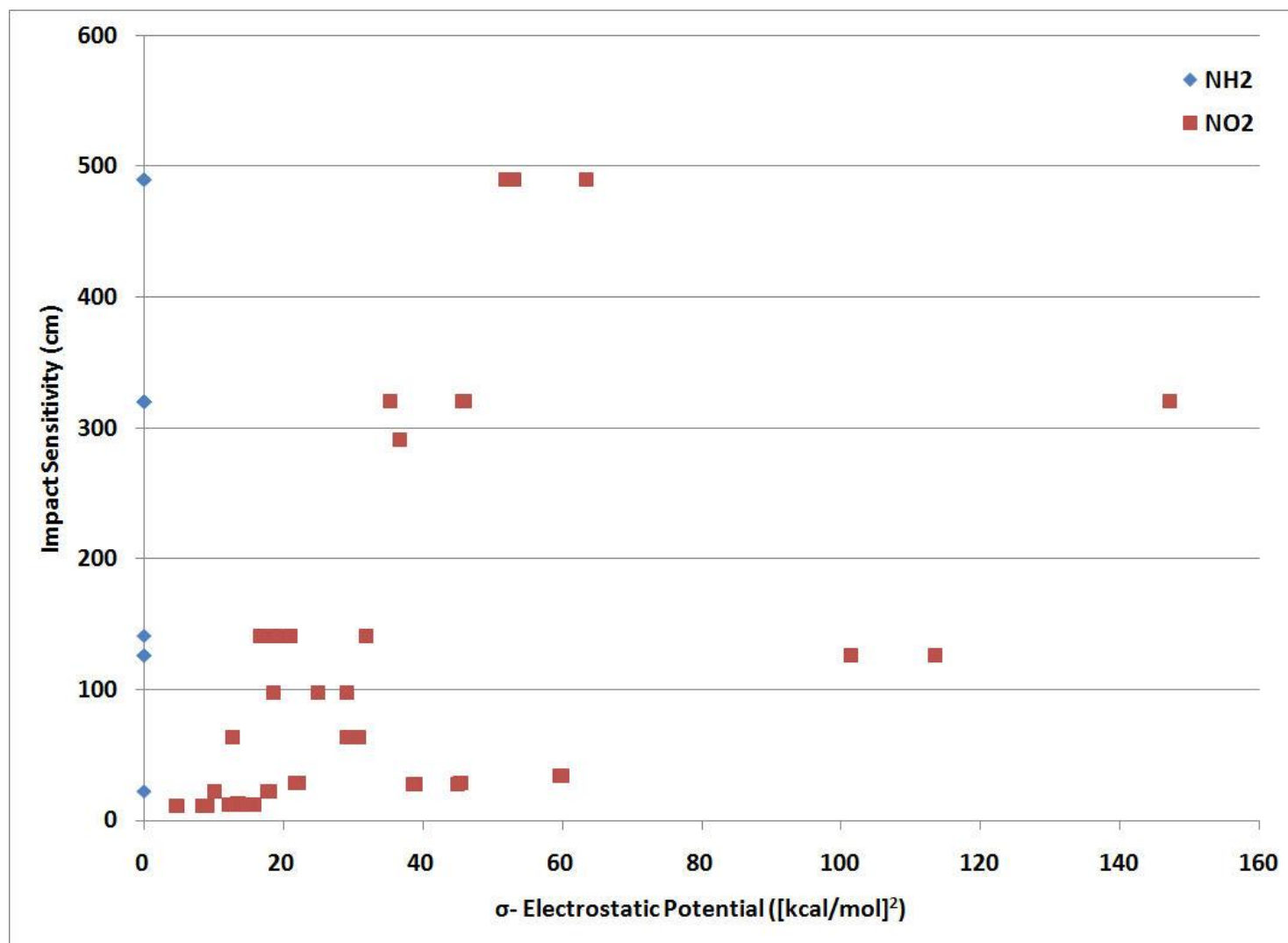


Figure A-74. Impact sensitivity (cm) vs. group σ^2 - electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

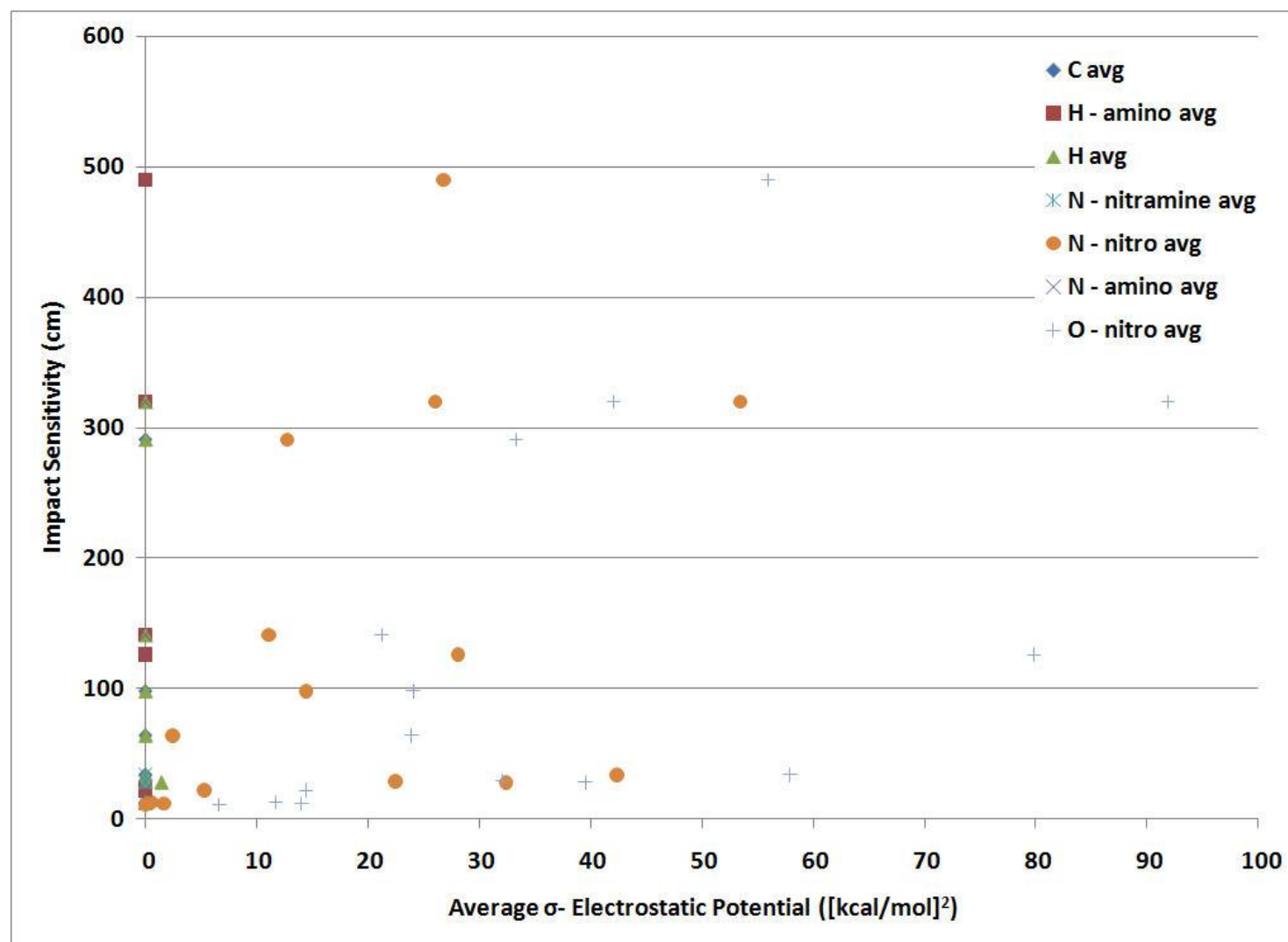


Figure A-75. Impact sensitivity (cm) vs. atomic average σ^2 - electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

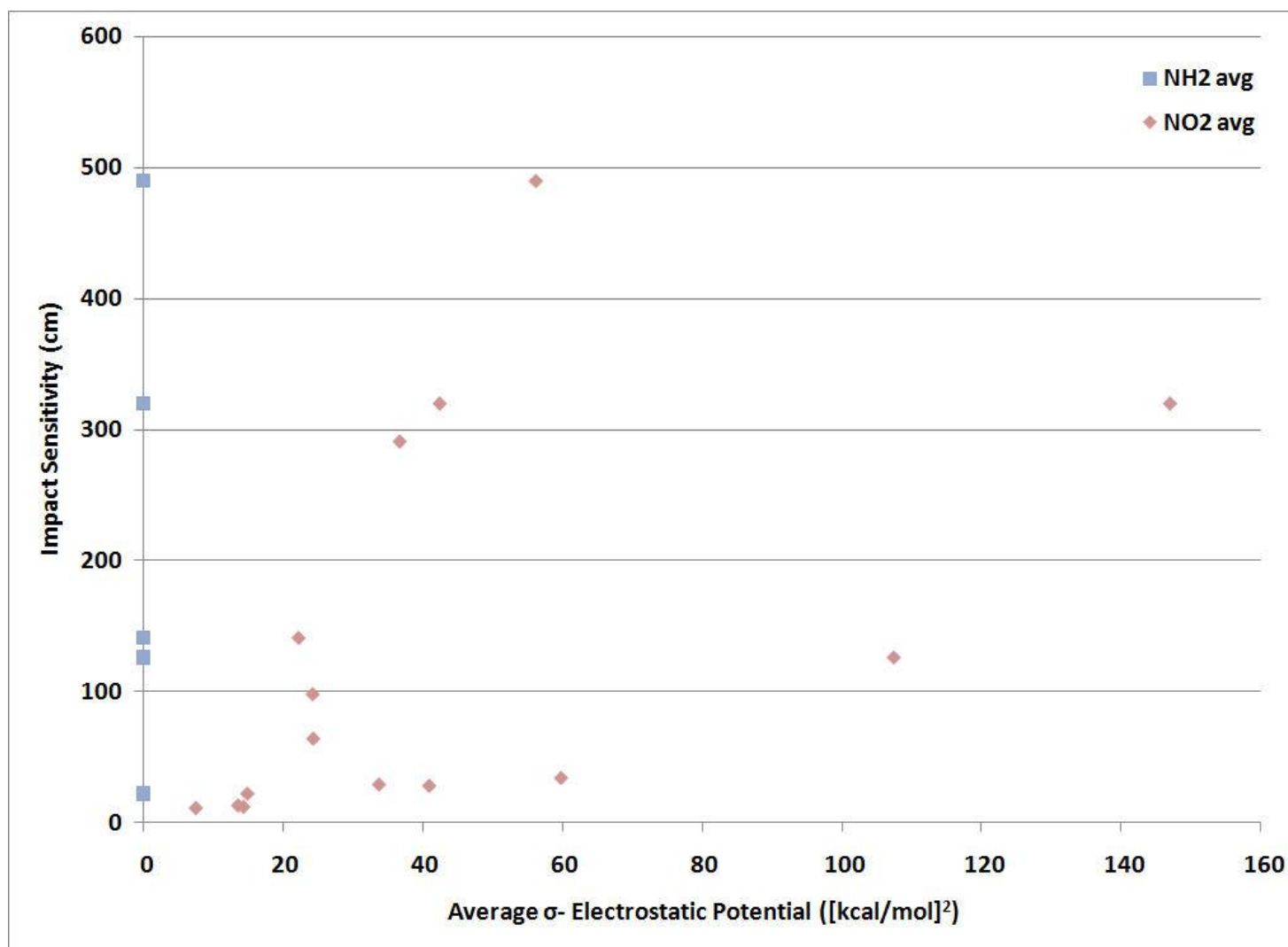


Figure A-76. Impact sensitivity (cm) vs. group average σ^2 - electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

Figure A-77. Impact sensitivity (cm) vs. atomic maximum σ^2 -electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

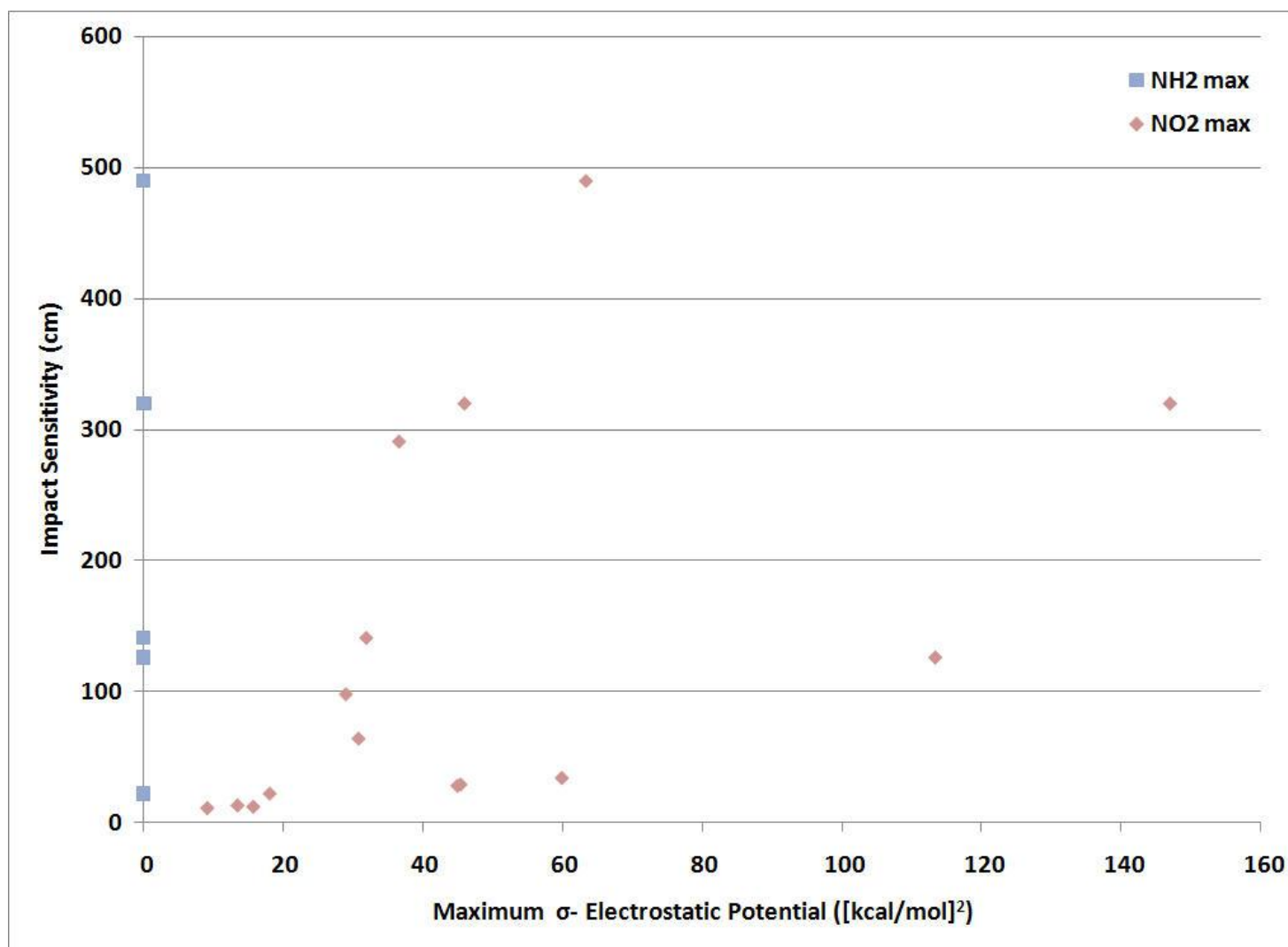


Figure A-78. Impact sensitivity (cm) vs. group maximum σ^2 -electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

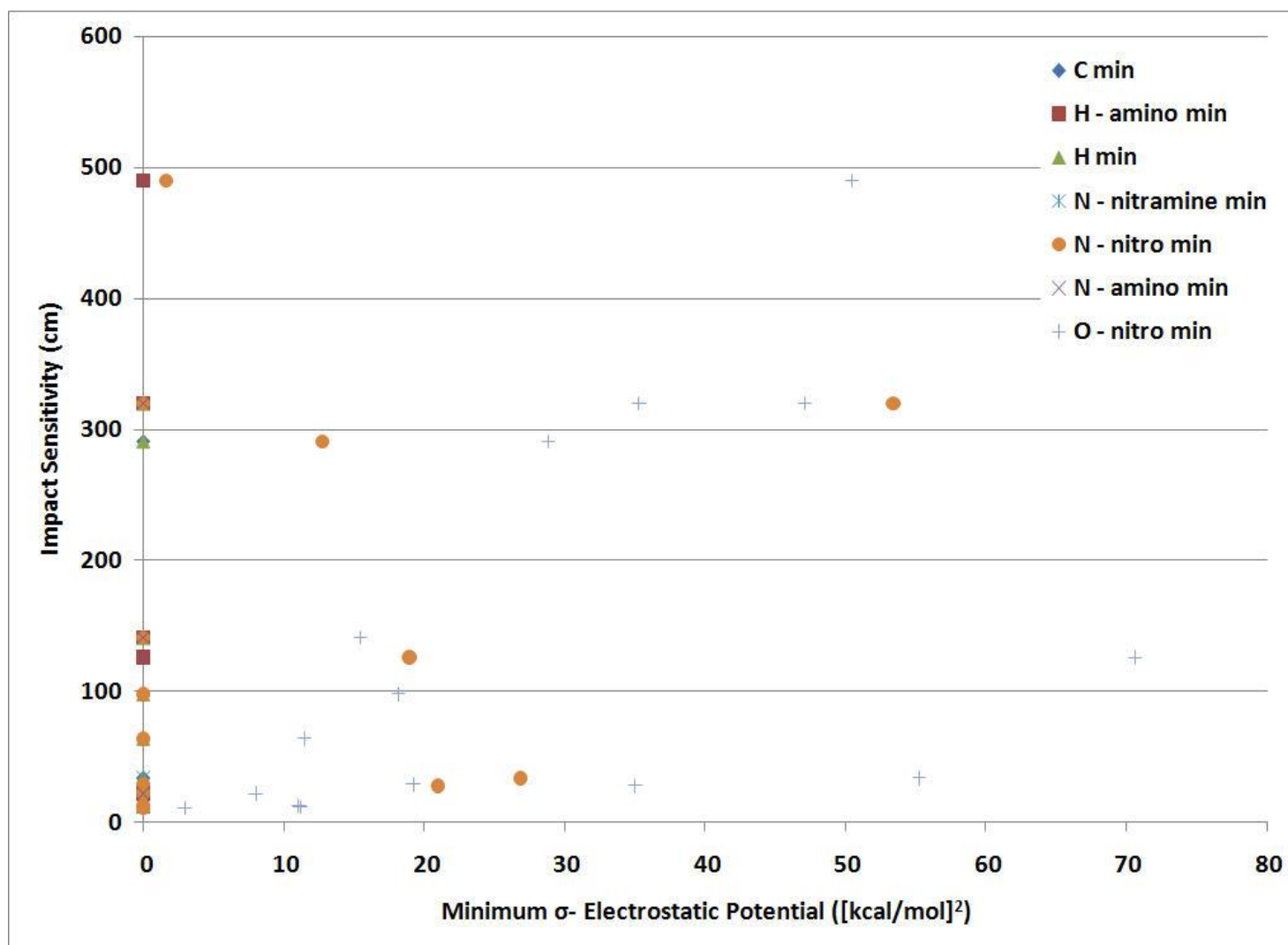


Figure A-79. Impact sensitivity (cm) vs. atomic minimum σ^2 - electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

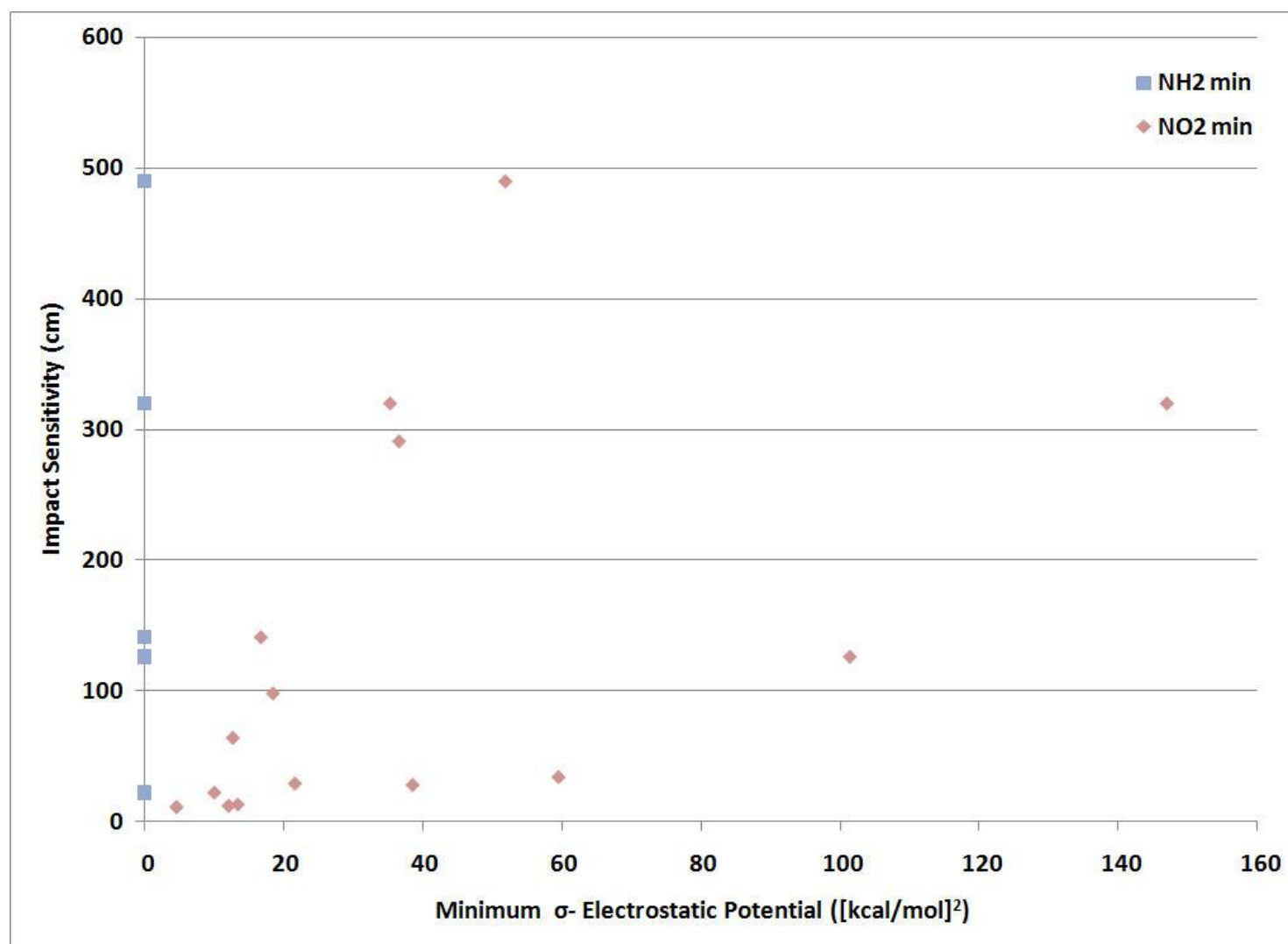


Figure A-80. Impact sensitivity (cm) vs. group minimum σ^2 -electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

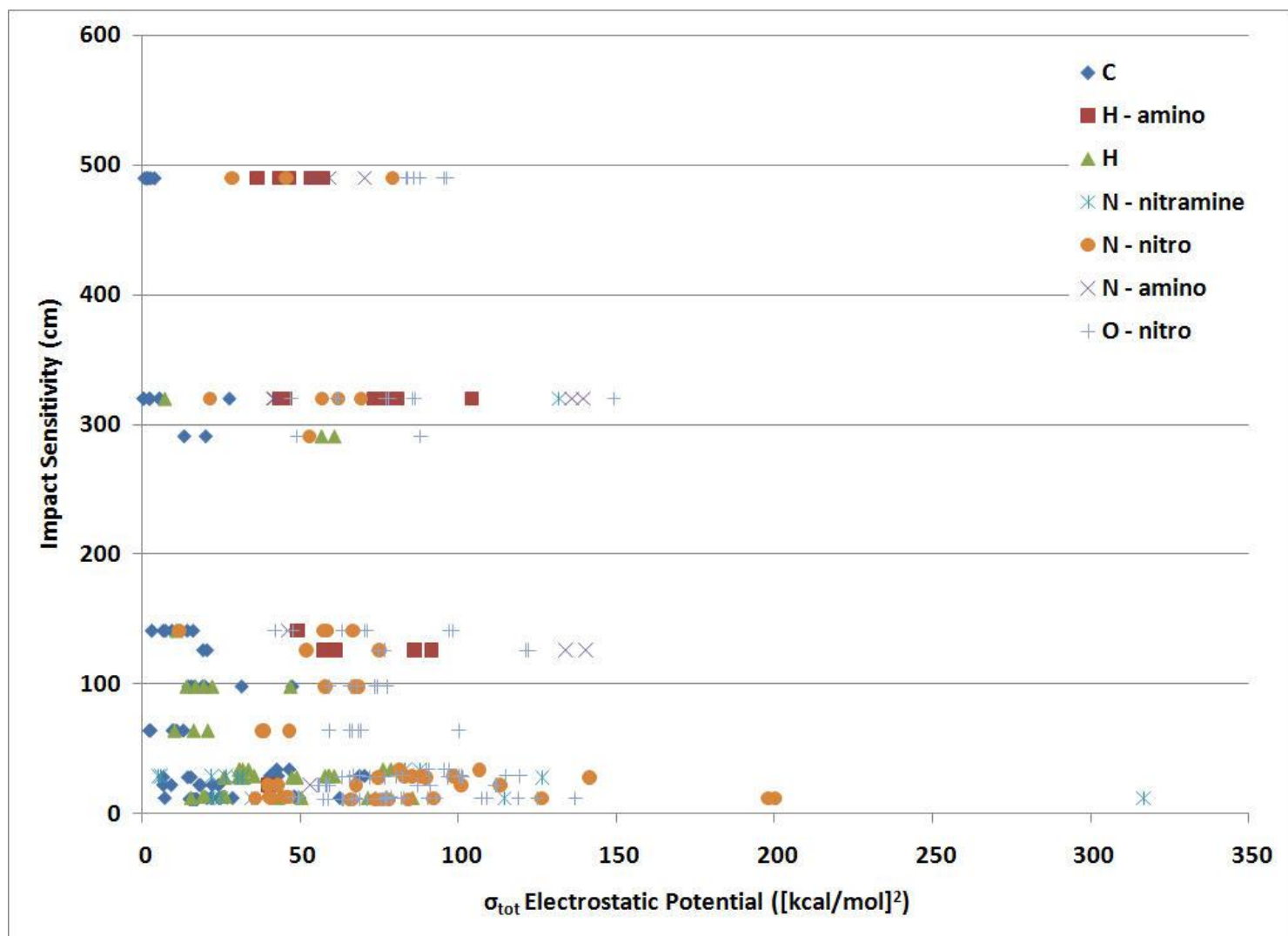


Figure A-81. Impact sensitivity (cm) vs. atomic σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

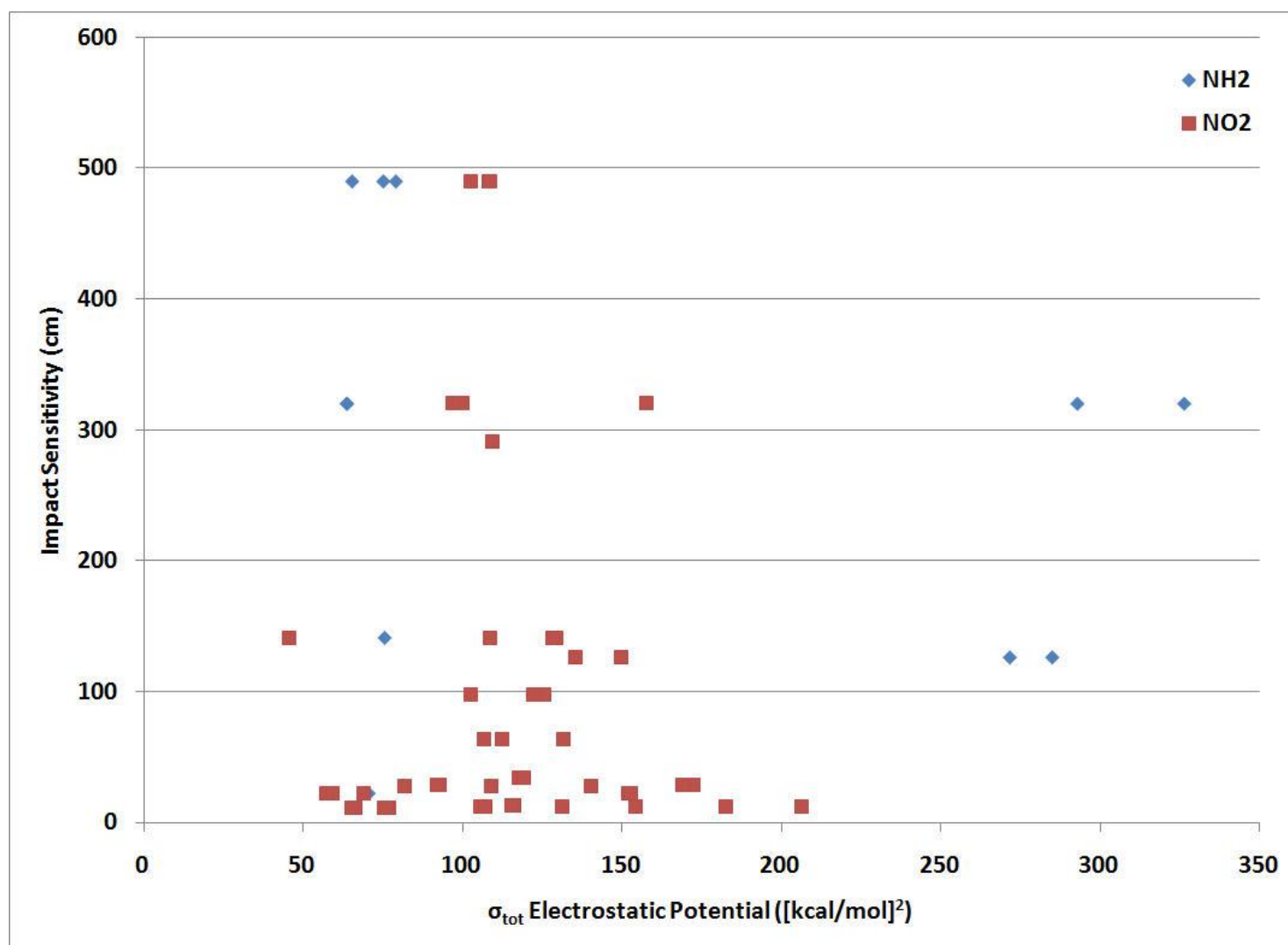


Figure A-82. Impact sensitivity (cm) vs. group σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

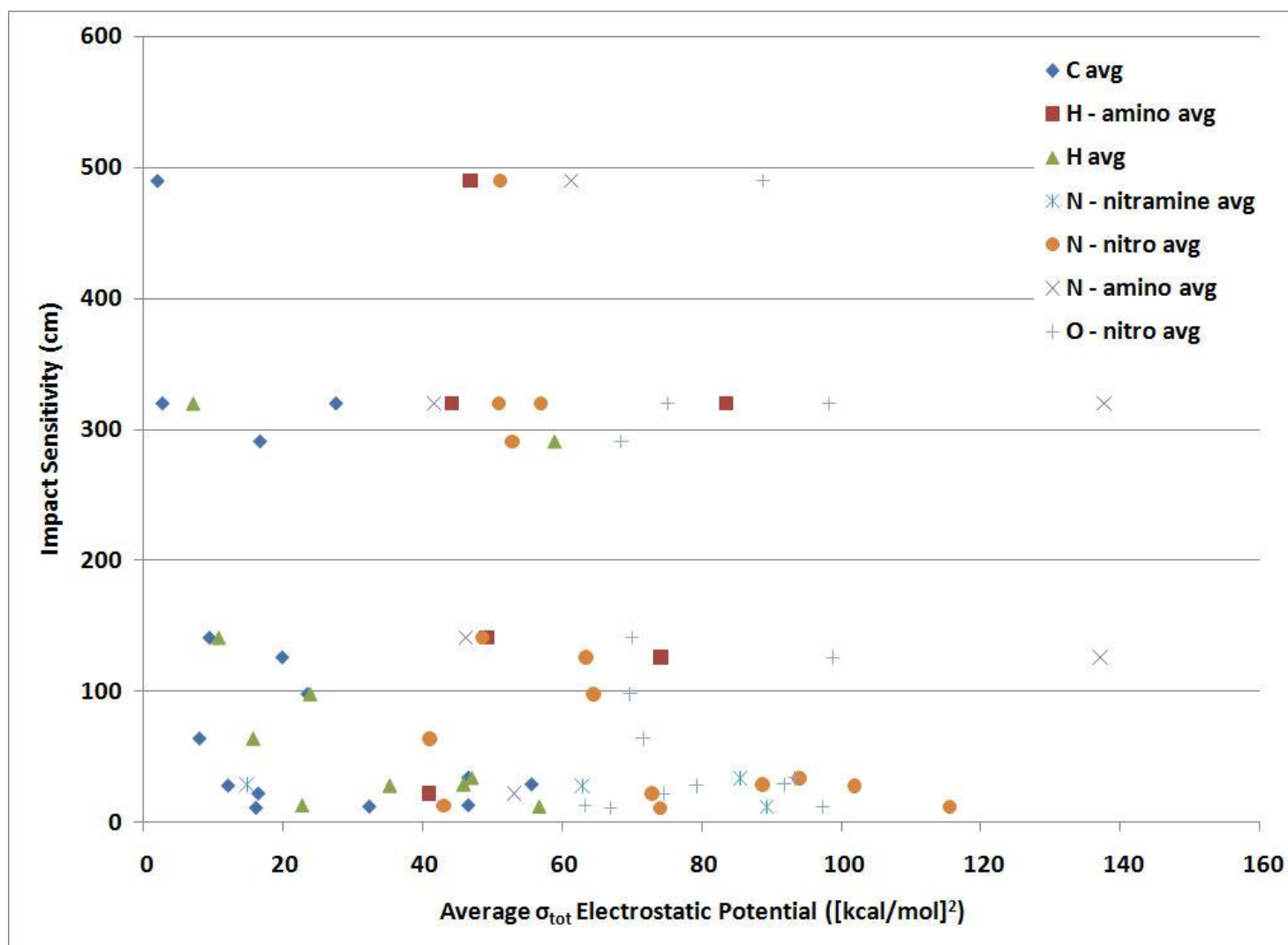


Figure A-83. Impact sensitivity (cm) vs. atomic average σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

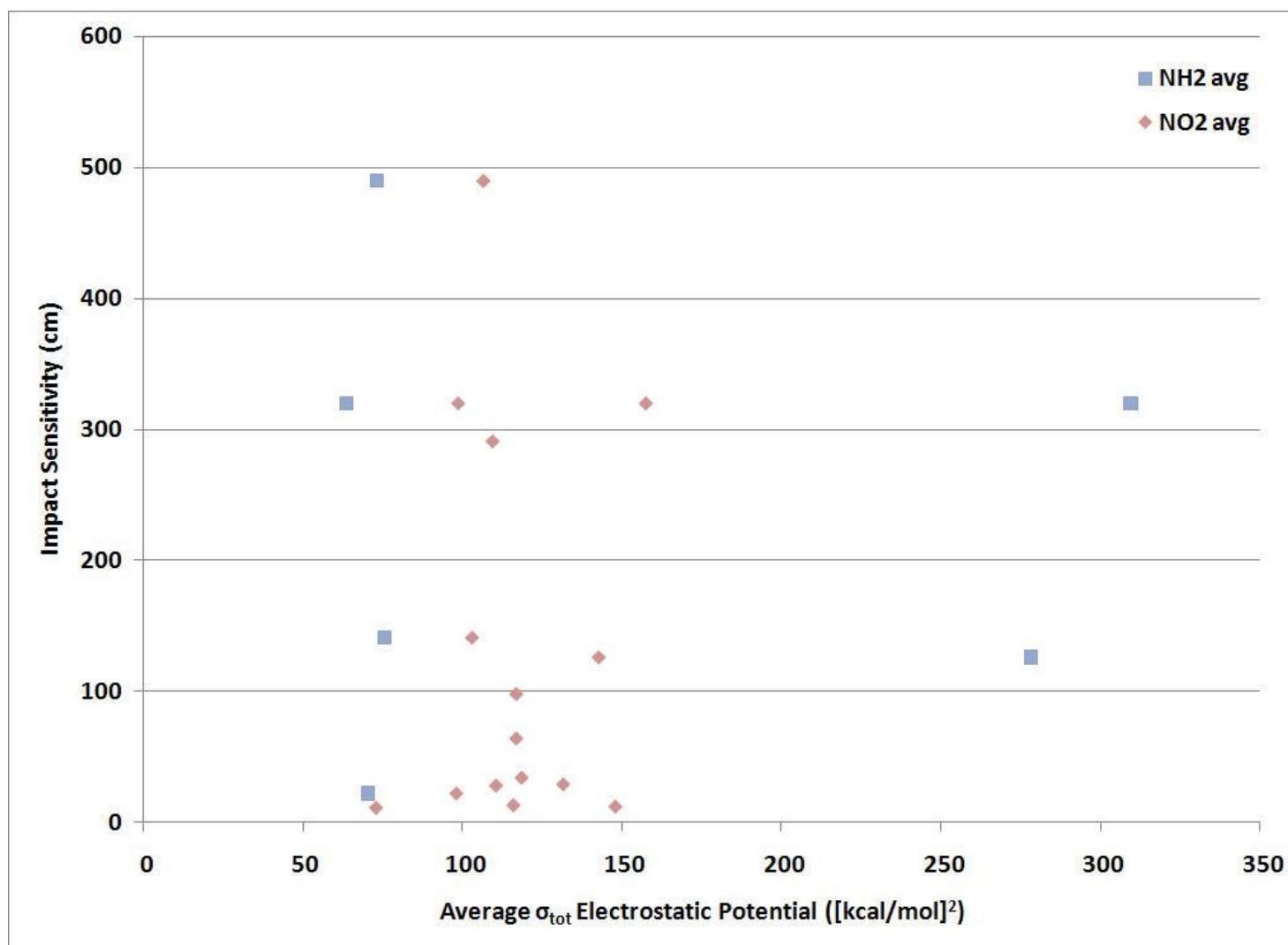


Figure A-84. Impact sensitivity (cm) vs. group average σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

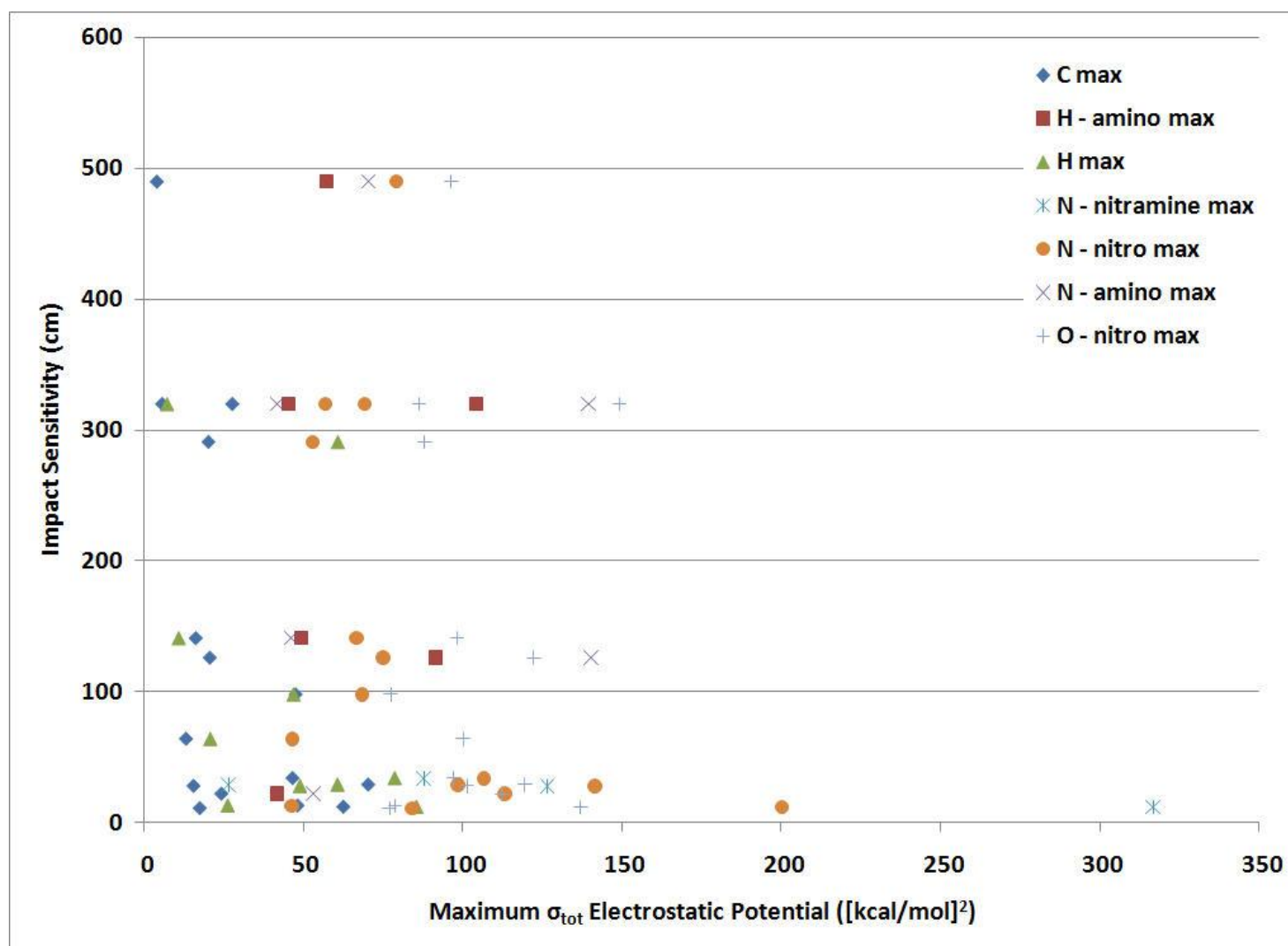


Figure A-85. Impact sensitivity (cm) vs. atomic maximum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for PBE/6-31G**.

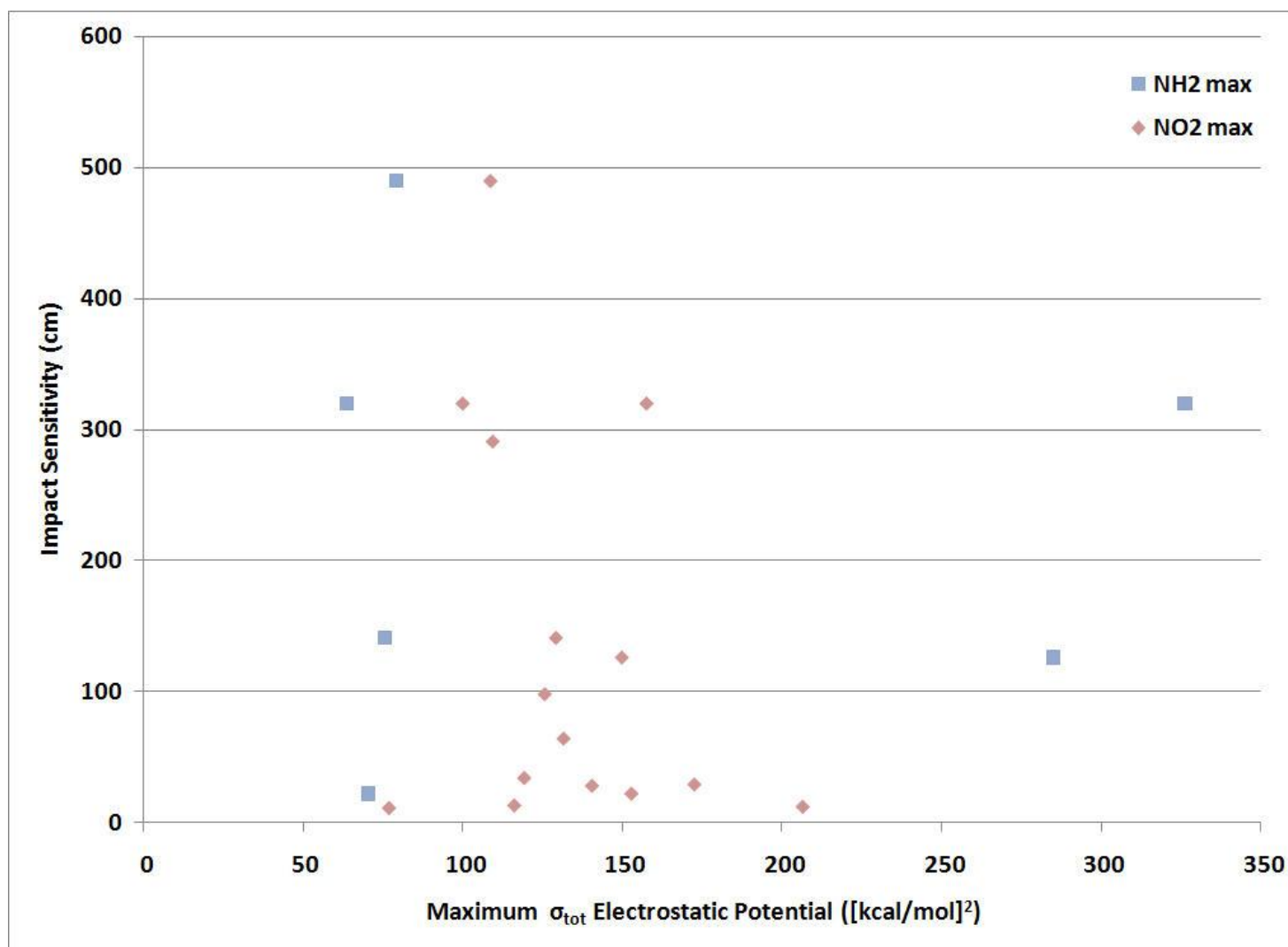


Figure A-86. Impact sensitivity (cm) vs. group maximum σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

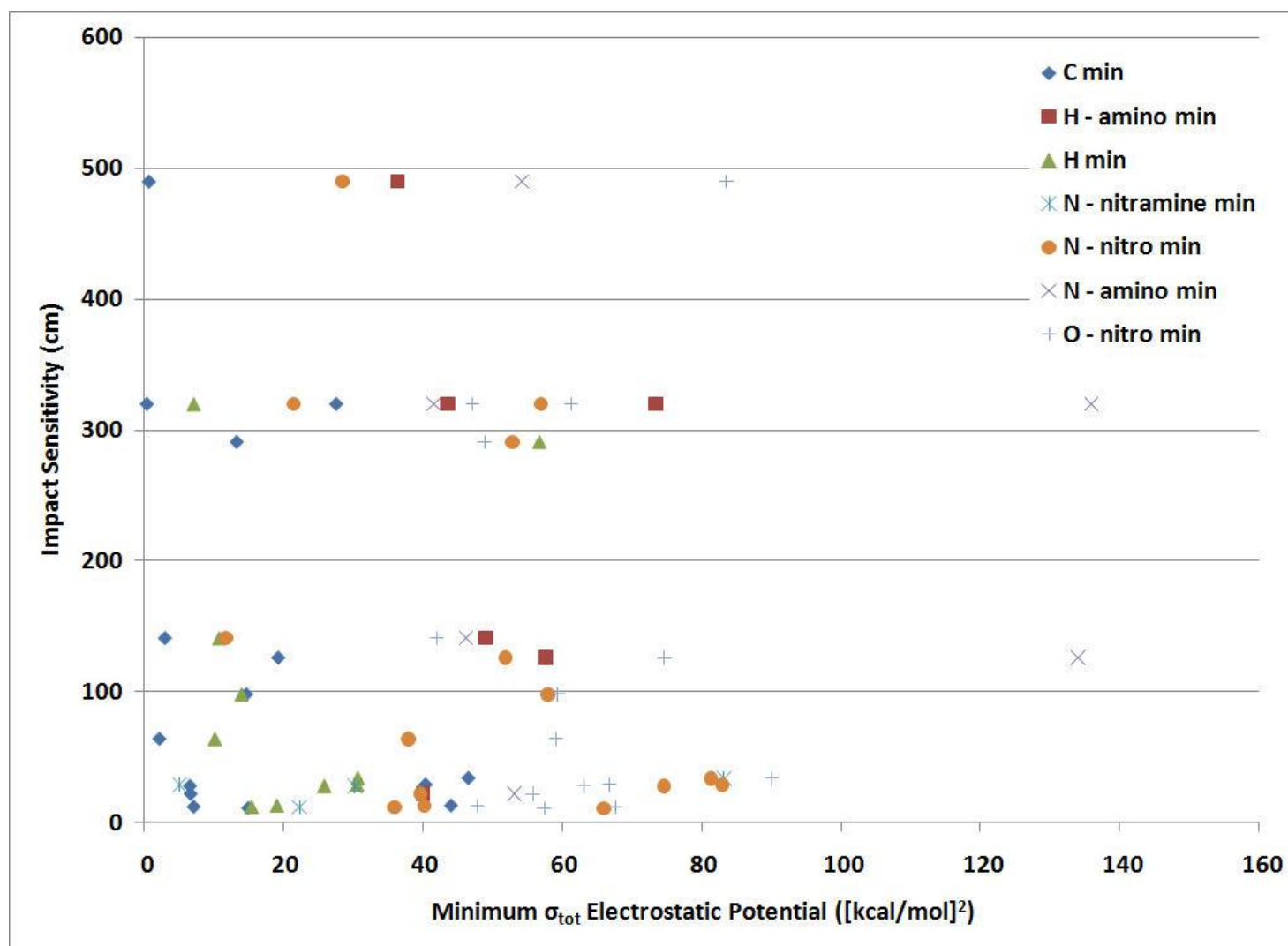


Figure A-87. Impact sensitivity (cm) vs. atomic minimum σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

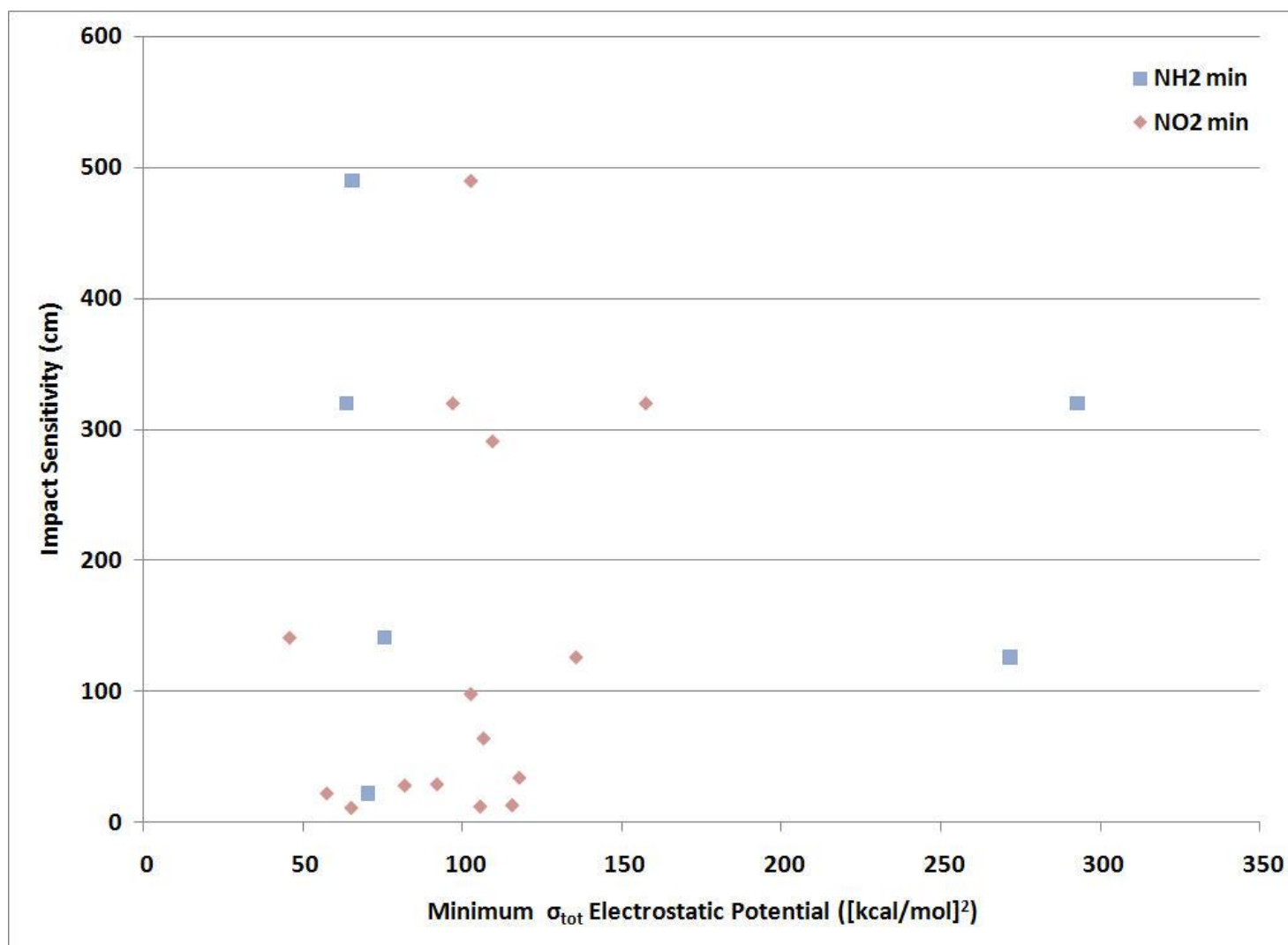


Figure A-88. Impact sensitivity (cm) vs. group minimum σ_{tot}^2 electrostatic potential ($[\text{kcal/mol}]^2$) for PBE/6-31G**.

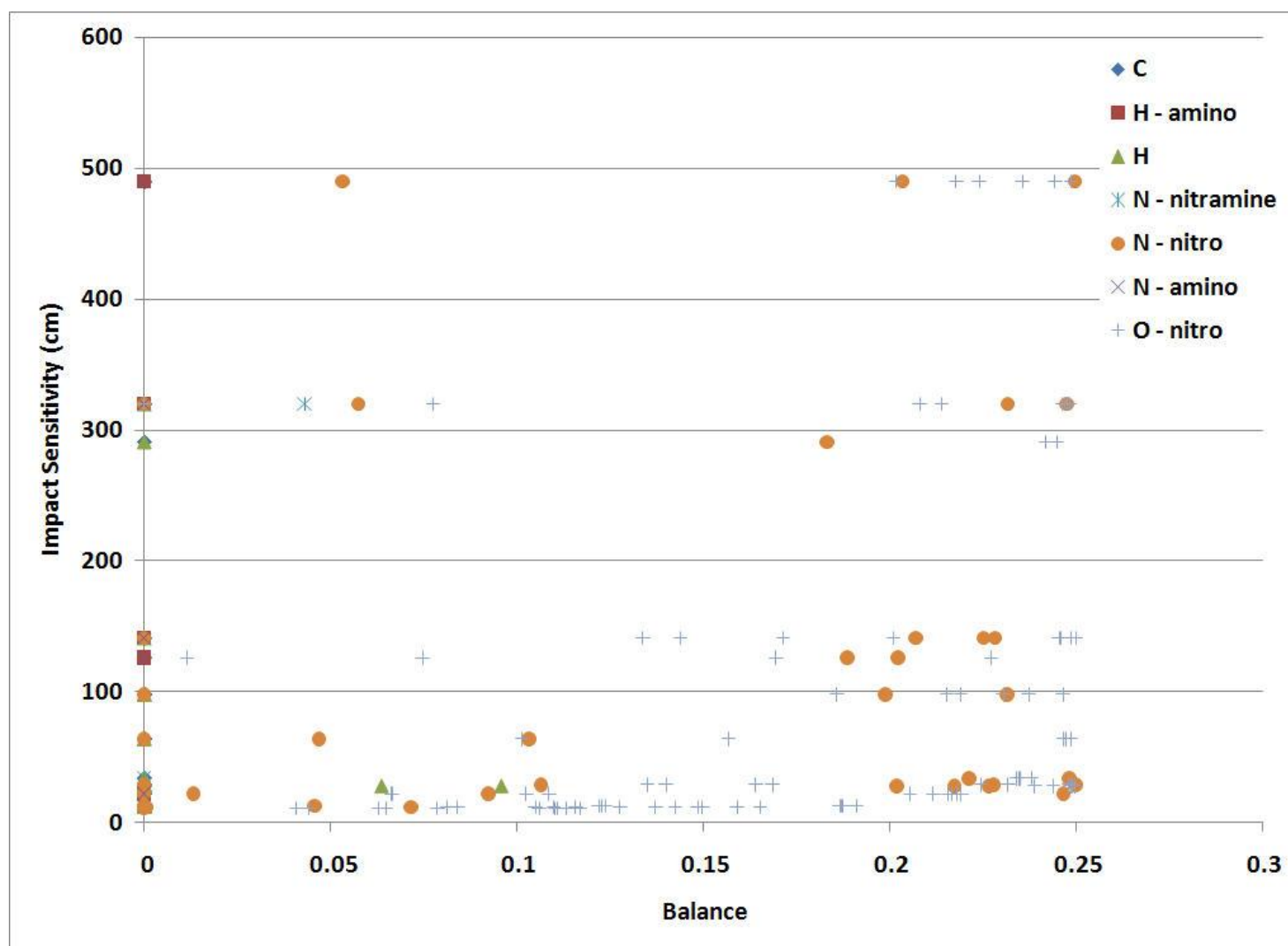


Figure A-89. Impact sensitivity (cm) vs. atomic balance electrostatic potential for PBE/6-31G**.

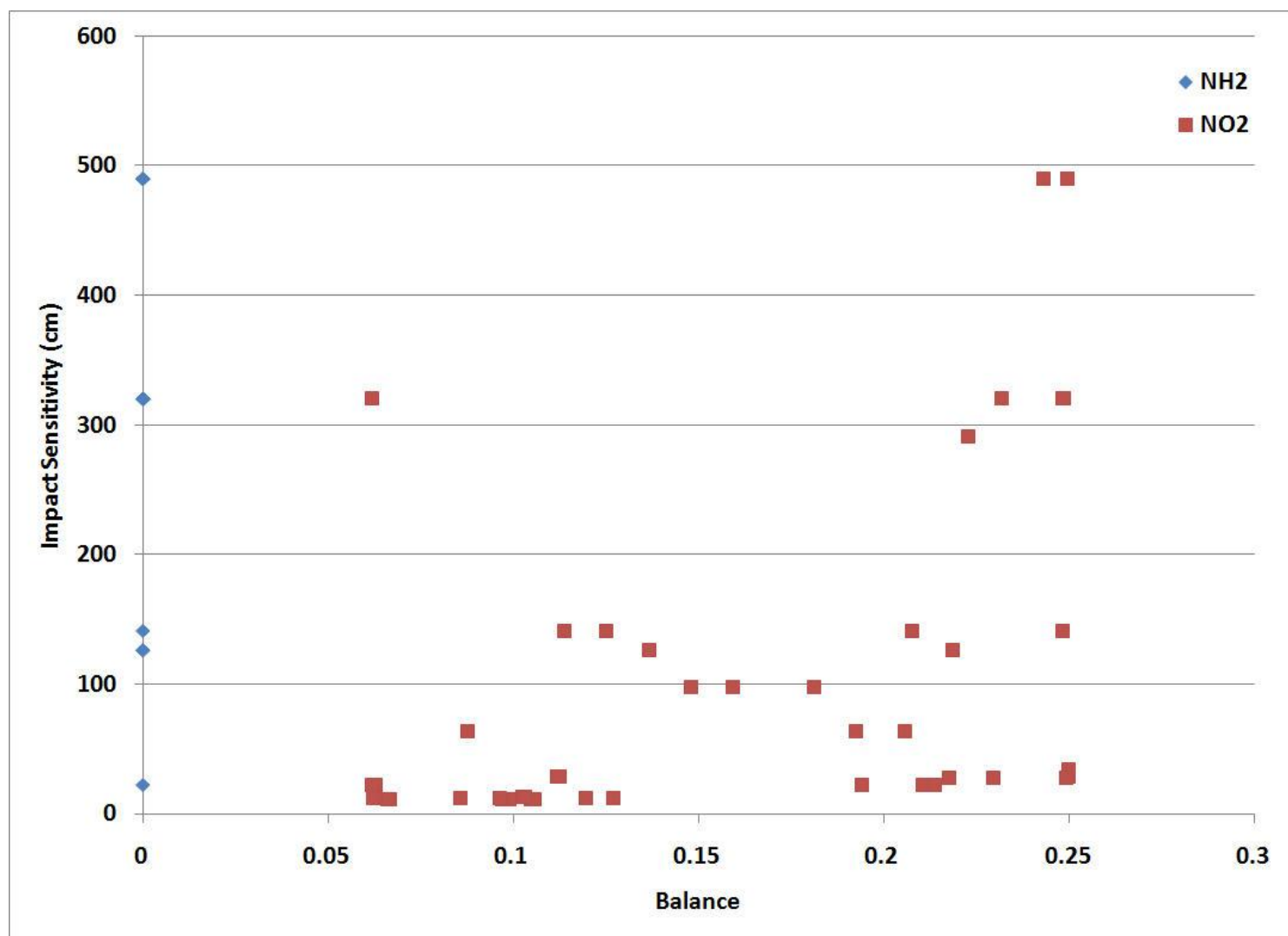


Figure A-90. Impact sensitivity (cm) vs. group balance electrostatic potential for PBE/6-31G**.

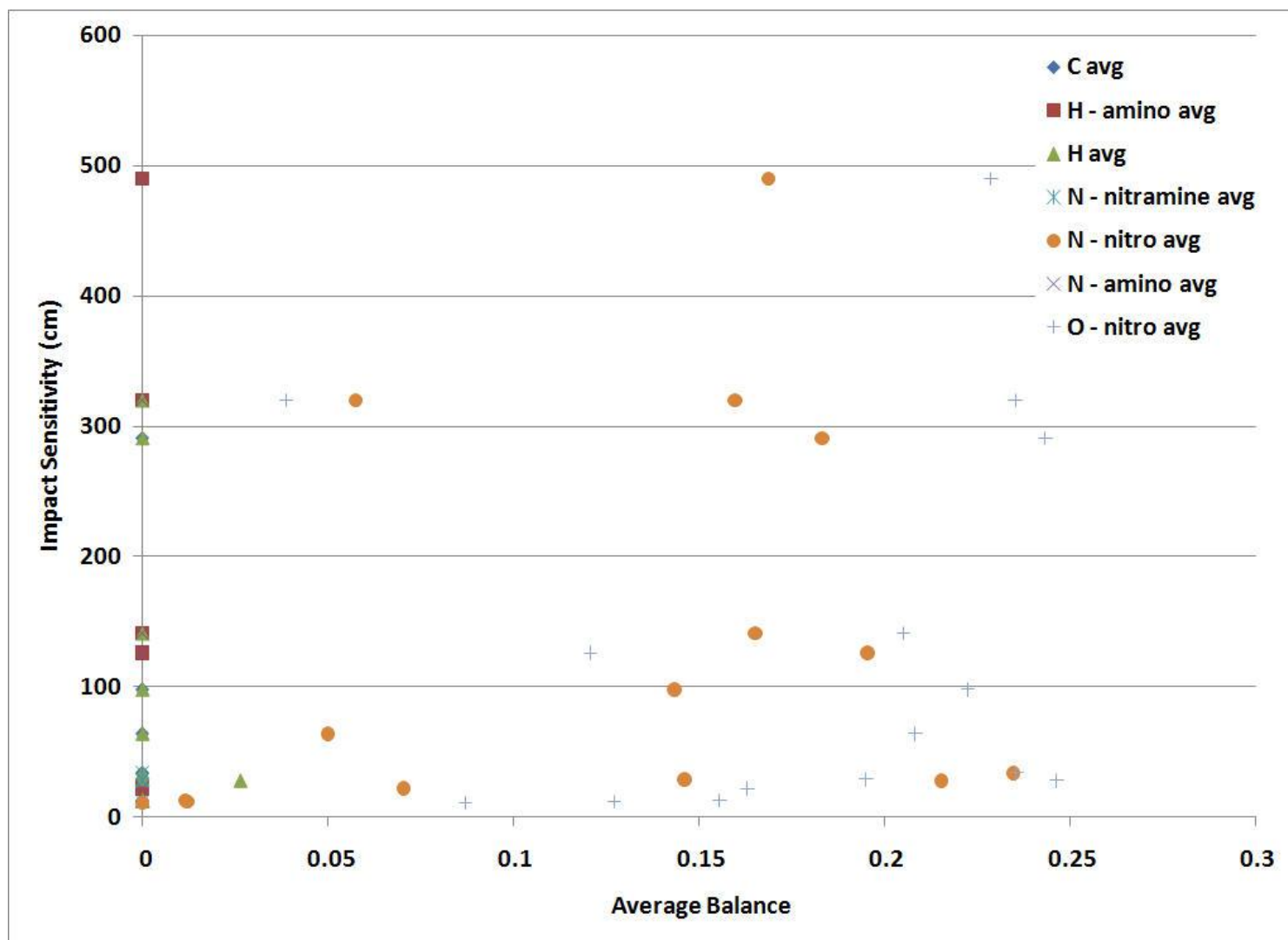


Figure A-91. Impact sensitivity (cm) vs. atomic average balance electrostatic potential for PBE/6-31G**.

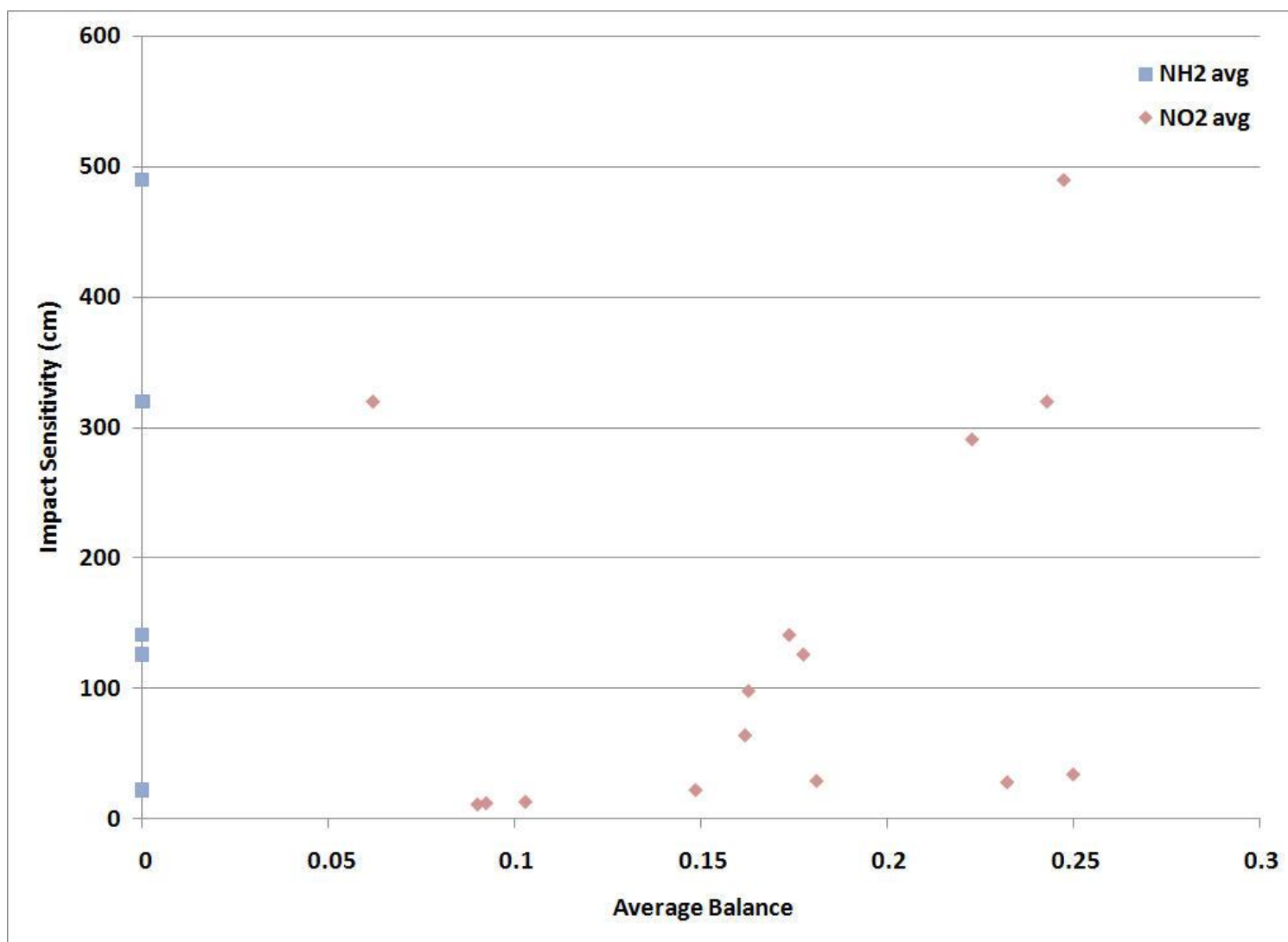


Figure A-92. Impact sensitivity (cm) vs. group average balance electrostatic potential for PBE/6-31G**.

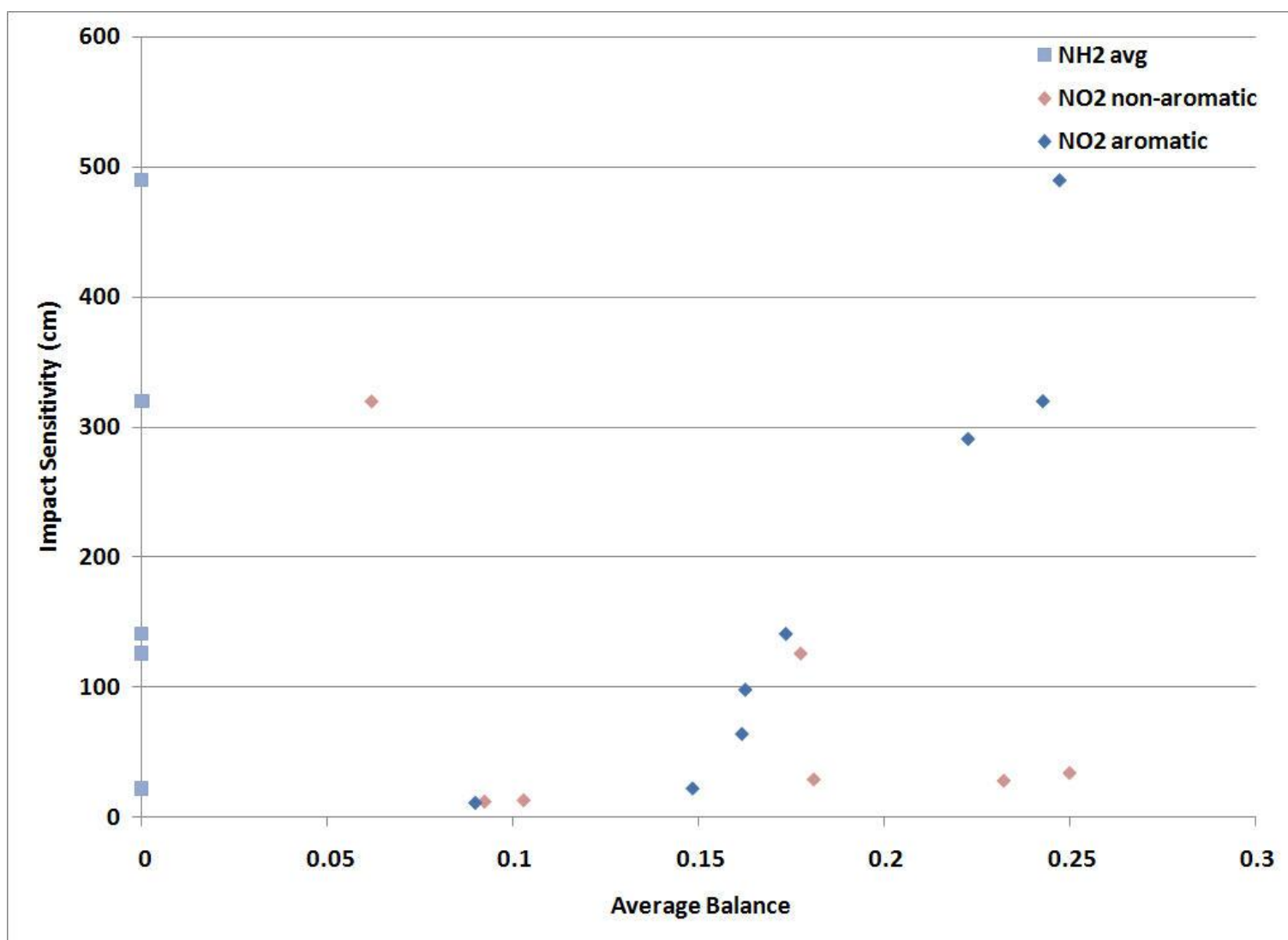


Figure A-93. Impact sensitivity (cm) vs. amino, non-aromatic and aromatic nitro group average balance electrostatic potential for PBE/6-31G**.

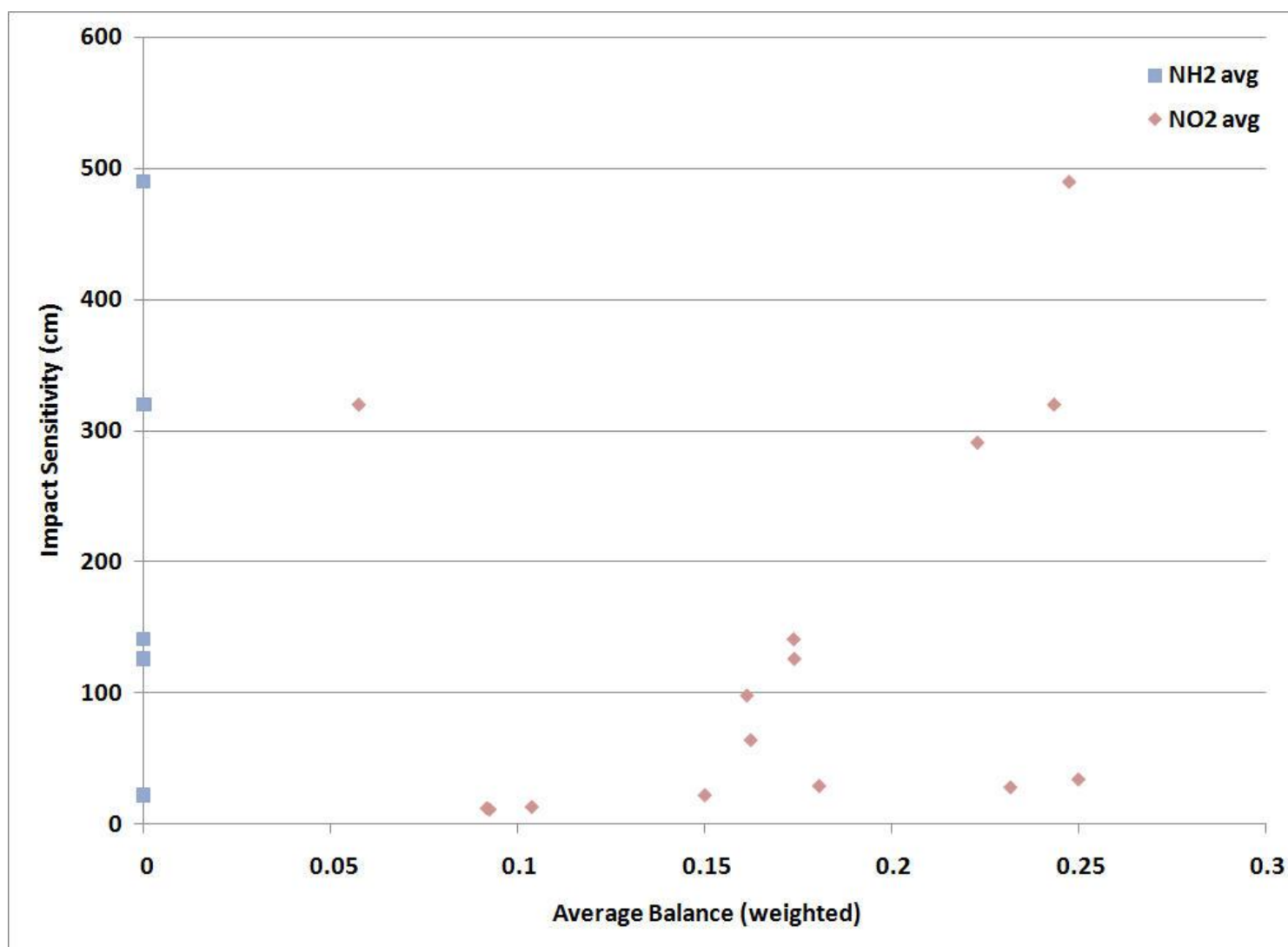


Figure A-94. Impact sensitivity (cm) vs. area weighted group average balance electrostatic potential for PBE/6-31G**.

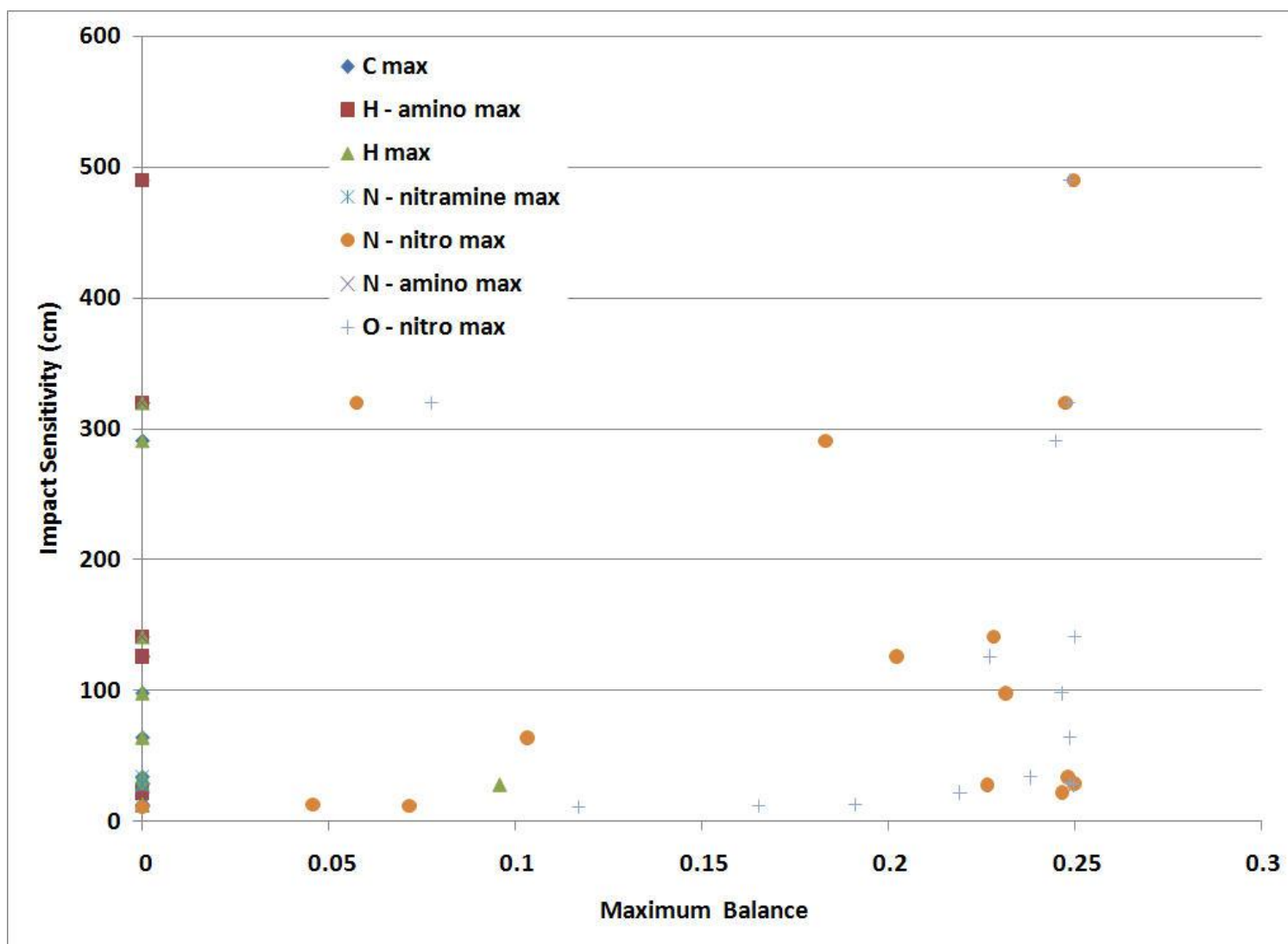


Figure A-95. Impact sensitivity (cm) vs. atomic maximum balance electrostatic potential for PBE/6-31G**.

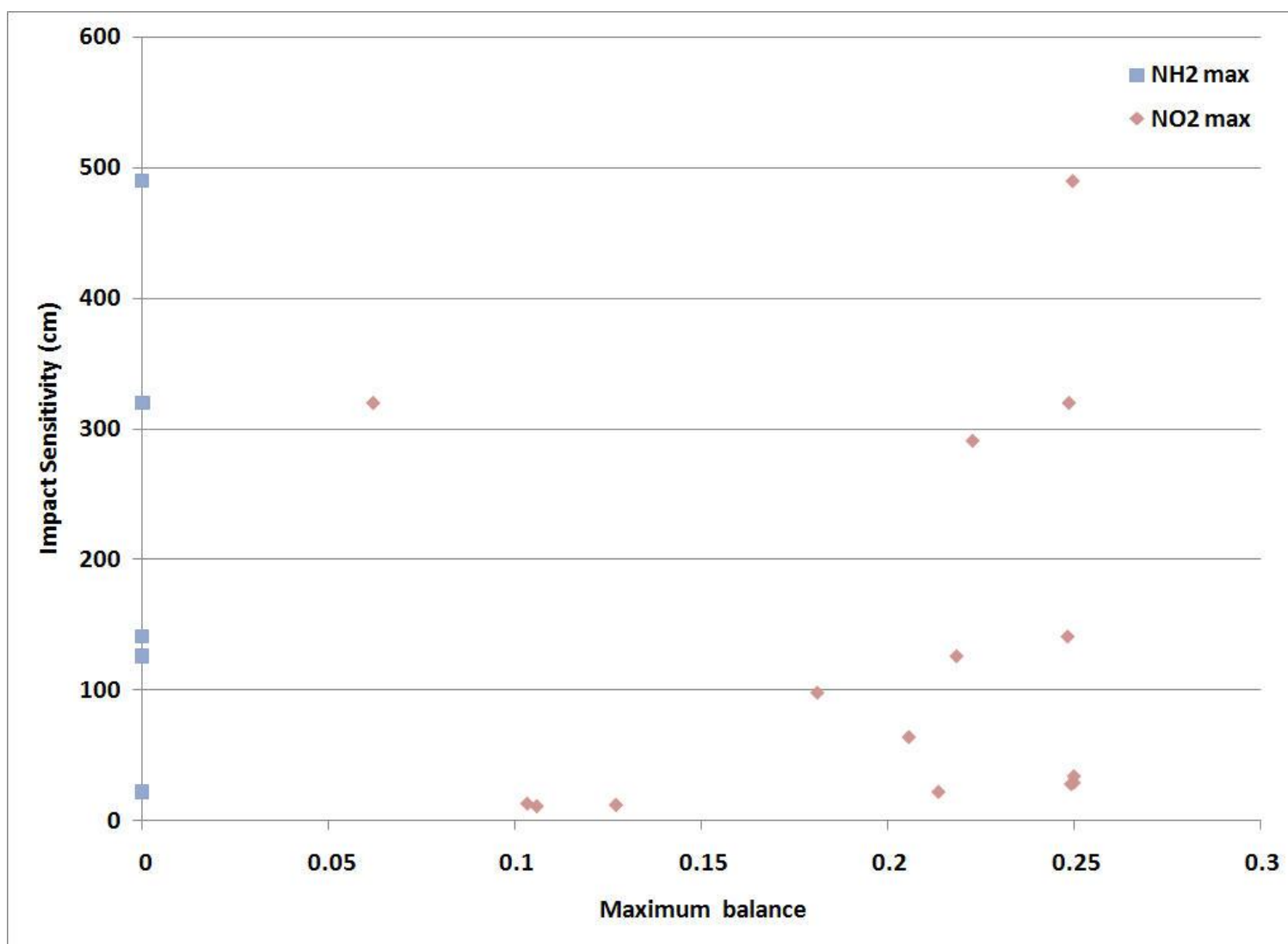


Figure A-96. Impact sensitivity (cm) vs. group maximum balance electrostatic potential for PBE/6-31G**.

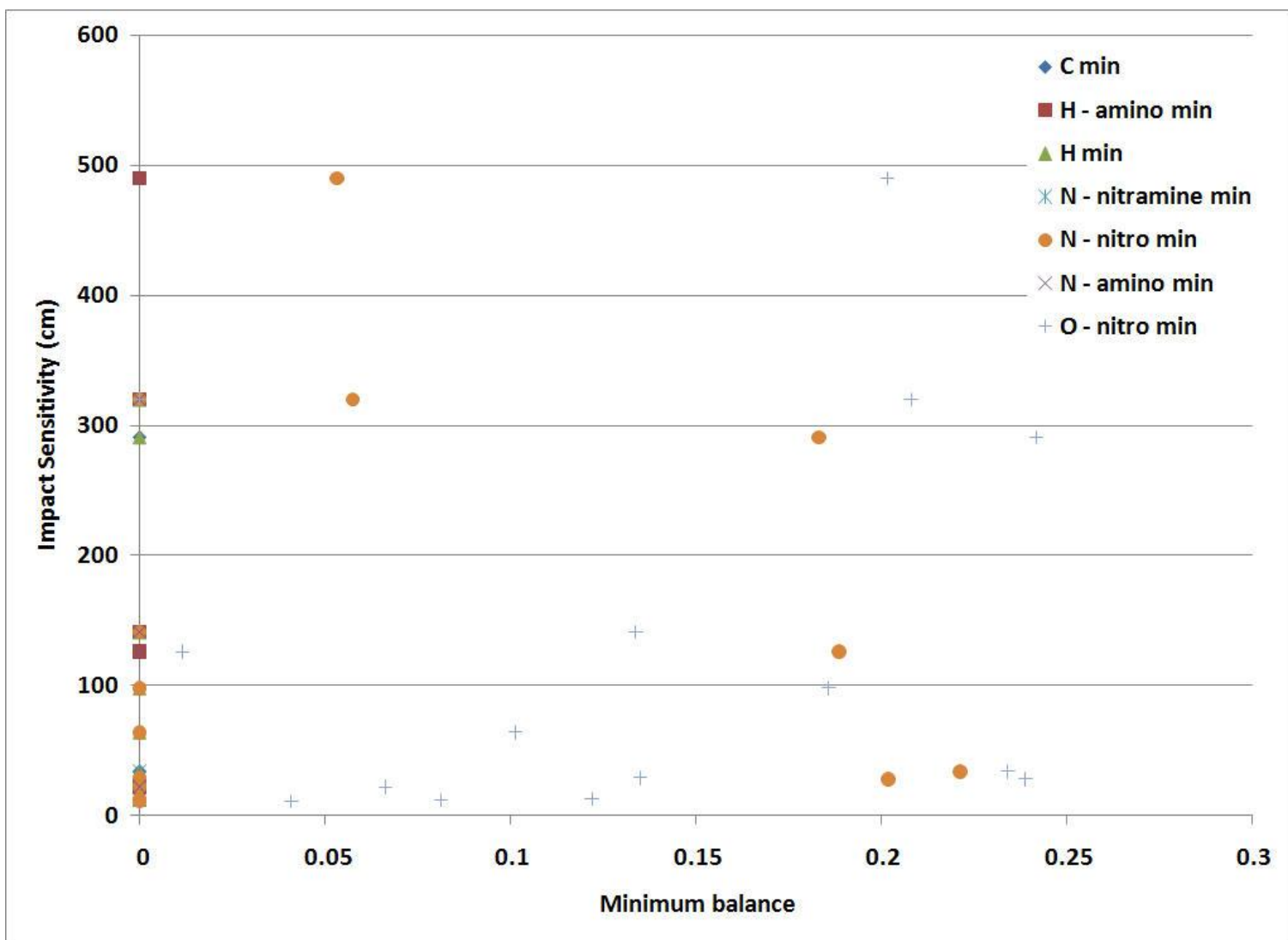


Figure A-97. Impact sensitivity (cm) vs. atomic minimum balance electrostatic potential for PBE/6-31G**.

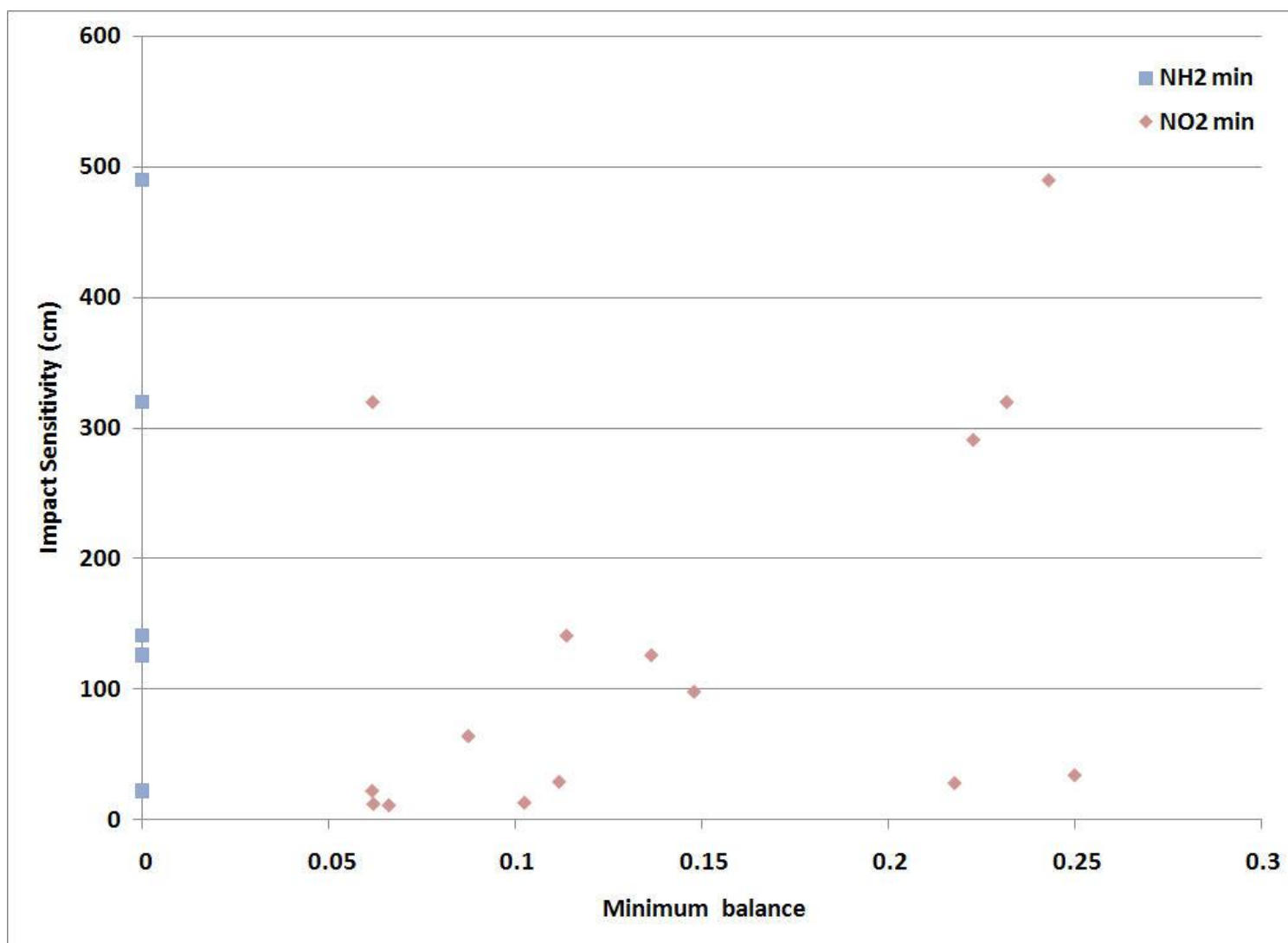


Figure A-98. Impact sensitivity (cm) vs. atomic minimum balance electrostatic potential for PBE/6-31G**.

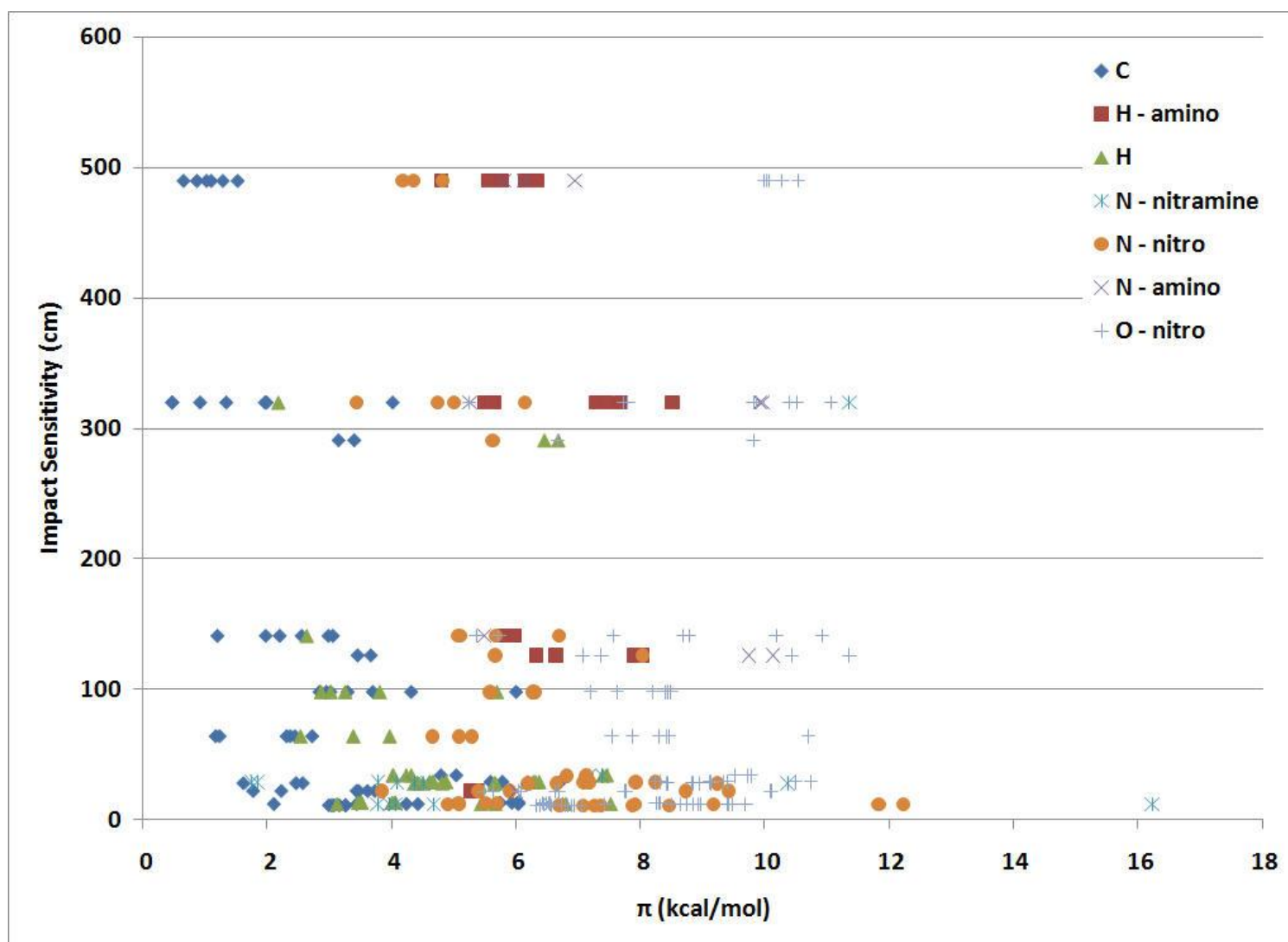


Figure A-99. Impact sensitivity (cm) vs. atomic Π (kcal/mol) electrostatic potential for PBE/6-31G**.

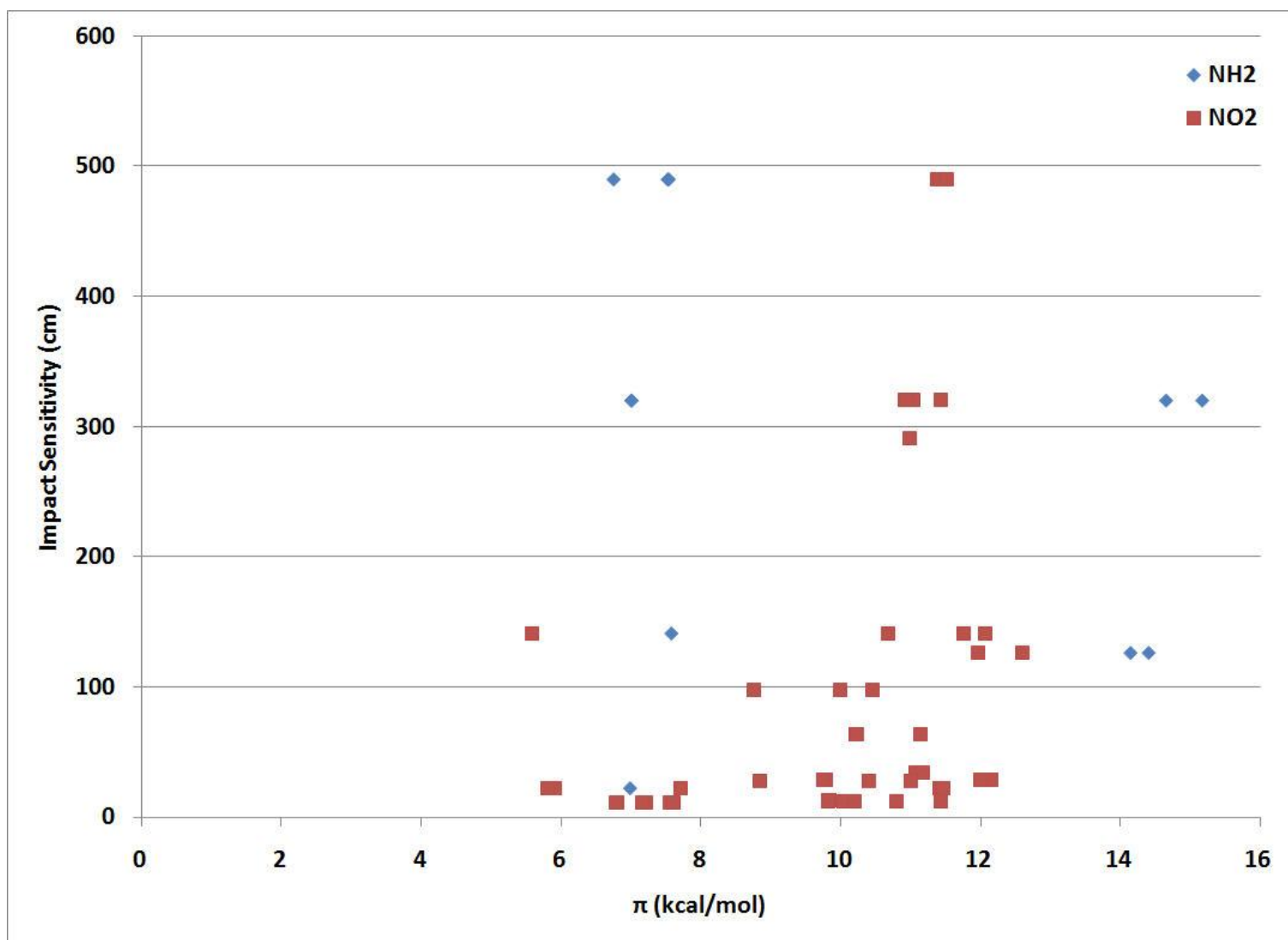


Figure A-100. Impact sensitivity (cm) vs. group II (kcal/mol) electrostatic potential for PBE/6-31G**.

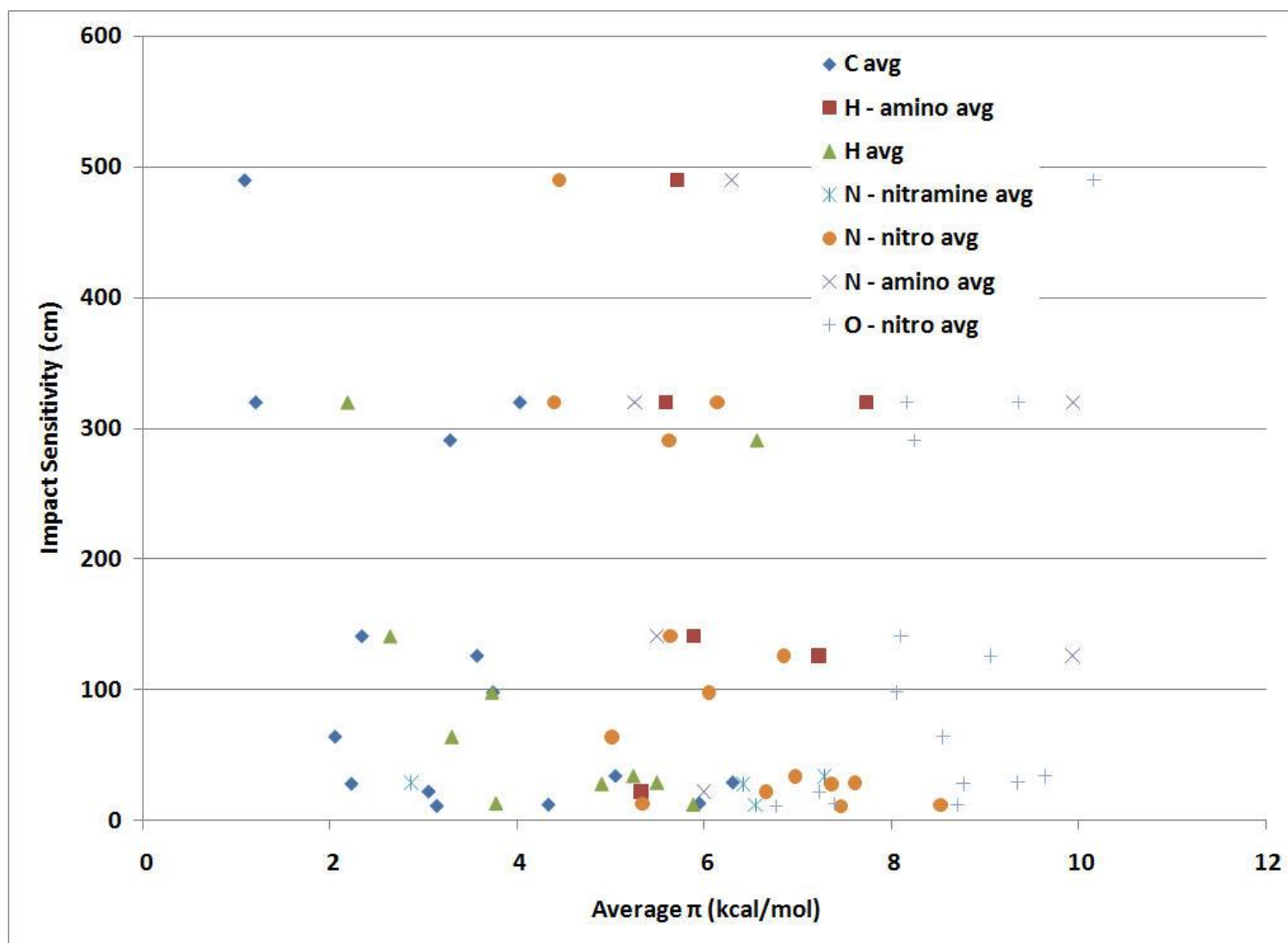


Figure A-101. Impact sensitivity (cm) vs. atomic average Π (kcal/mol) electrostatic potential for PBE/6-31G**.

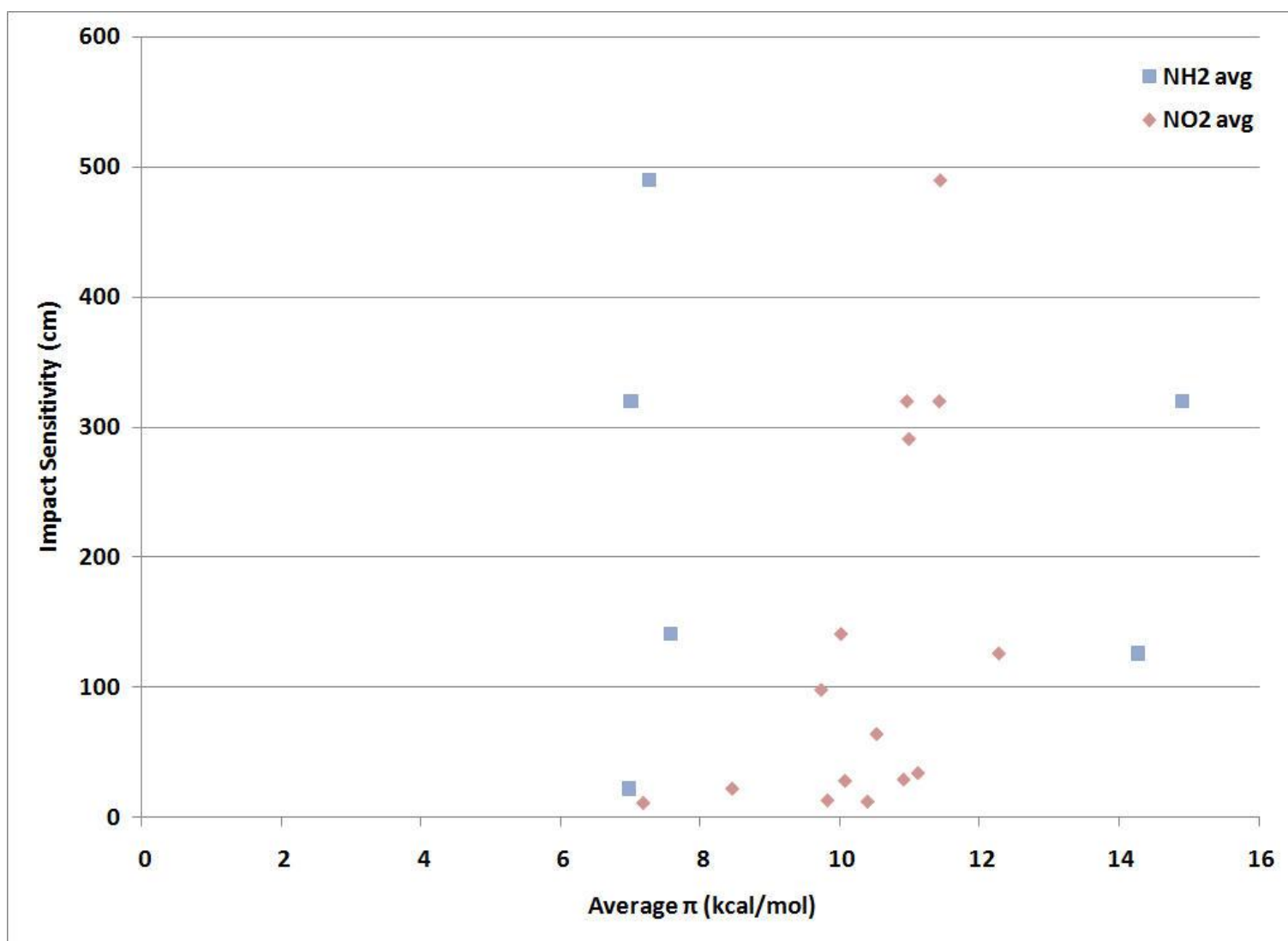


Figure A-102. Impact sensitivity (cm) vs. group average π (kcal/mol) electrostatic potential for PBE/6-31G**.

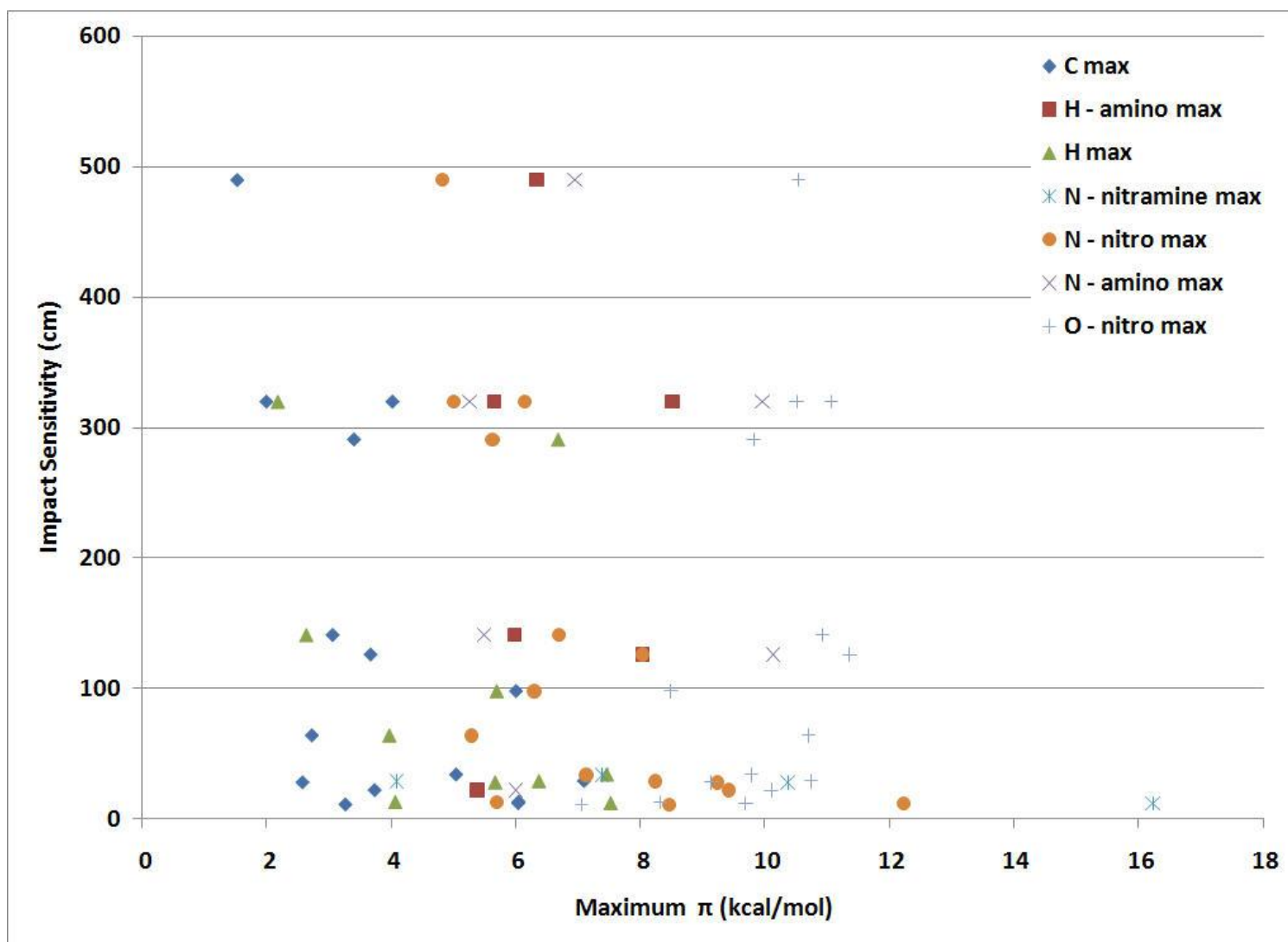


Figure A-103. Impact sensitivity (cm) vs. atomic maximum π (kcal/mol) electrostatic potential for PBE/6-31G**.

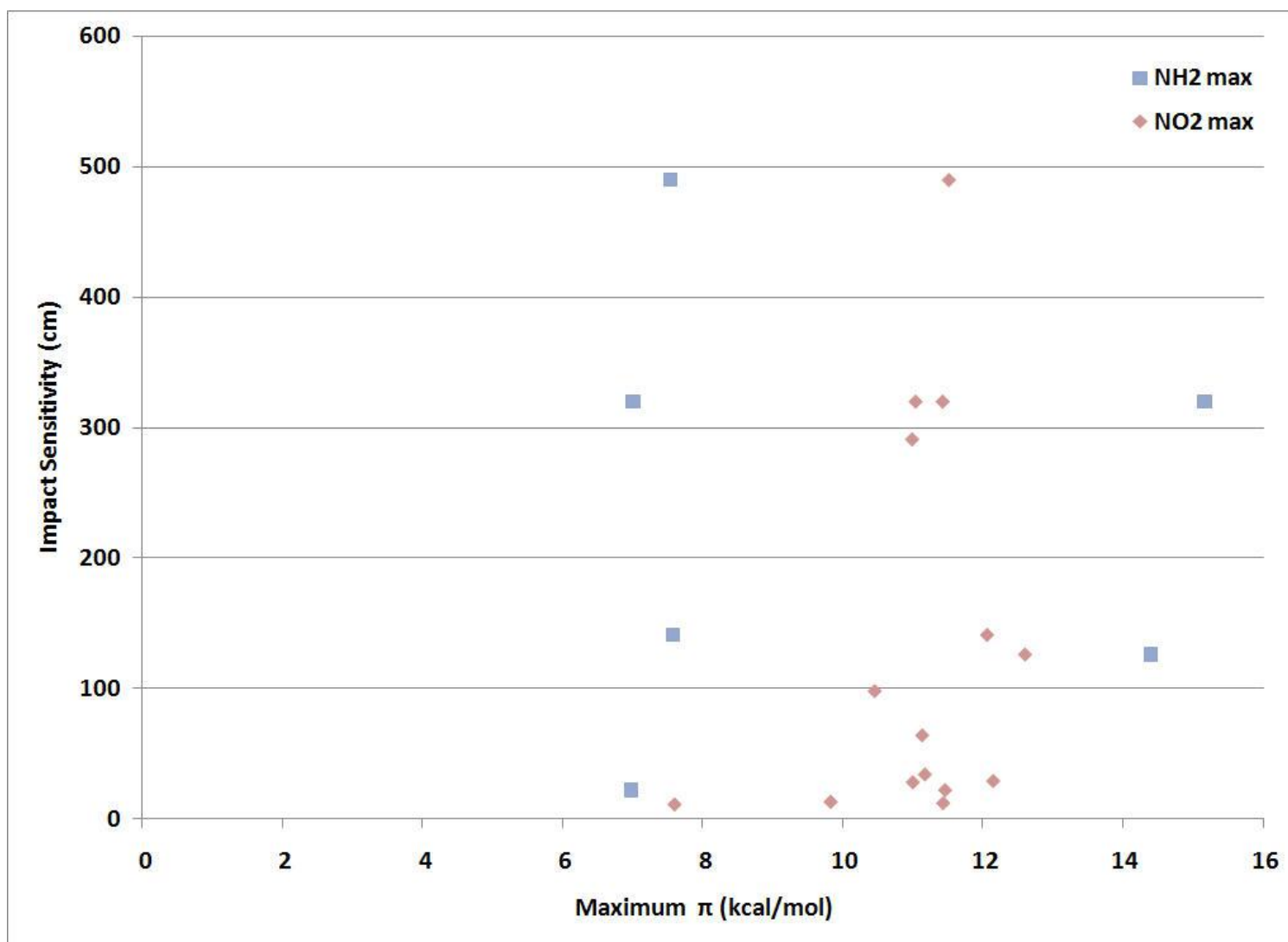


Figure A-104. Impact sensitivity (cm) vs. group maximum π (kcal/mol) electrostatic potential for PBE/6-31G**.

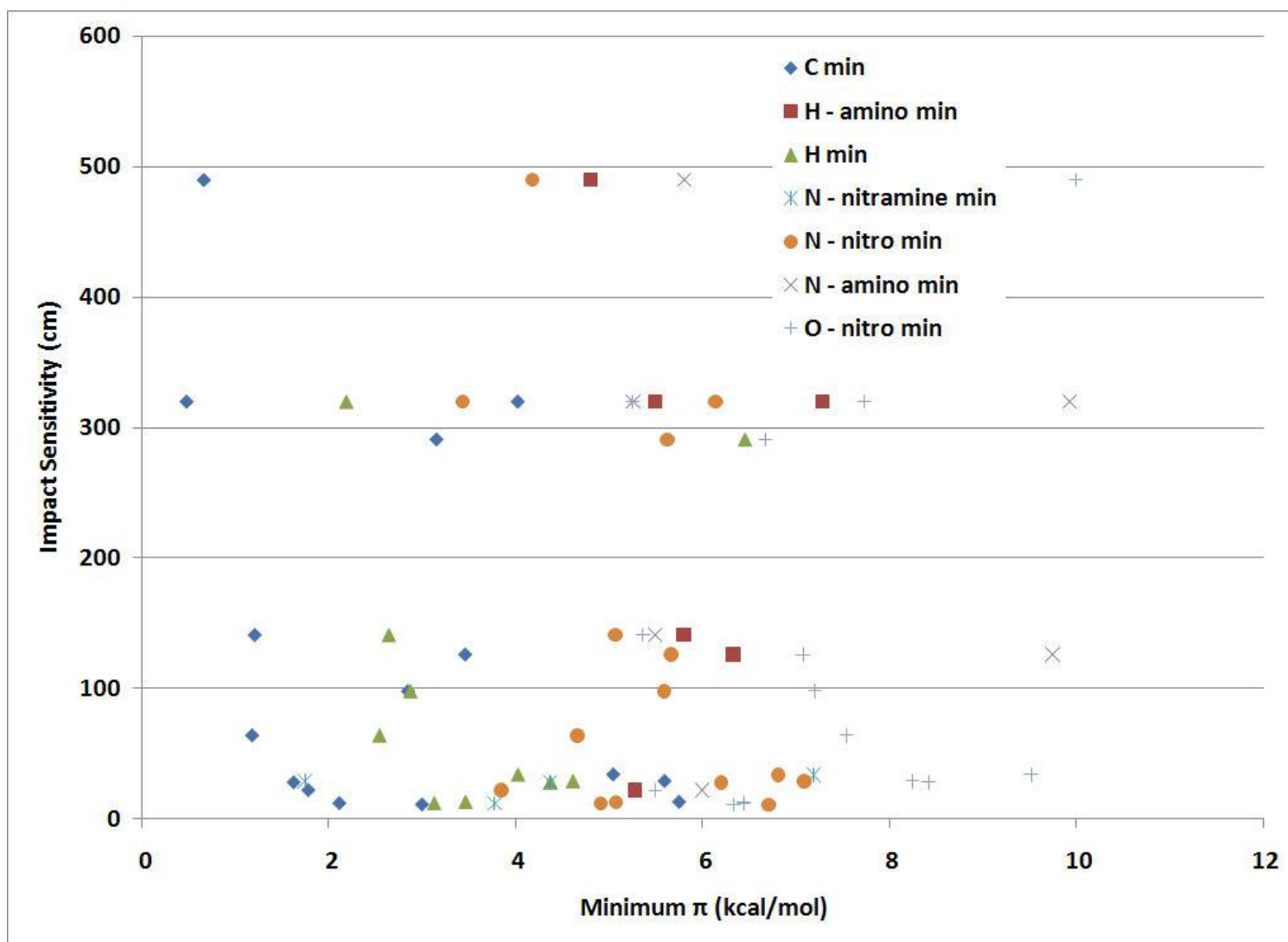


Figure A-105. Impact sensitivity (cm) vs. atomic minimum π (kcal/mol) electrostatic potential for PBE/6-31G**.

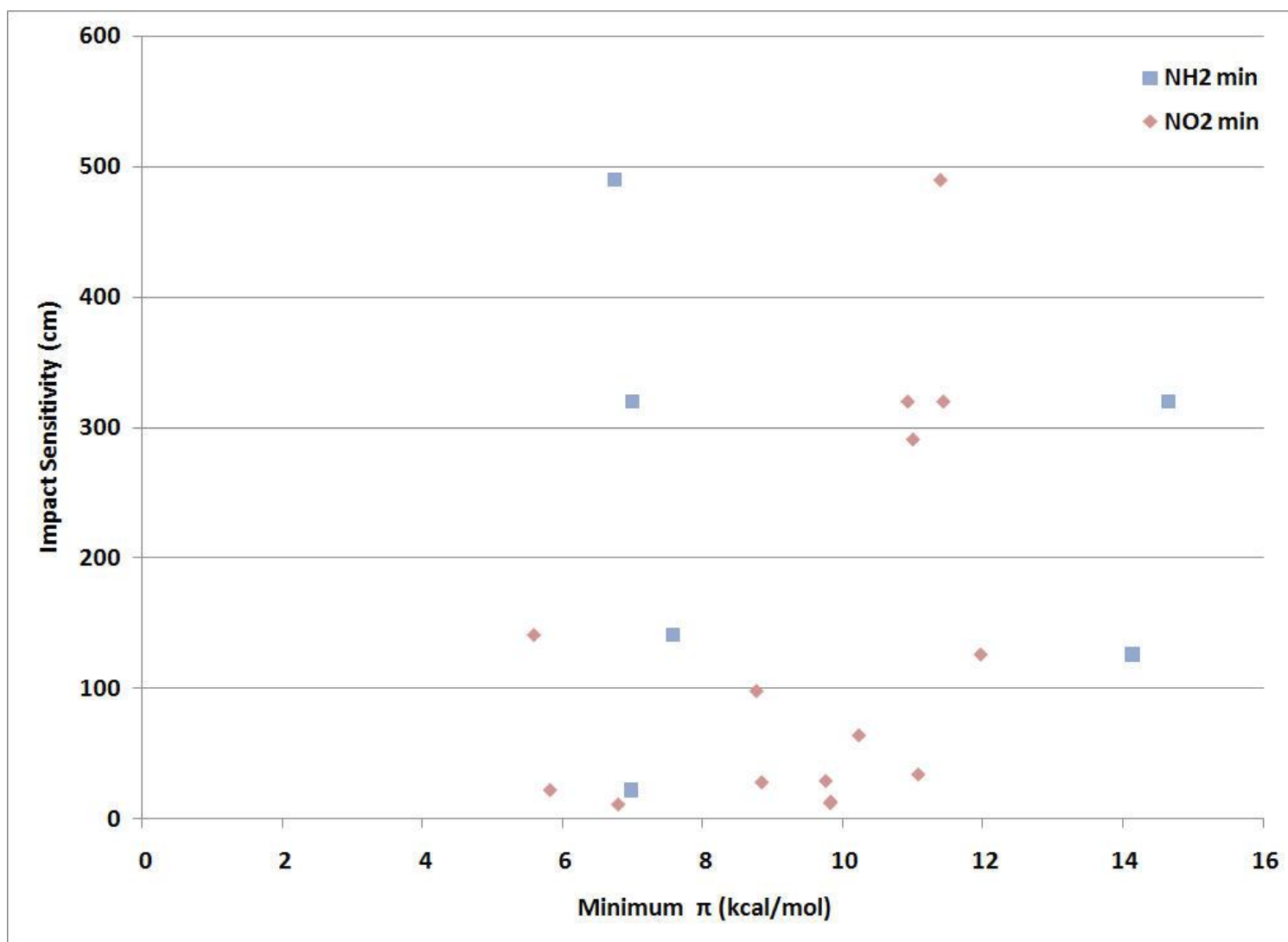


Figure A-106. Impact sensitivity (cm) vs. group minimum π (kcal/mol) electrostatic potential for PBE/6-31G**.

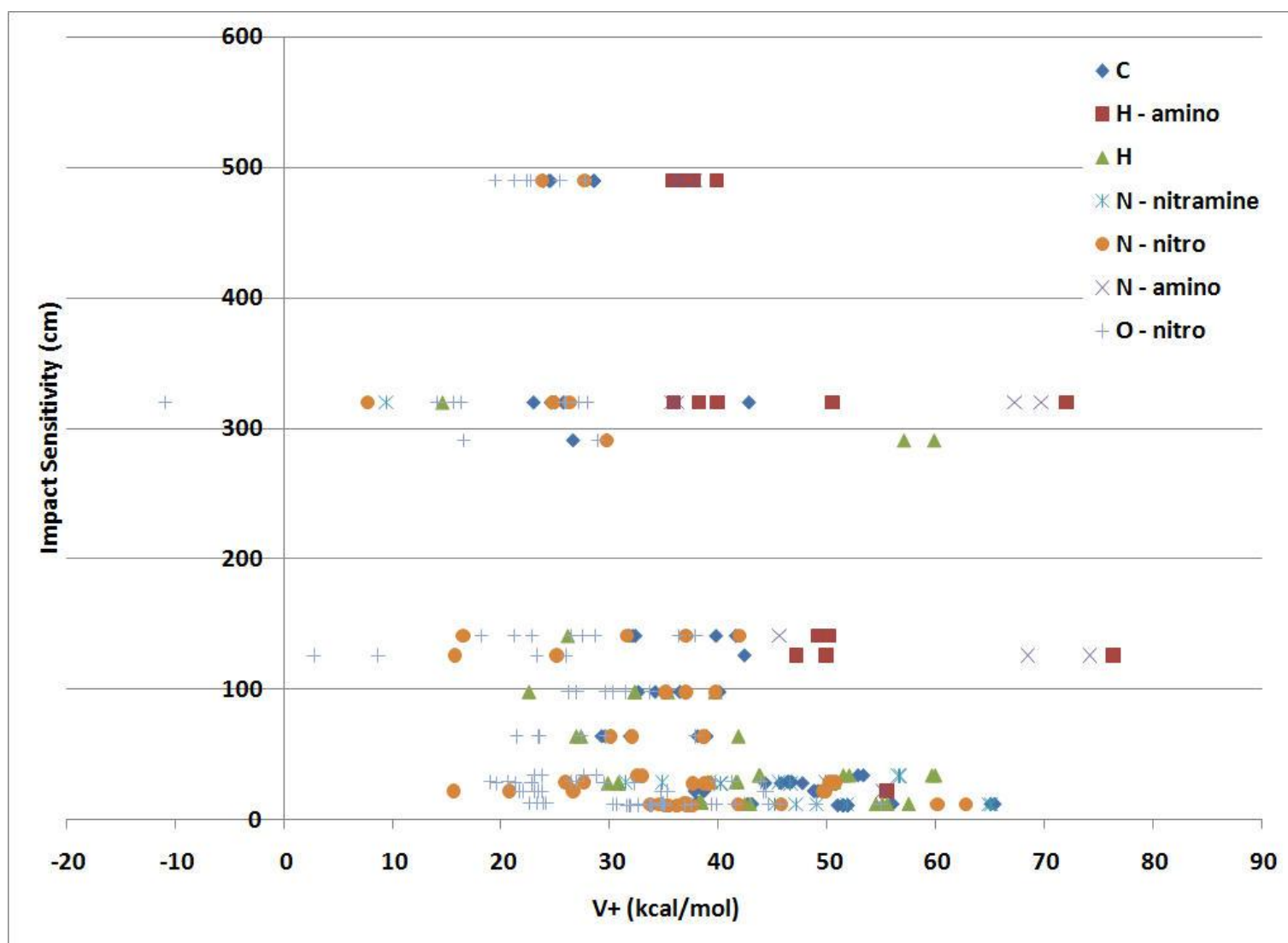


Figure A-107. Impact sensitivity (cm) vs. atomic V^+ (kcal/mol) electrostatic potential for PBE/6-31G**.

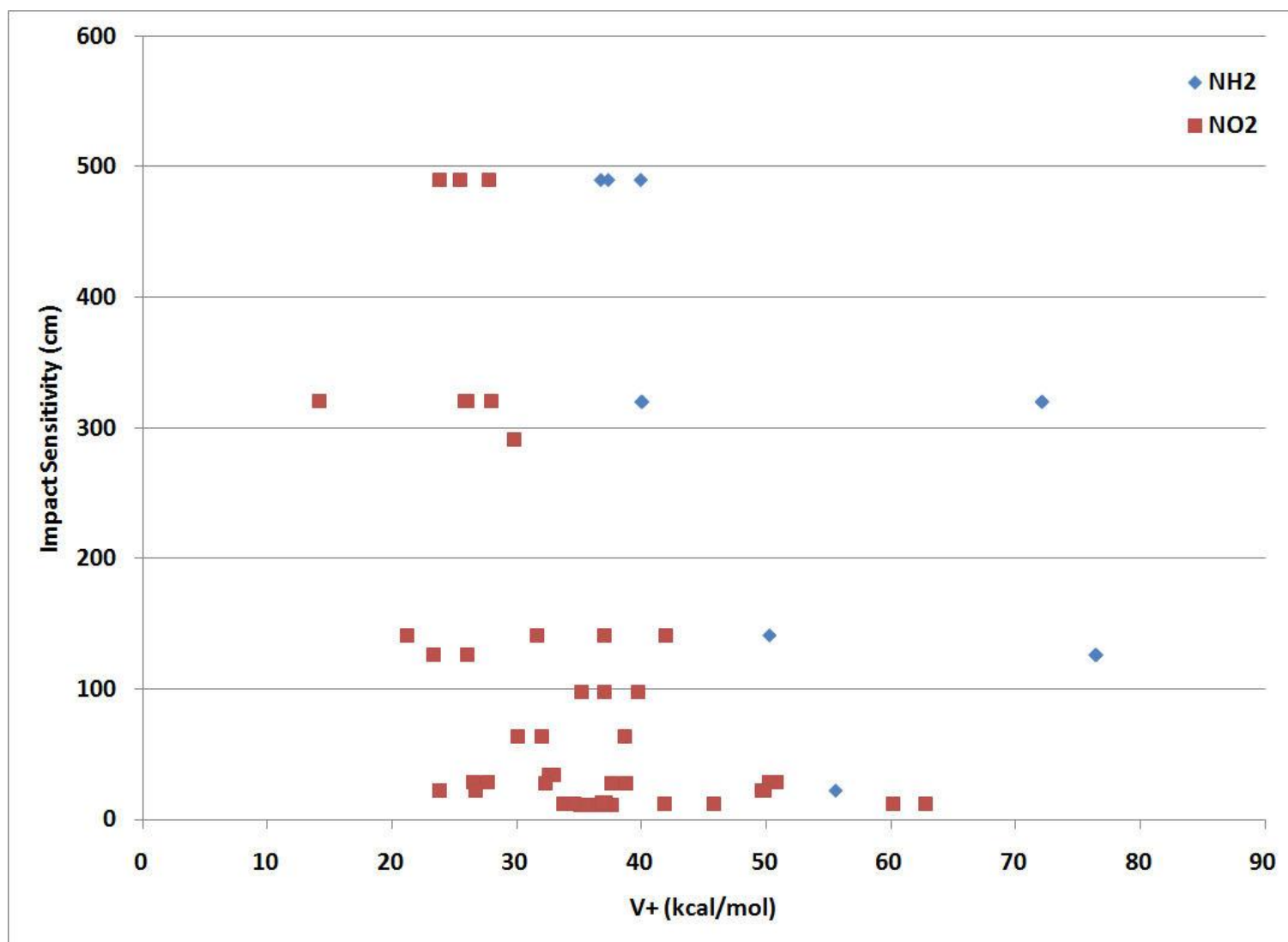


Figure A-108. Impact sensitivity (cm) vs. group V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

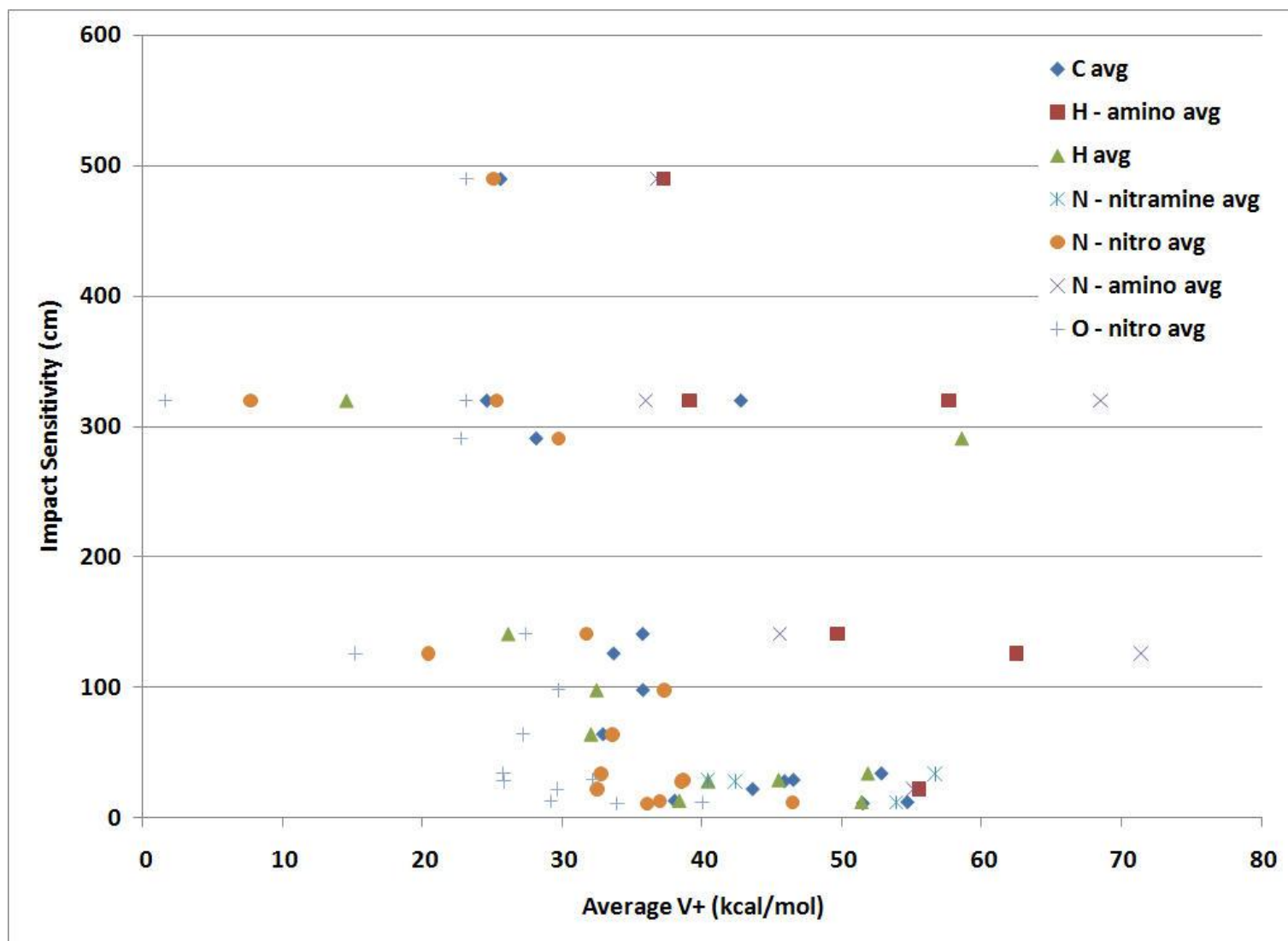


Figure A-109. Impact sensitivity (cm) vs. atomic average V^+ (kcal/mol) electrostatic potential for PBE/6-31G**.

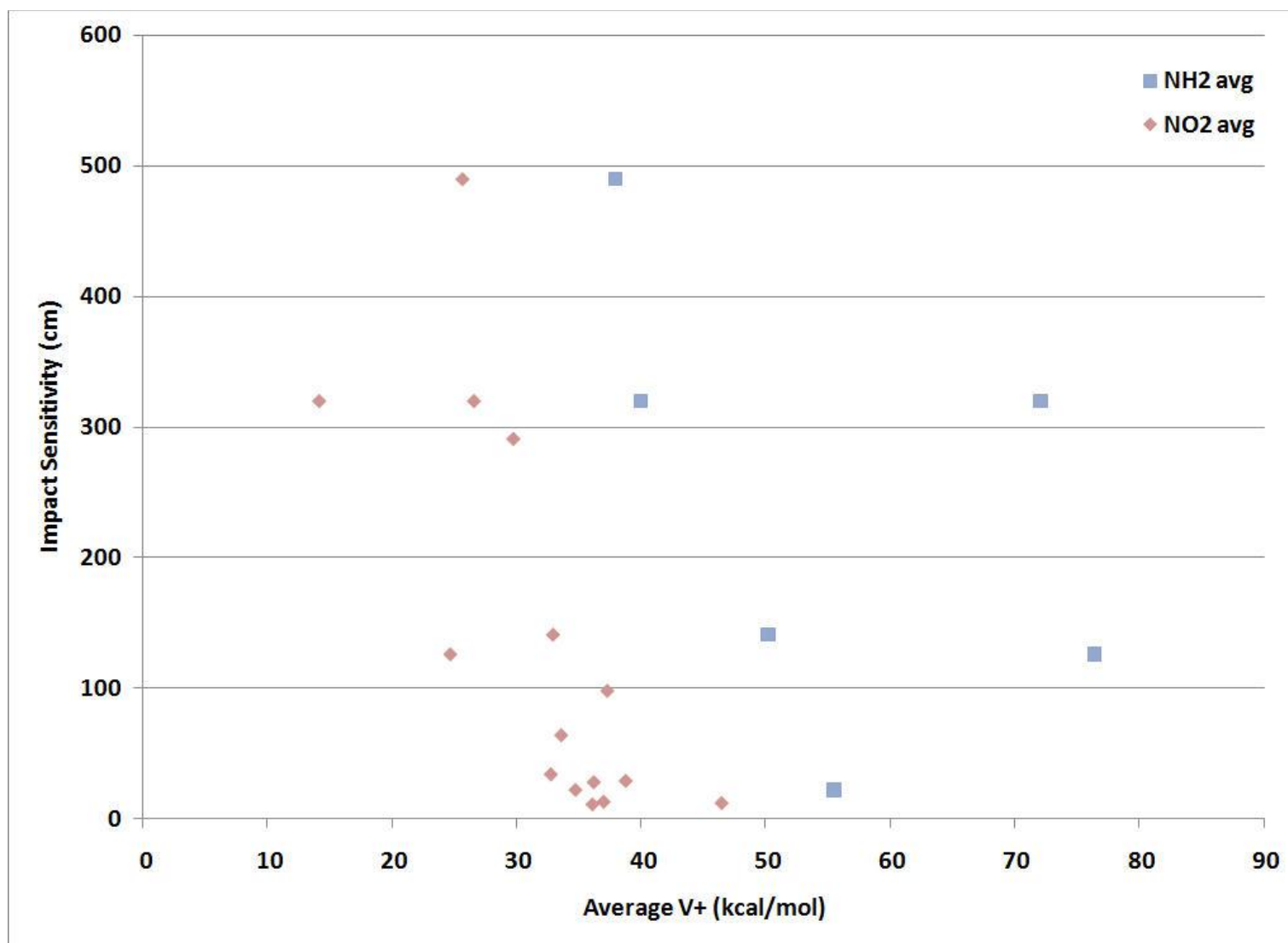


Figure A-110. Impact sensitivity (cm) vs. group average V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

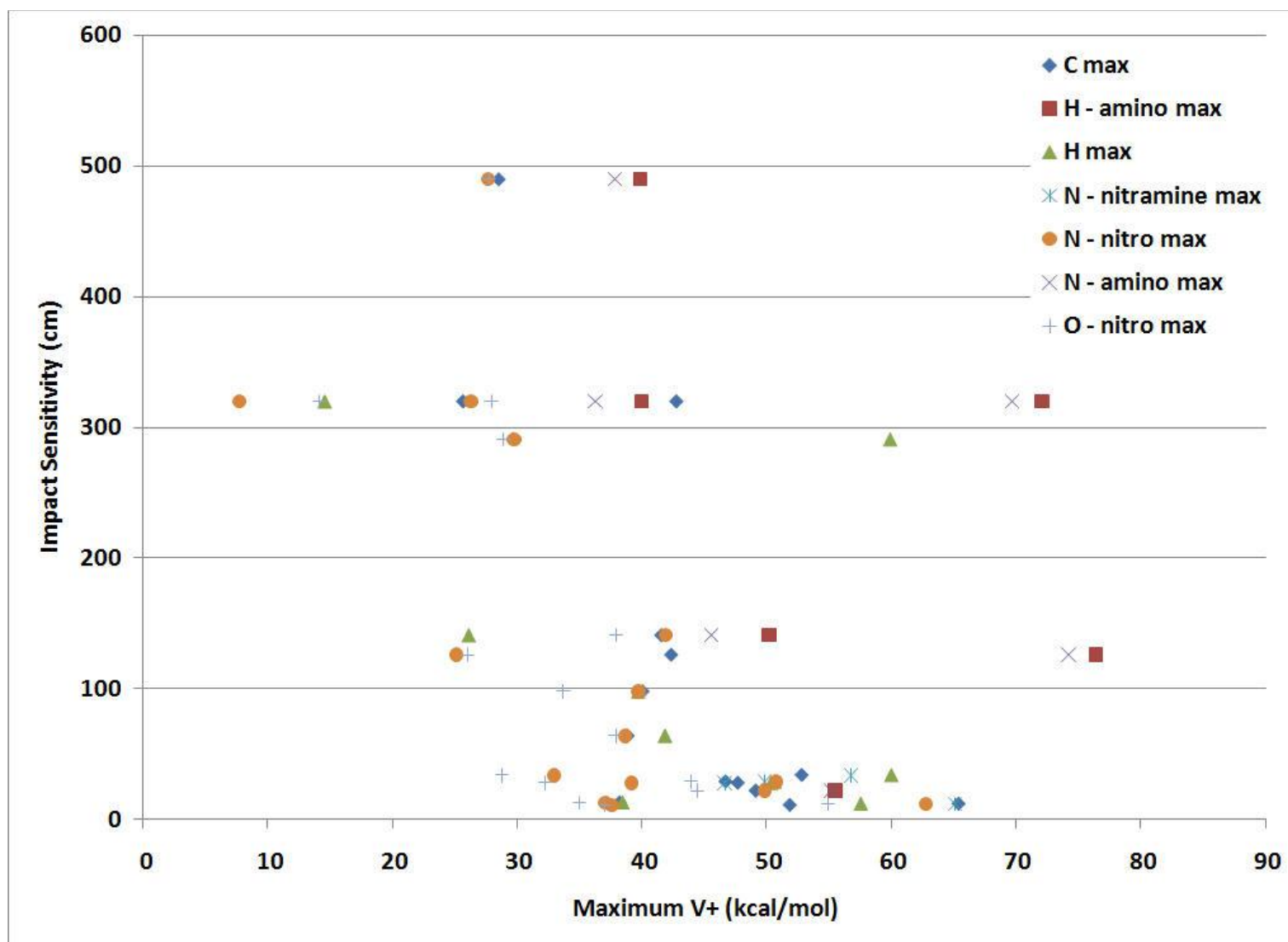


Figure A-111. Impact sensitivity (cm) vs. atomic maximum V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

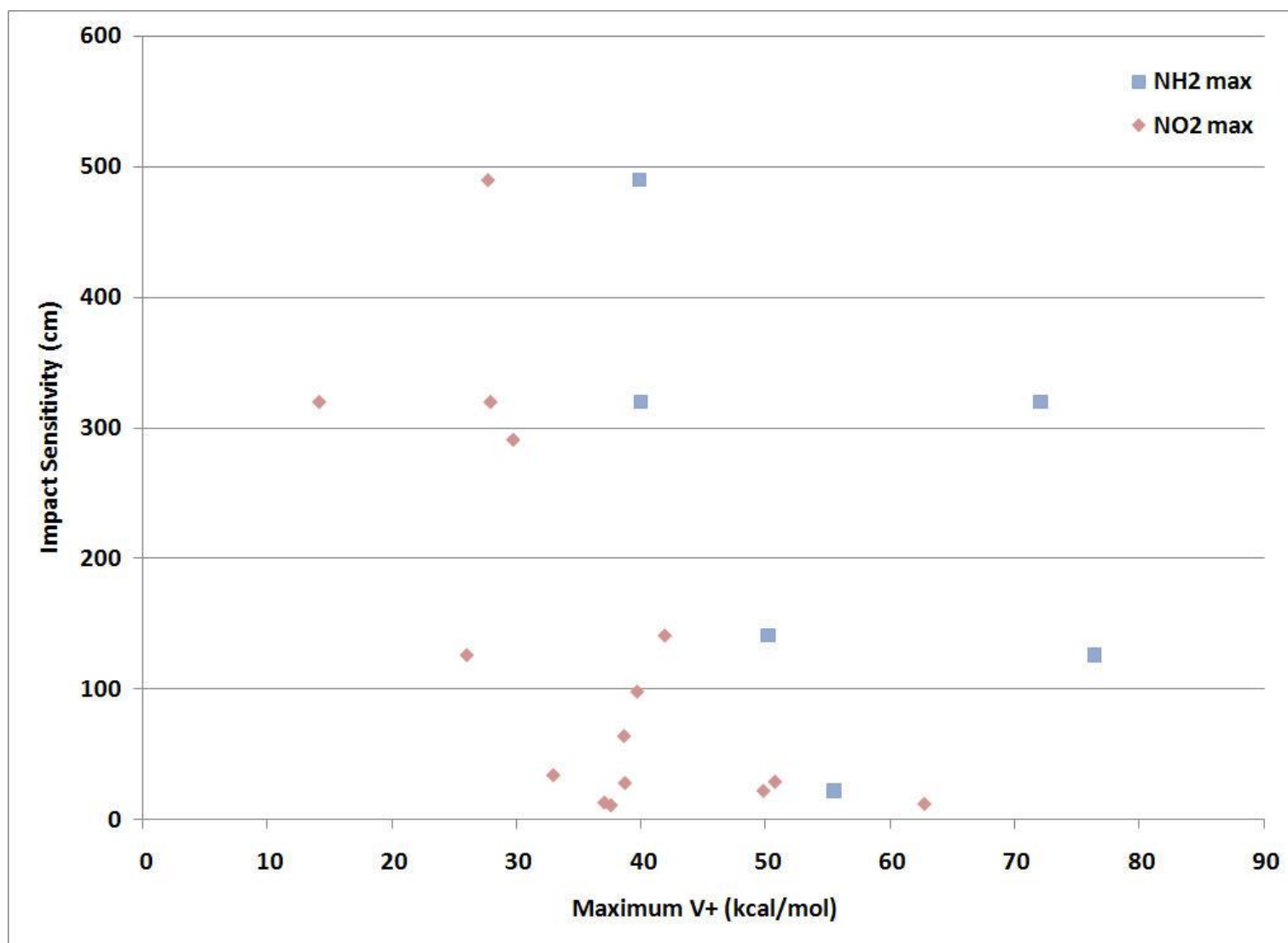


Figure A-112. Impact sensitivity (cm) vs. group maximum V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

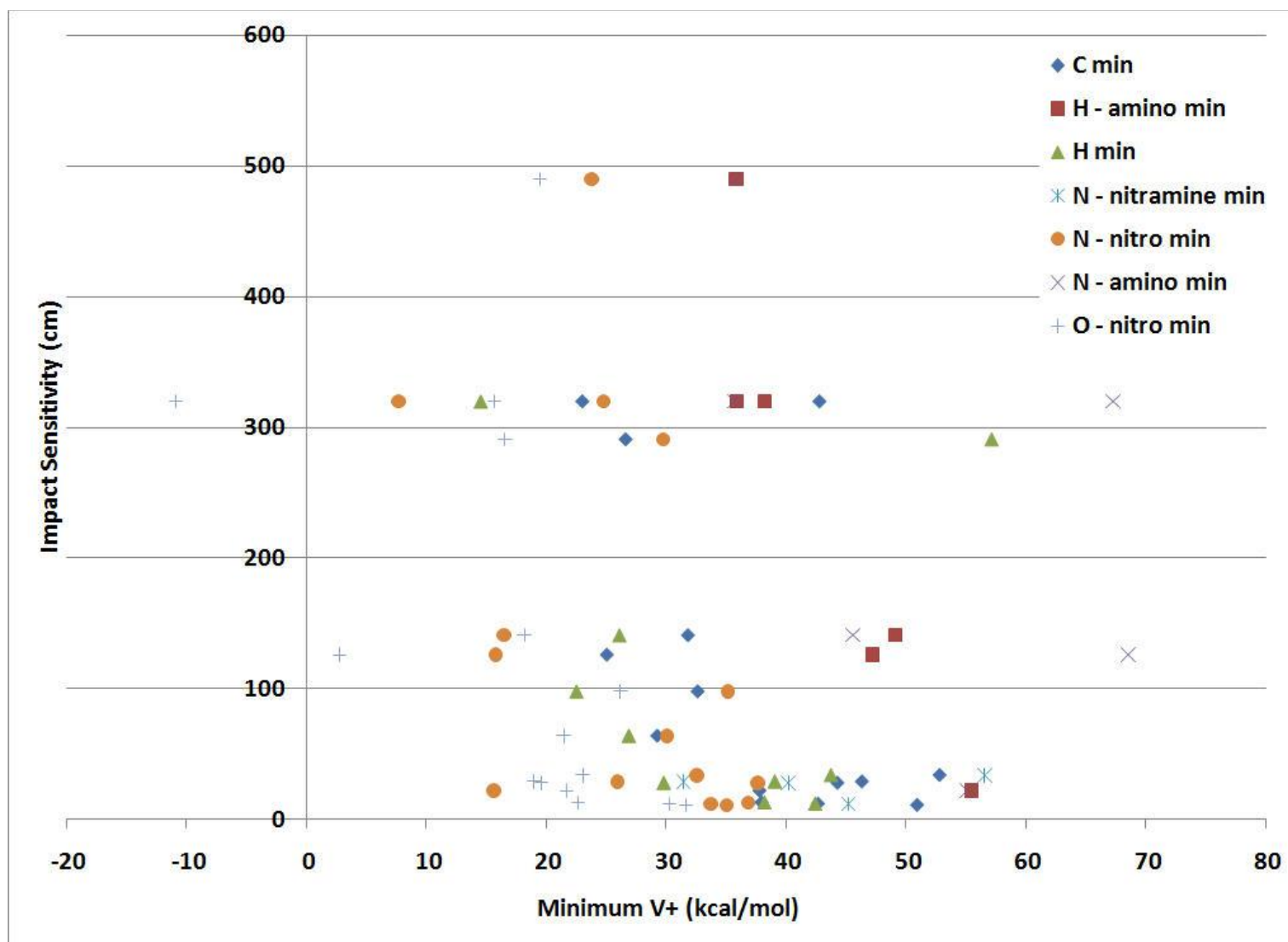


Figure A-113. Impact sensitivity (cm) vs. atomic minimum V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

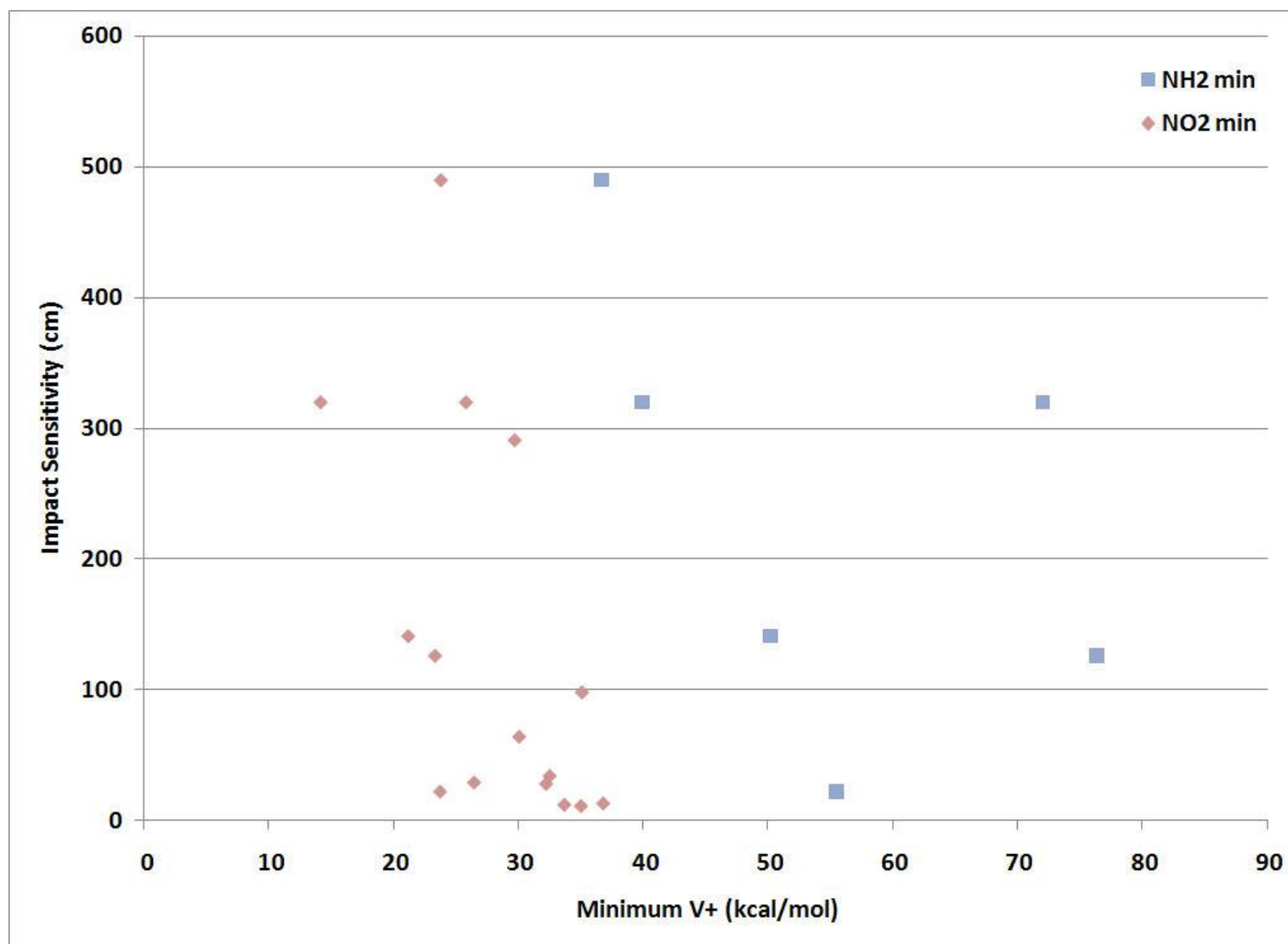


Figure A-114. Impact sensitivity (cm) vs. group minimum V+ (kcal/mol) electrostatic potential for PBE/6-31G**.

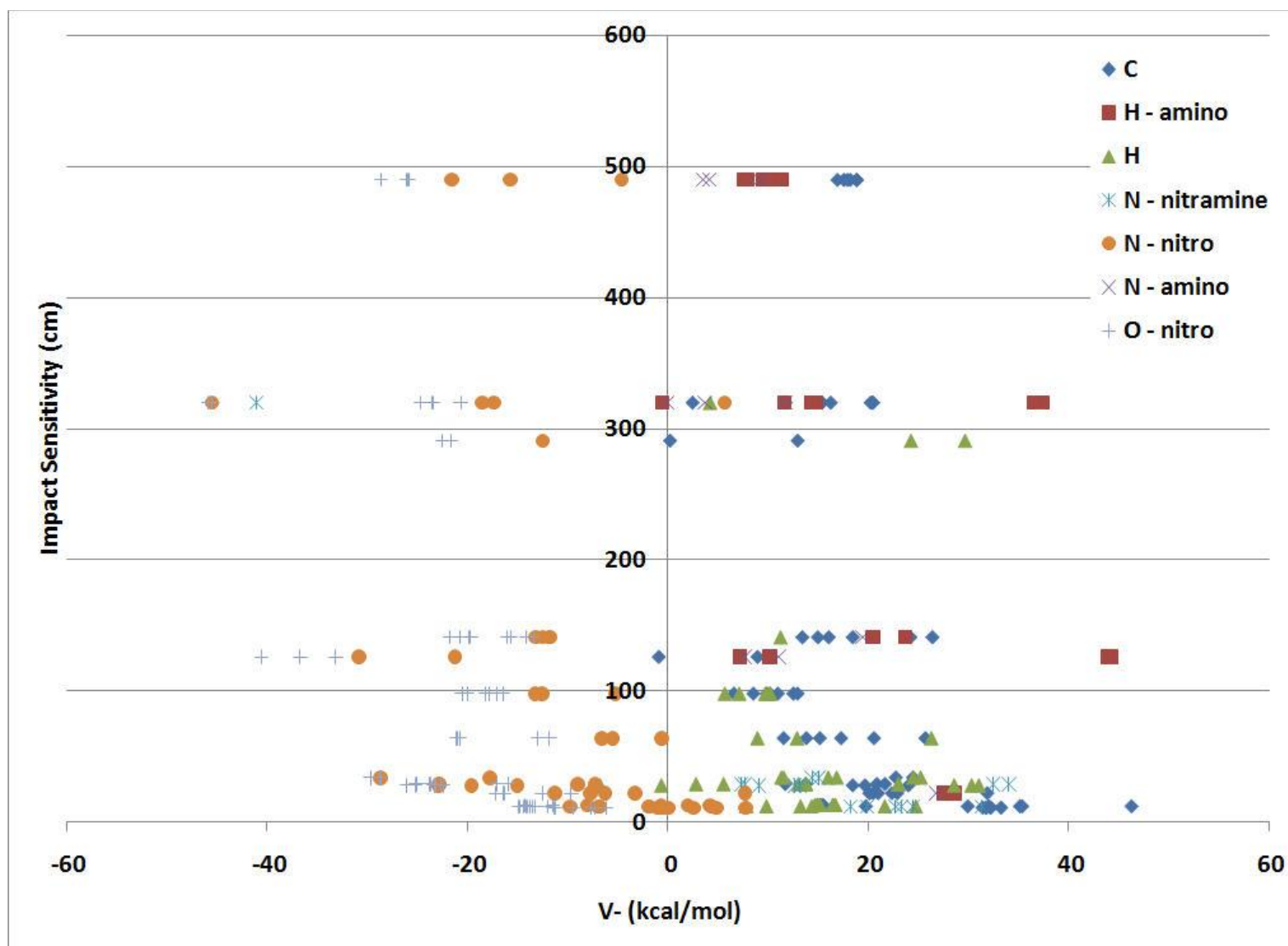


Figure A-115. Impact sensitivity (cm) vs. atomic V- (kcal/mol) electrostatic potential for PBE/6-31G**.

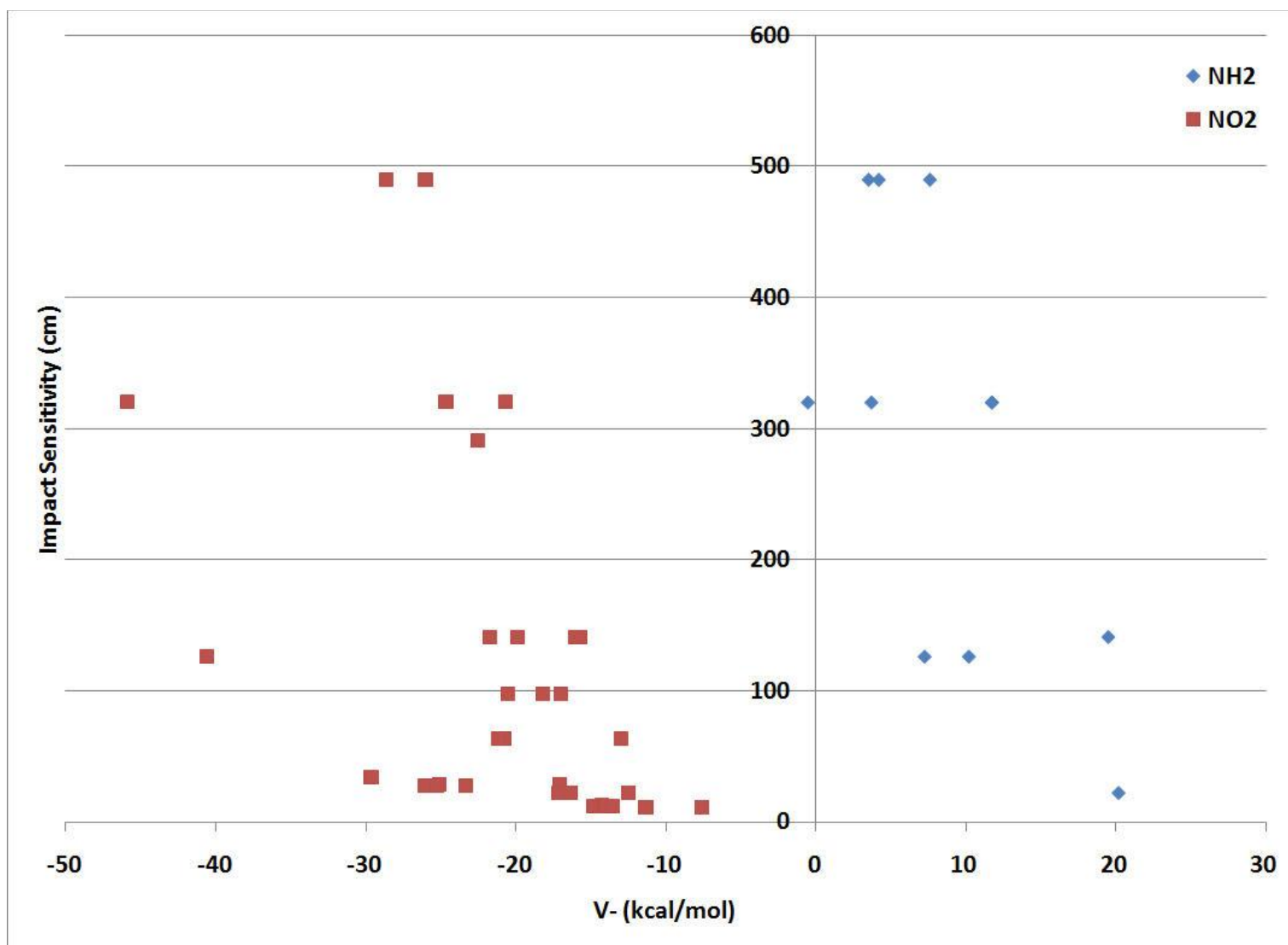


Figure A-116. Impact sensitivity (cm) vs. group V- (kcal/mol) electrostatic potential for PBE/6-31G**.

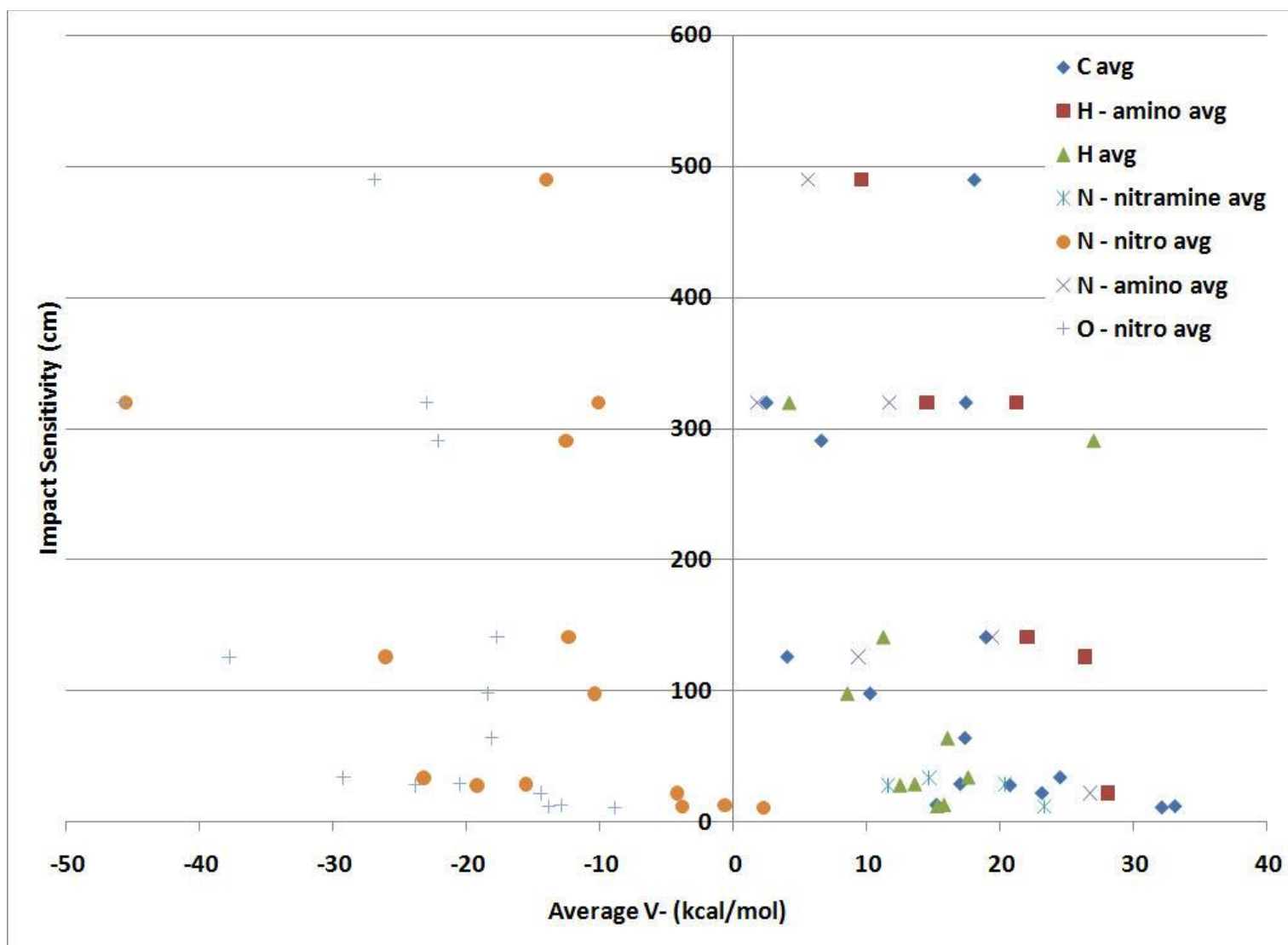


Figure A-117. Impact sensitivity (cm) vs. atomic average V- (kcal/mol) electrostatic potential for PBE/6-31G**.

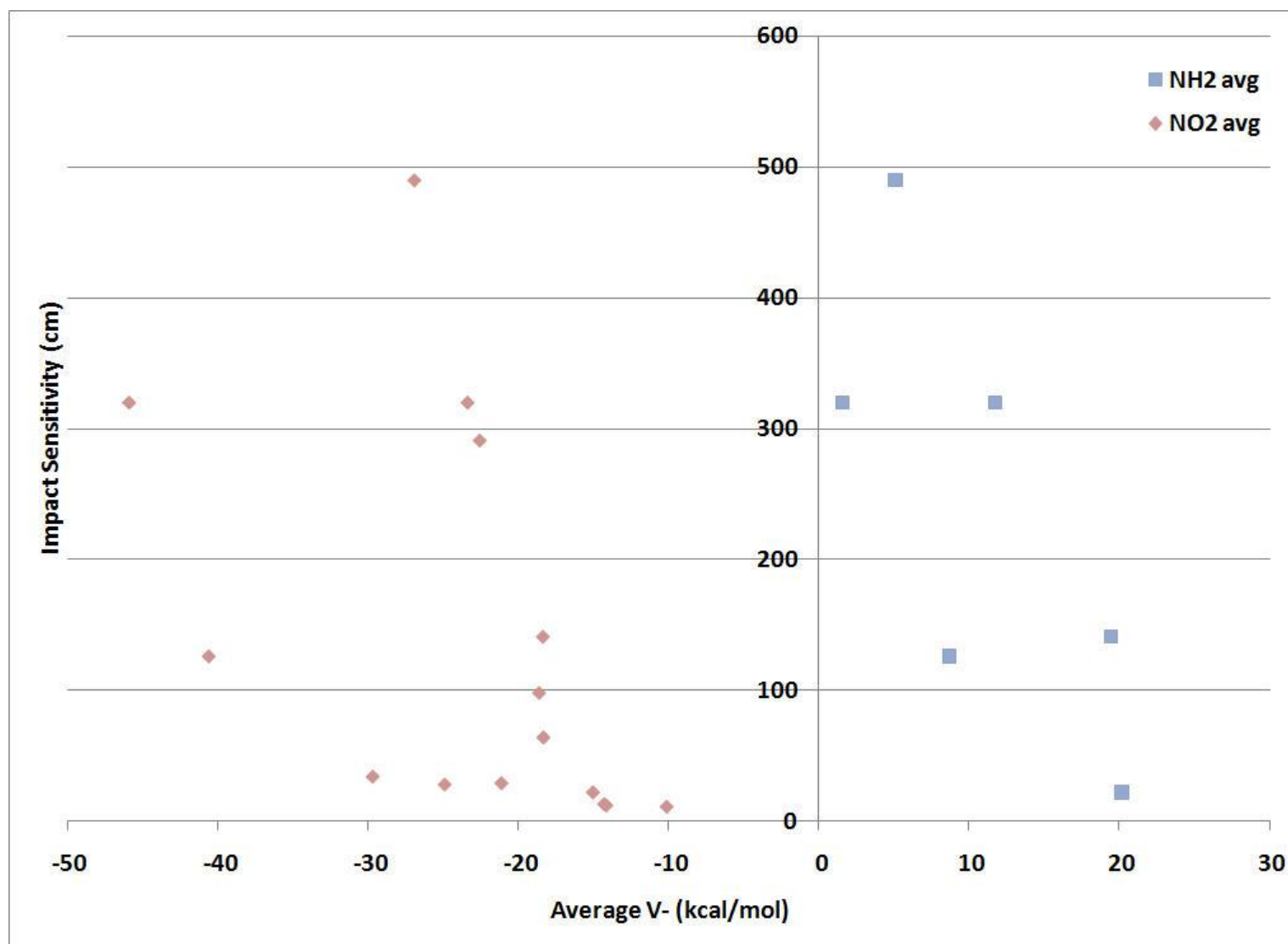


Figure A-118. Impact sensitivity (cm) vs. group average V- (kcal/mol) electrostatic potential for PBE/6-31G**.

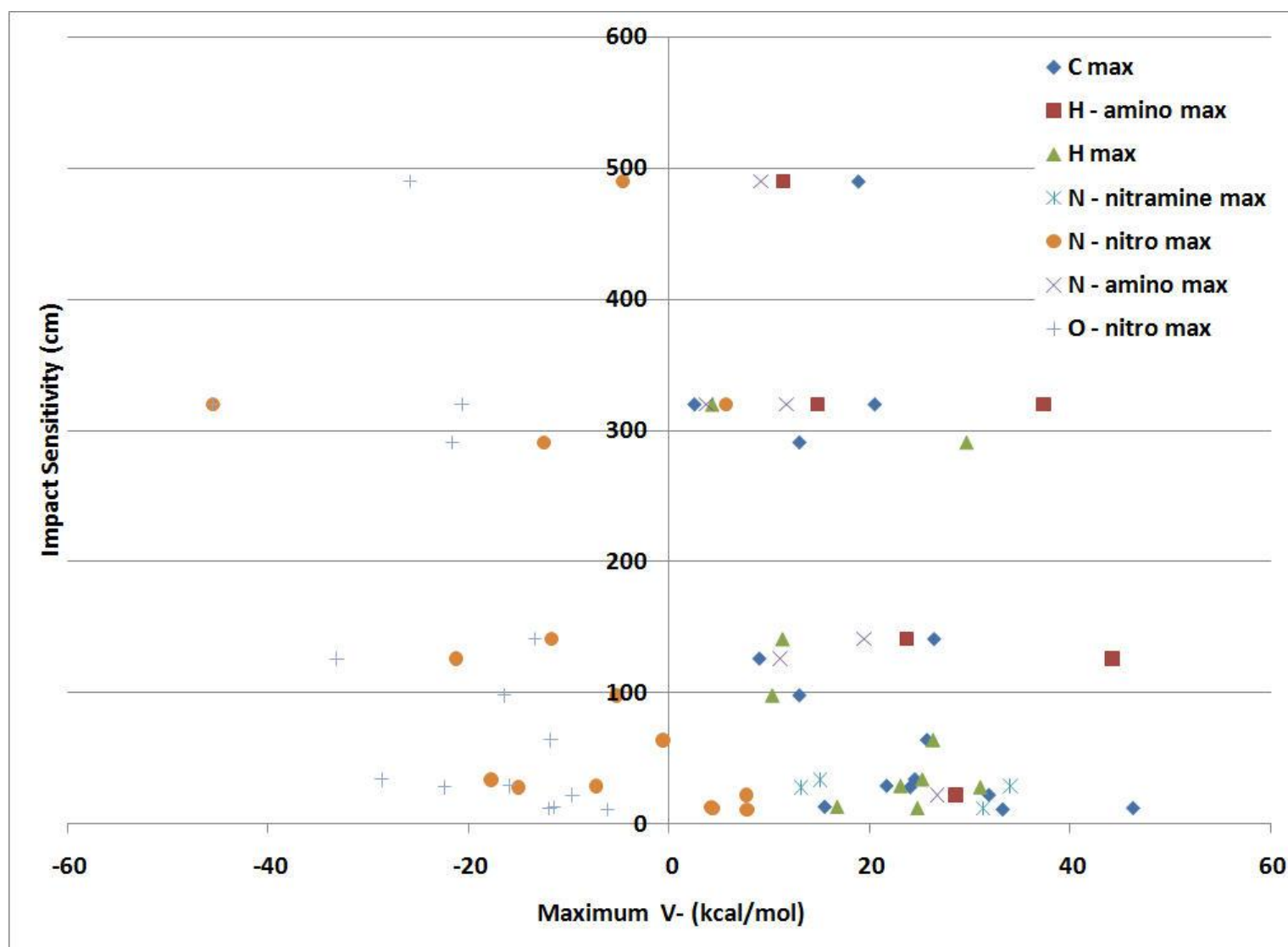


Figure A-119. Impact sensitivity (cm) vs. atomic maximum V- (kcal/mol) electrostatic potential for PBE/6-31G**.

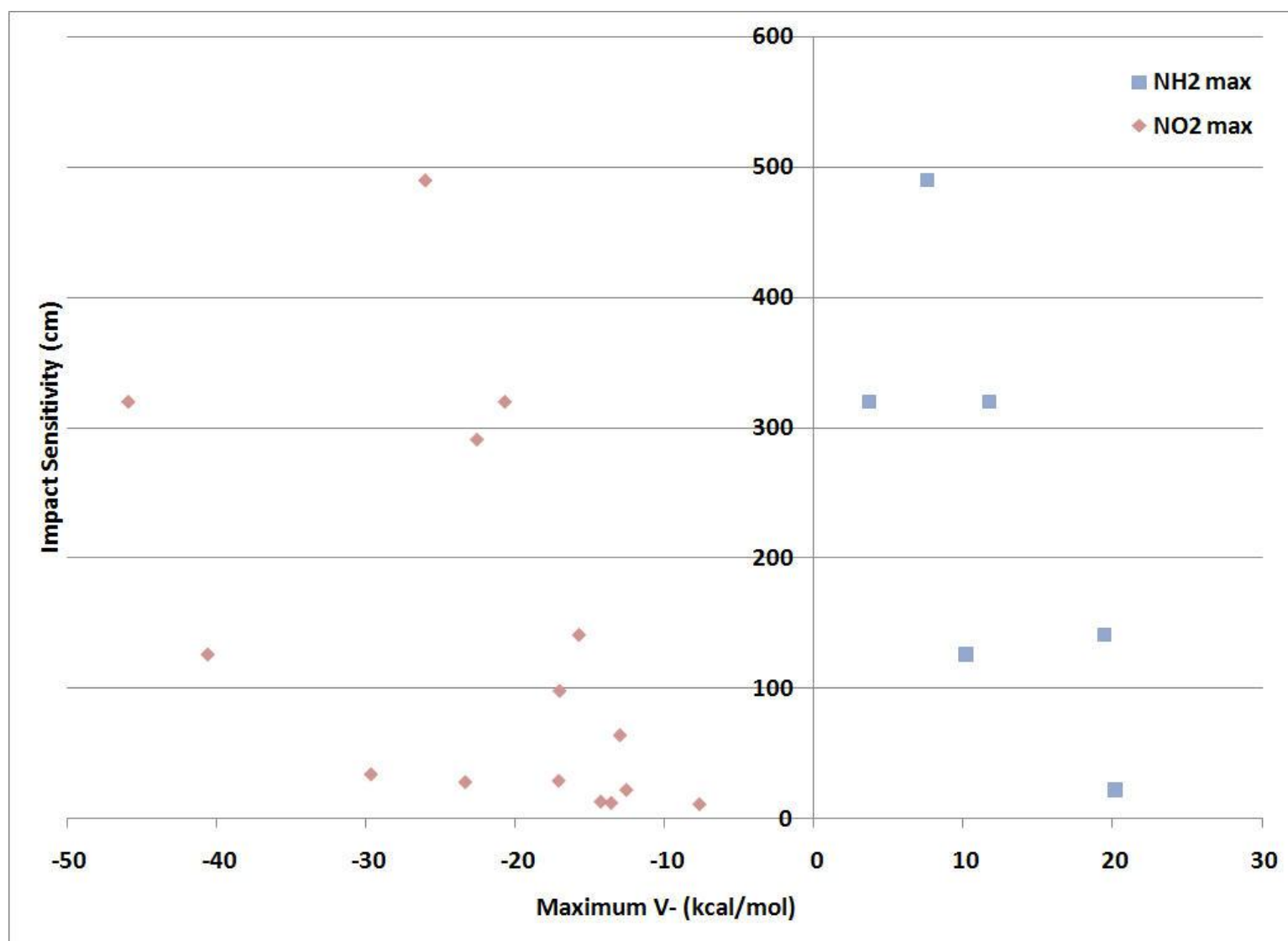


Figure A-120. Impact sensitivity (cm) vs. group maximum V- (kcal/mol) electrostatic potential for PBE/6-31G**.

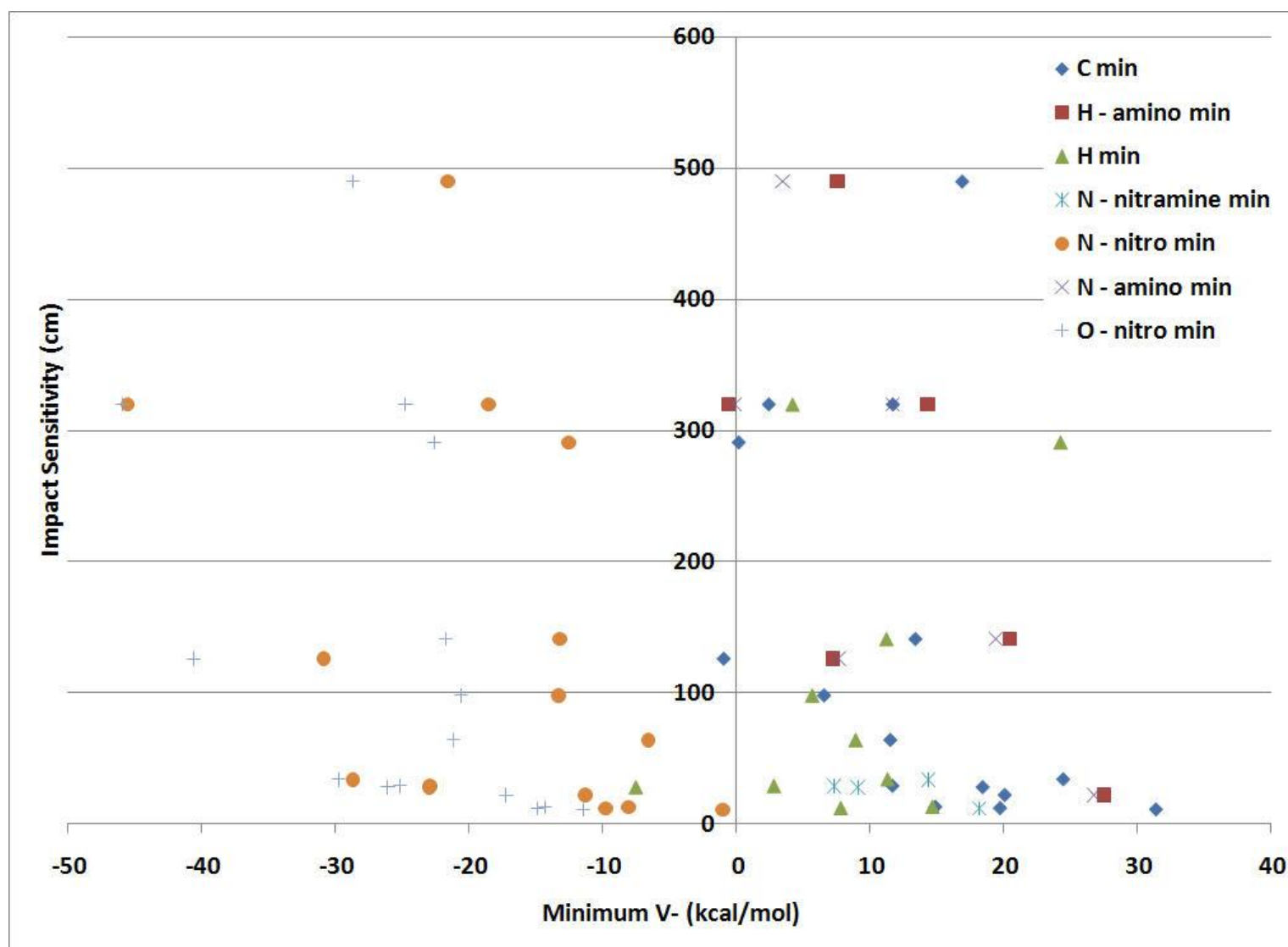


Figure A-121. Impact sensitivity (cm) vs. atomic minimum V- (kcal/mol) electrostatic potential for PBE/6-31G**.

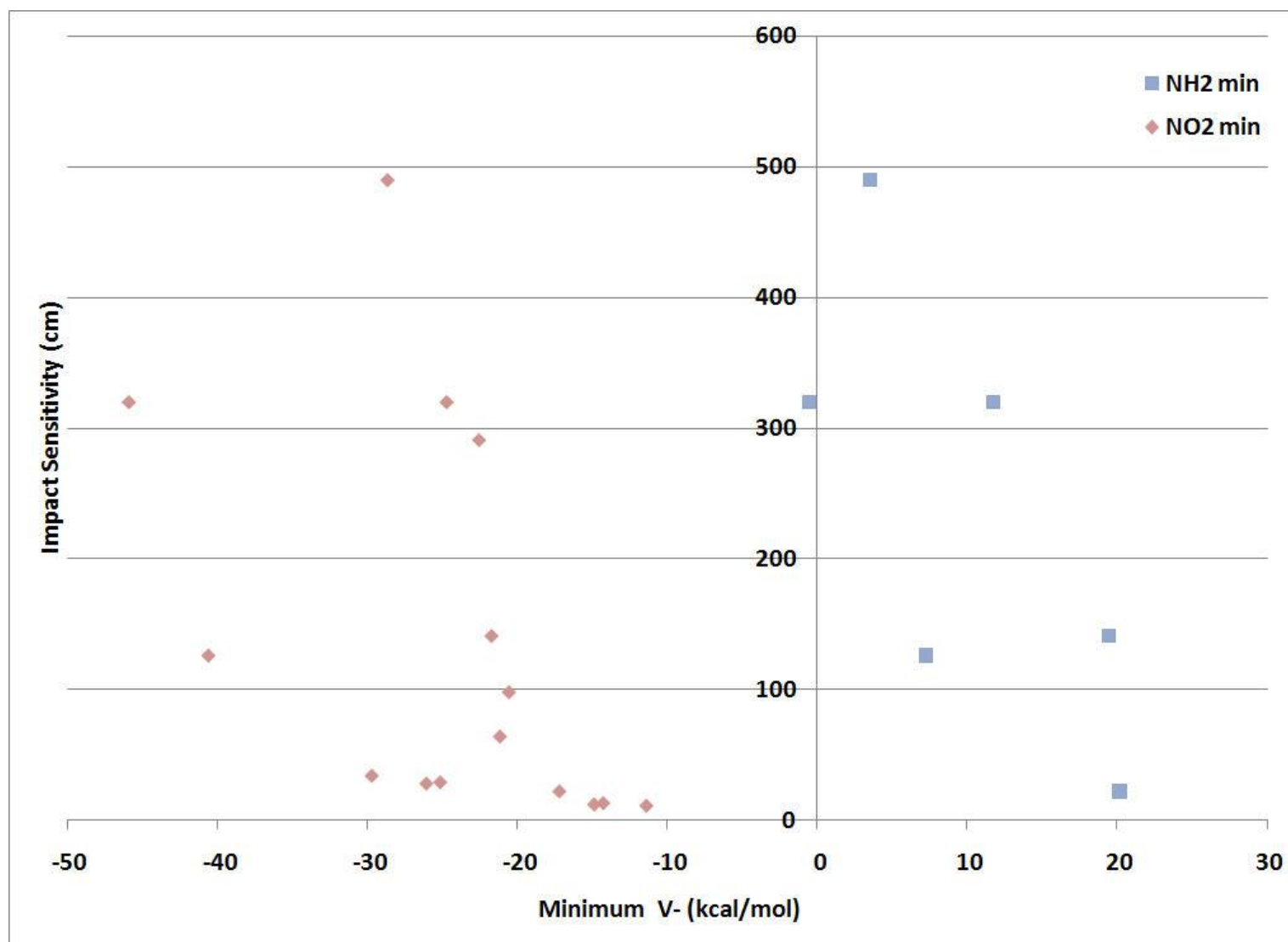


Figure A-122. Impact sensitivity (cm) vs. group minimum V- (kcal/mol) electrostatic potential for PBE/6-31G**.

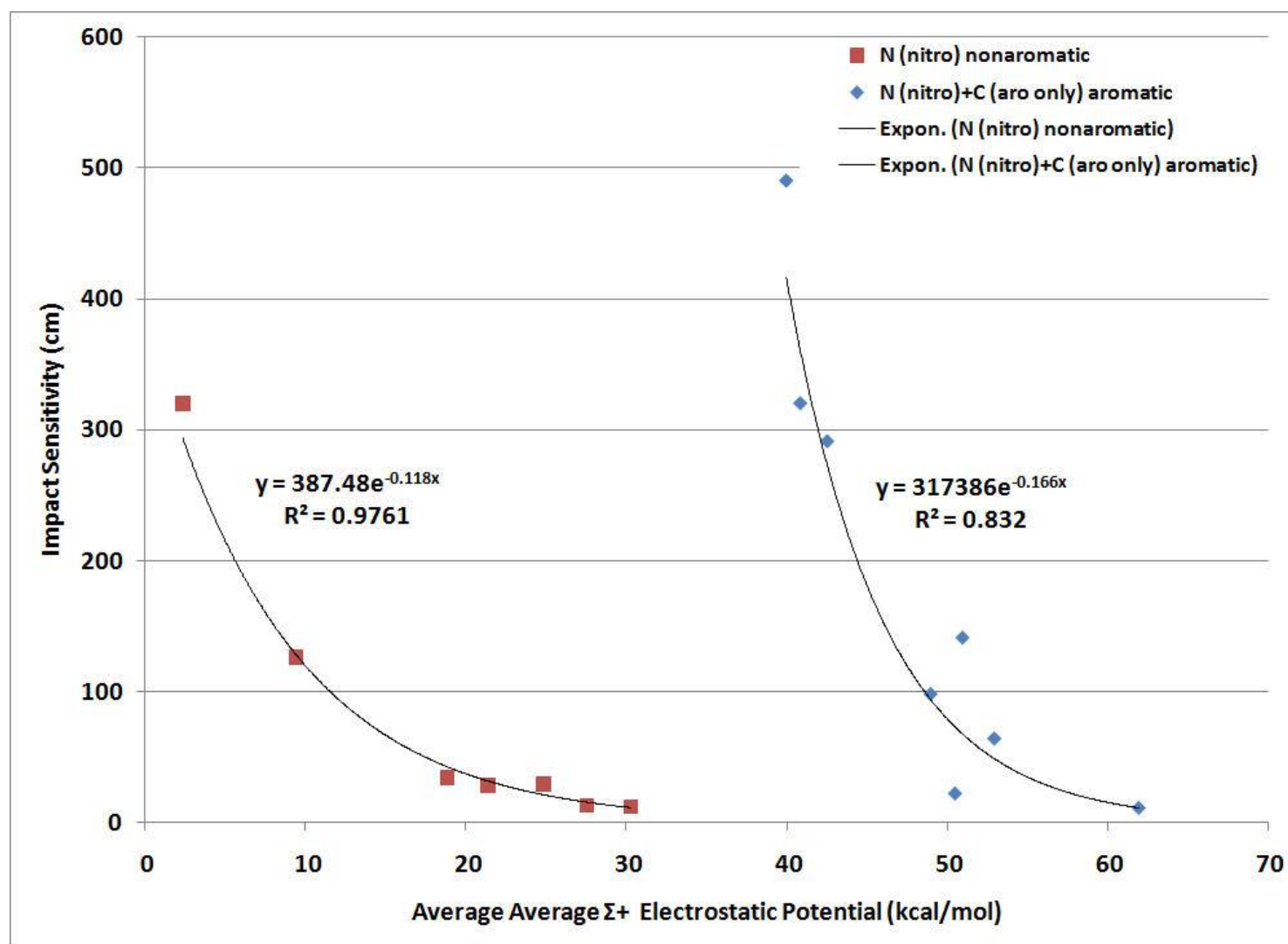


Figure A-123. Impact sensitivity (cm) vs. average average Σ^+ electrostatic potential (kcal/mol) for (1) nitro nitrogens for nonaromatic species and (2) nitro nitrogen plus associated aromatic carbons for aromatic species for PBE/6-31G**. Exponential fits with associated R^2 factors included.

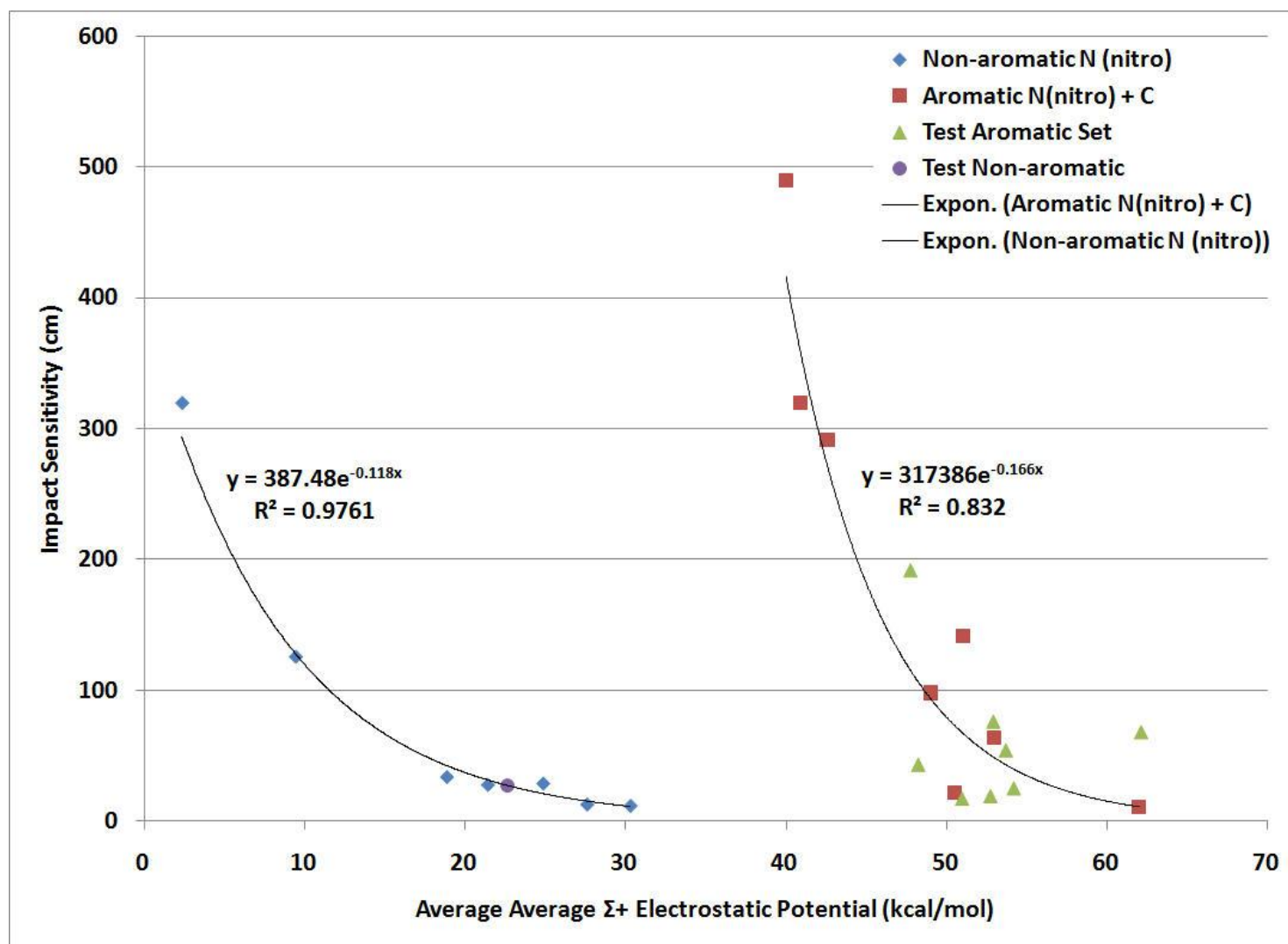


Figure A-124. Impact sensitivity (cm) vs. average average Σ^+ electrostatic potential (kcal/mol) for (1) nitro nitrogens for nonaromatic species and (2) nitro nitrogen plus associated aromatic carbons for aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

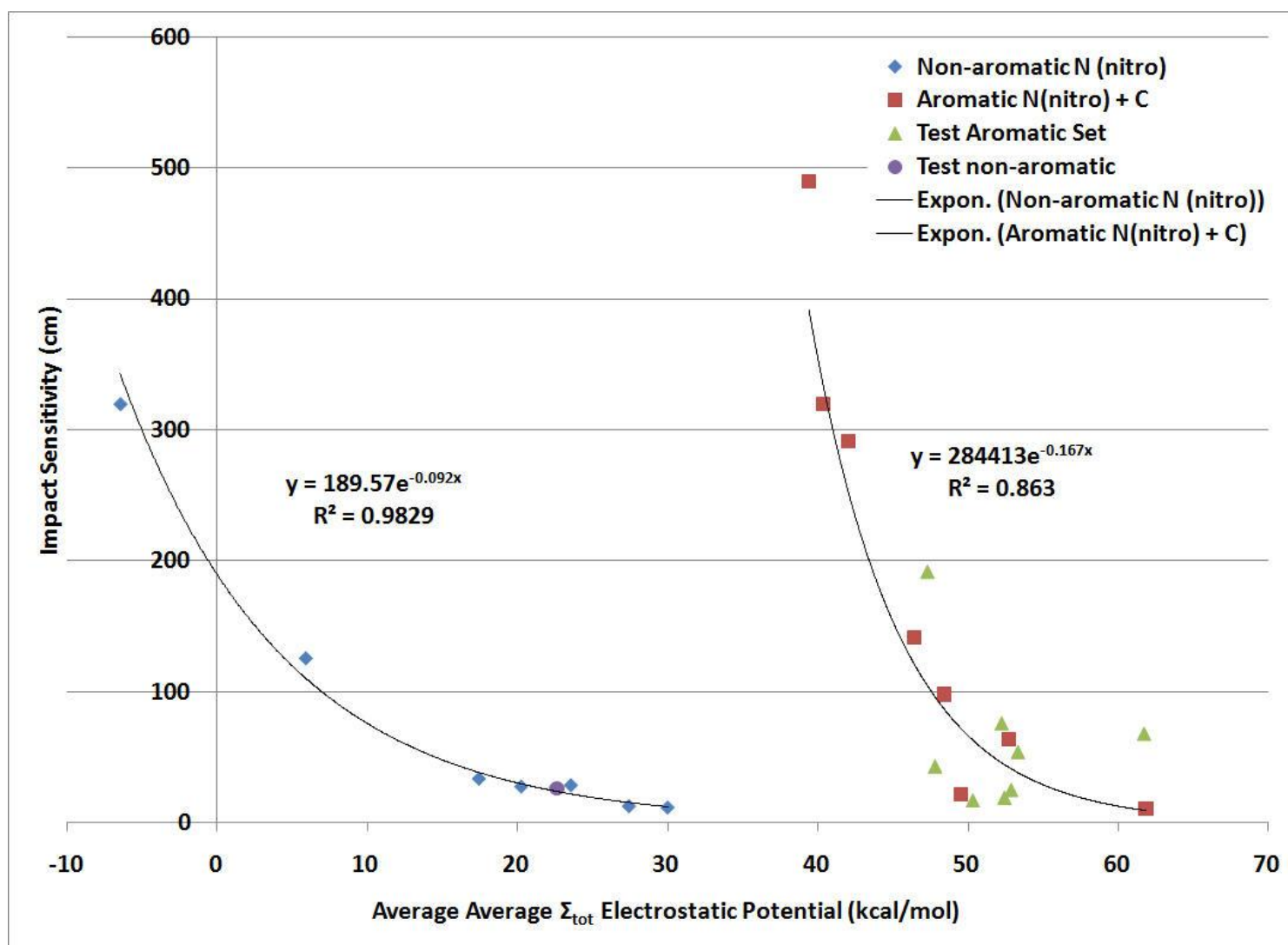


Figure A-125. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for nitro nitrogens for (1) nonaromatic and (2) nitro nitrogen plus associated aromatic carbons for aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

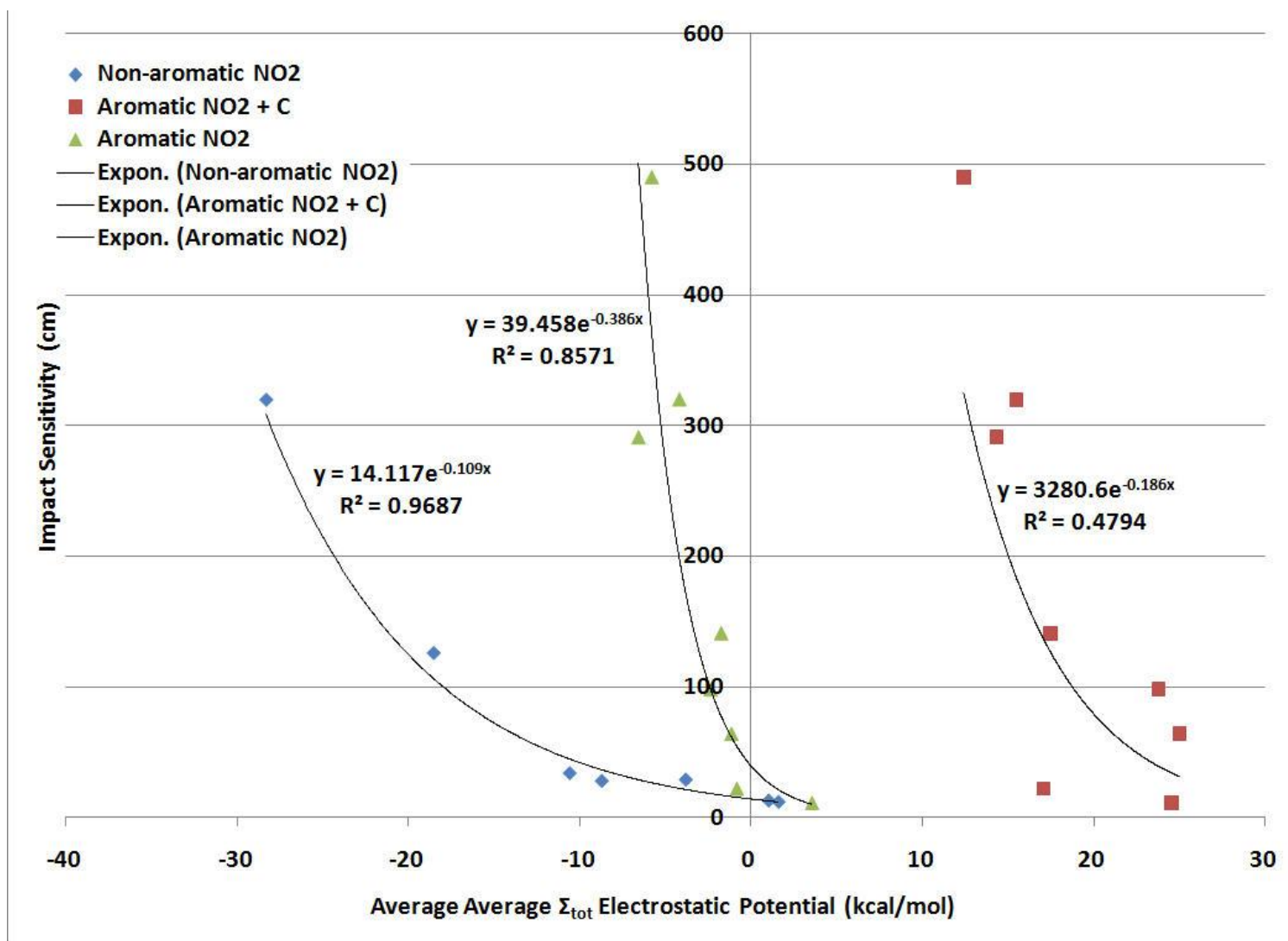


Figure A-126. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for (1) nitro groups for (1) nonaromatic and (2) aromatic species and (3) nitro groups plus associated aromatic carbons for aromatic species for PBE/6-31G**. Exponential fits with associated R^2 factors included.

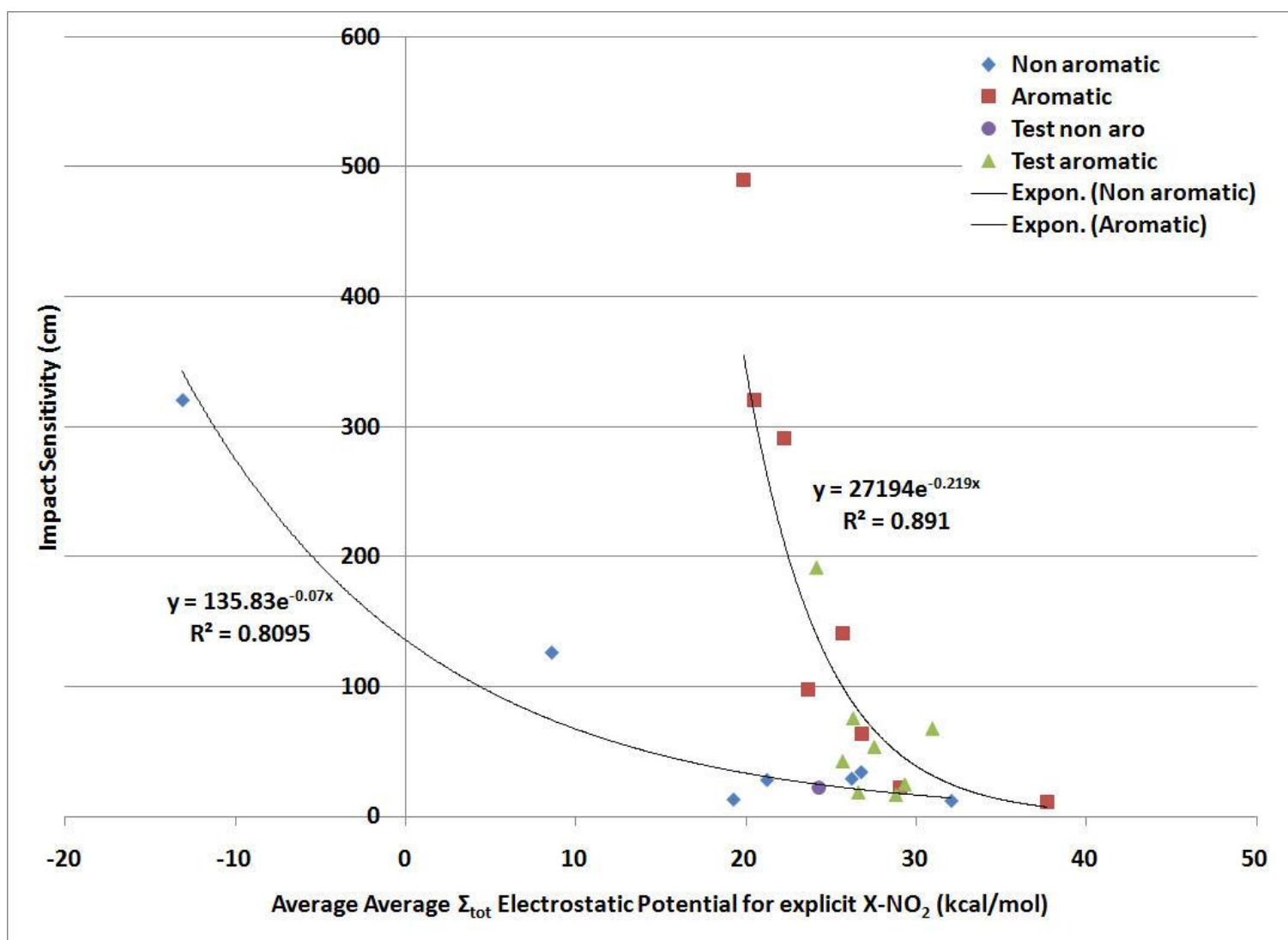


Figure A-127. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

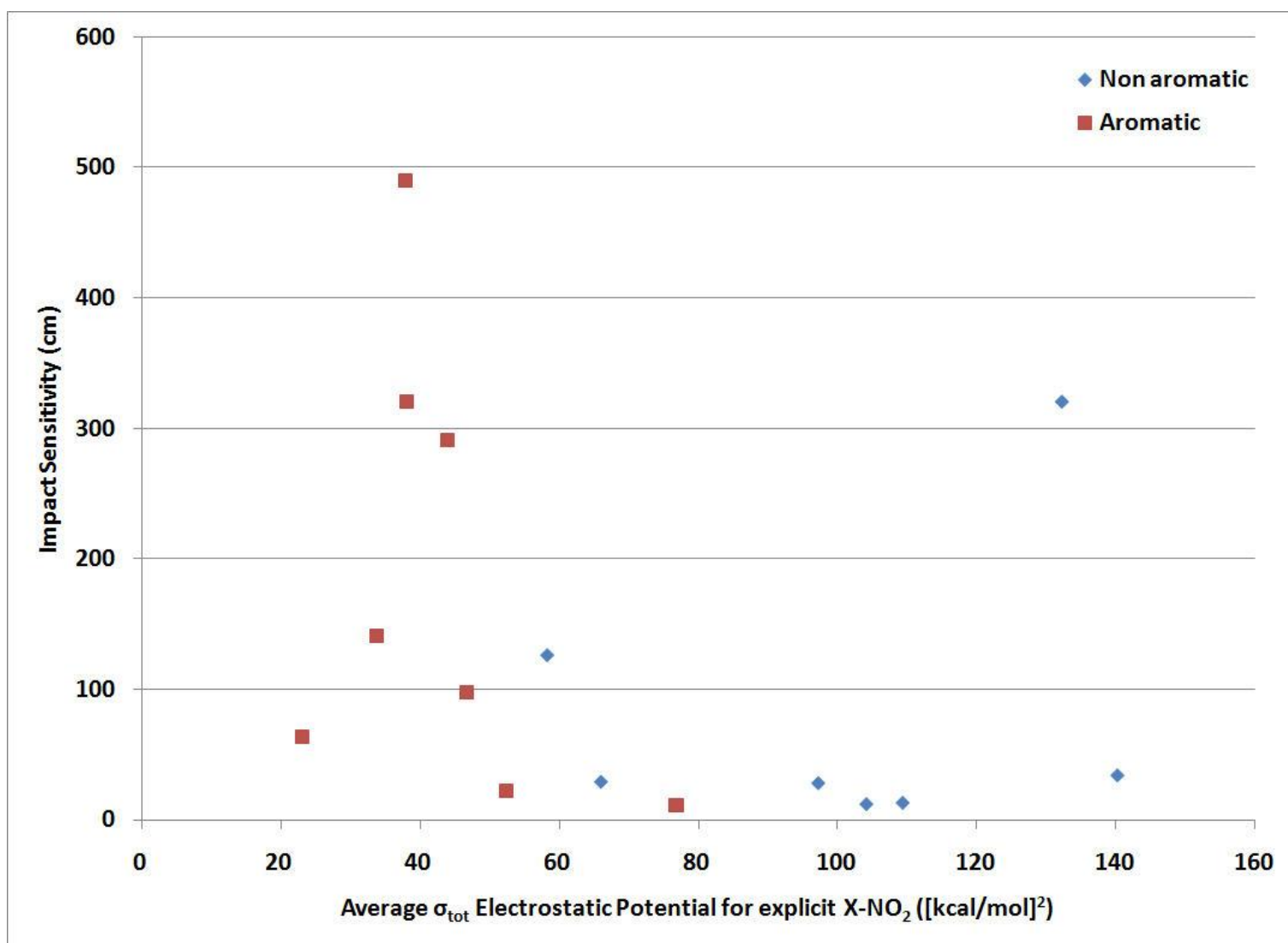


Figure A-128. Impact sensitivity (cm) vs. average σ_{tot}^2 electrostatic potential ([kcal/mol]²) for explicit X-N subgroups of the X-NO₂ for nonaromatic and aromatic species for PBE/6-31G**.

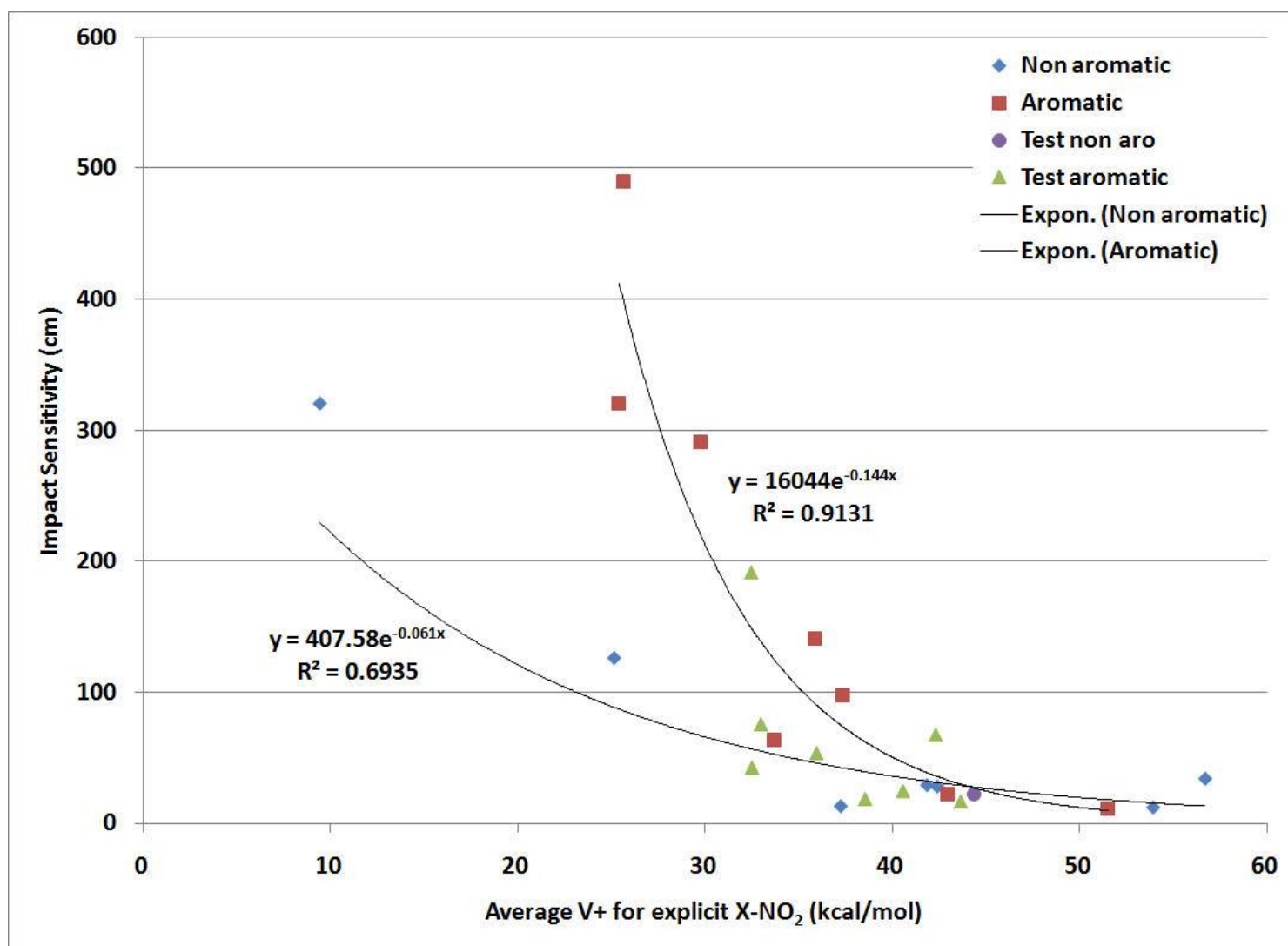


Figure A-129. Impact sensitivity (cm) vs. average V+ electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R² factors included.

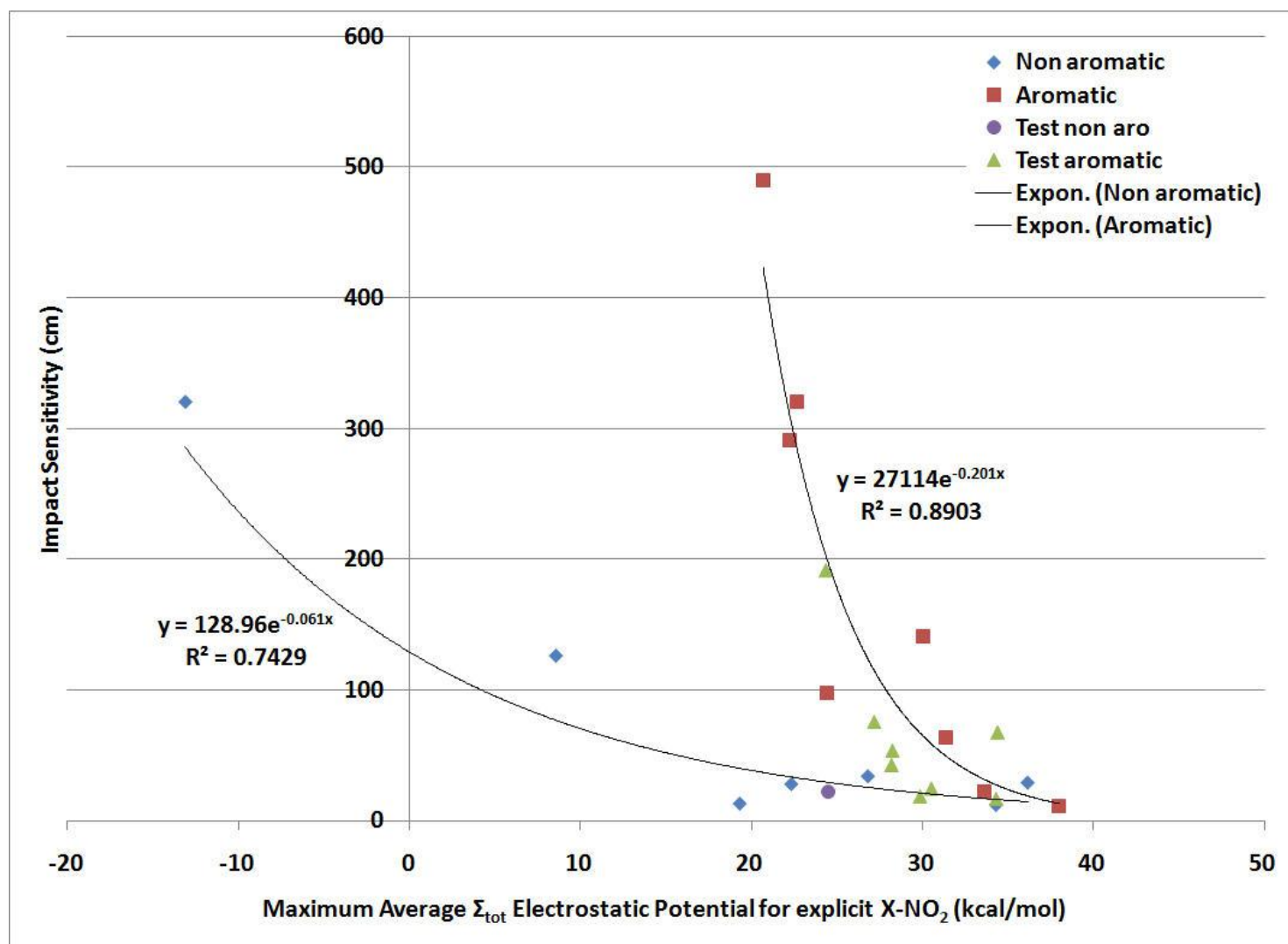


Figure A-130. Impact sensitivity (cm) vs. maximum average Σ_{tot} electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R² factors included.

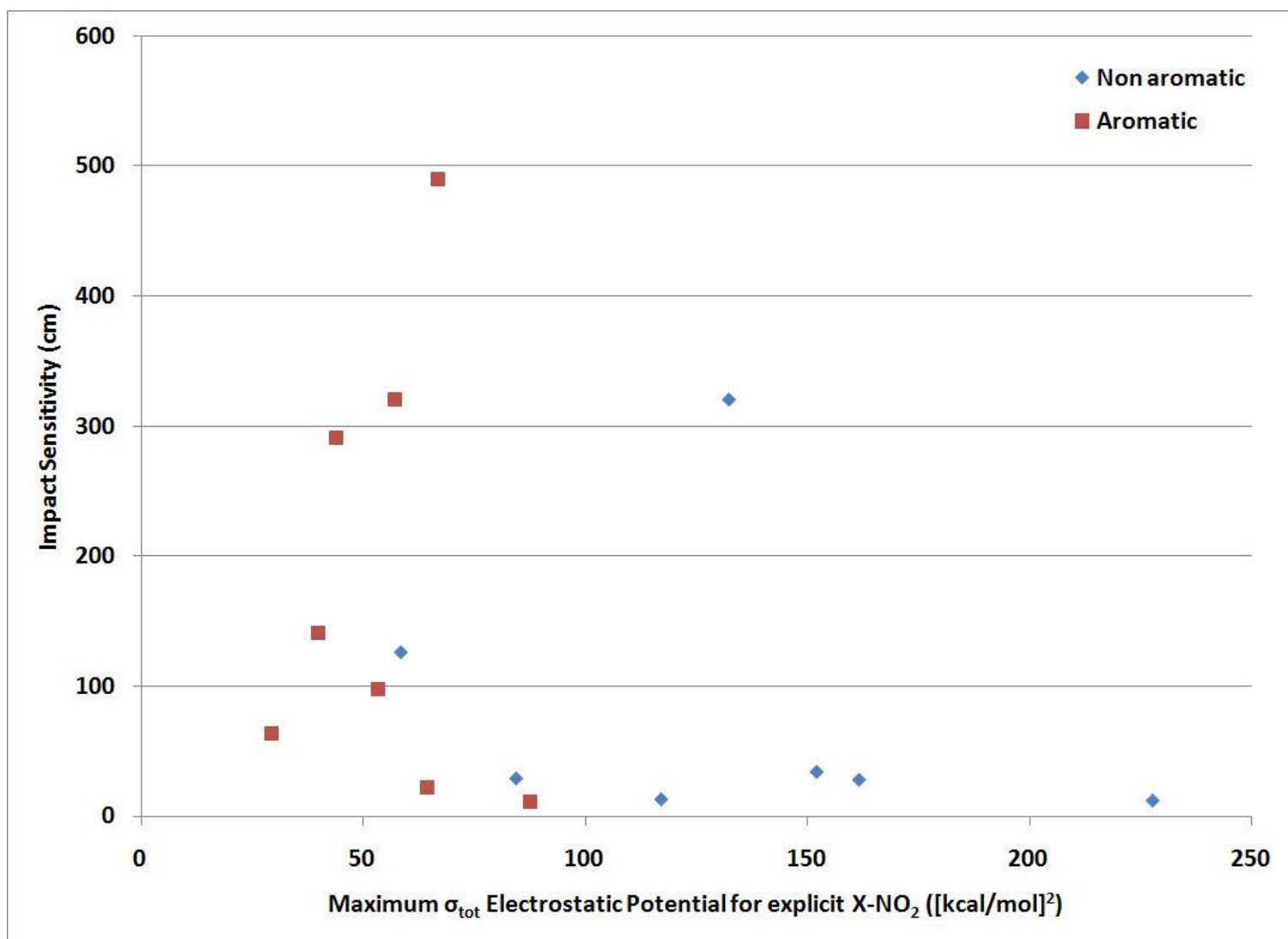


Figure A-131. Impact sensitivity (cm) vs. maximum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for explicit X-N subgroups of the X-NO₂ for nonaromatic and aromatic species for PBE/6-31G**.

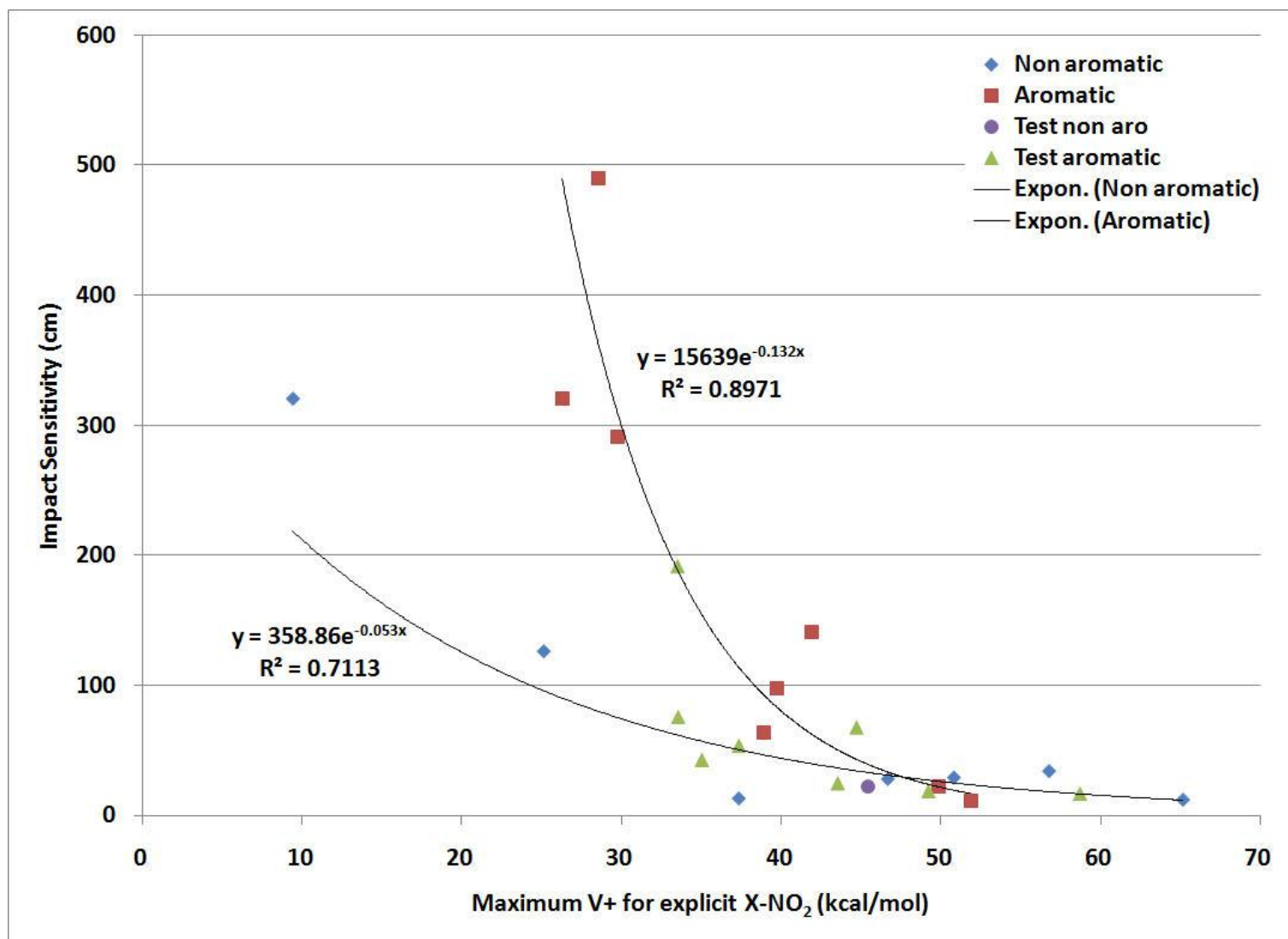


Figure A-132. Impact sensitivity (cm) vs. maximum V+ electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R² factors included.

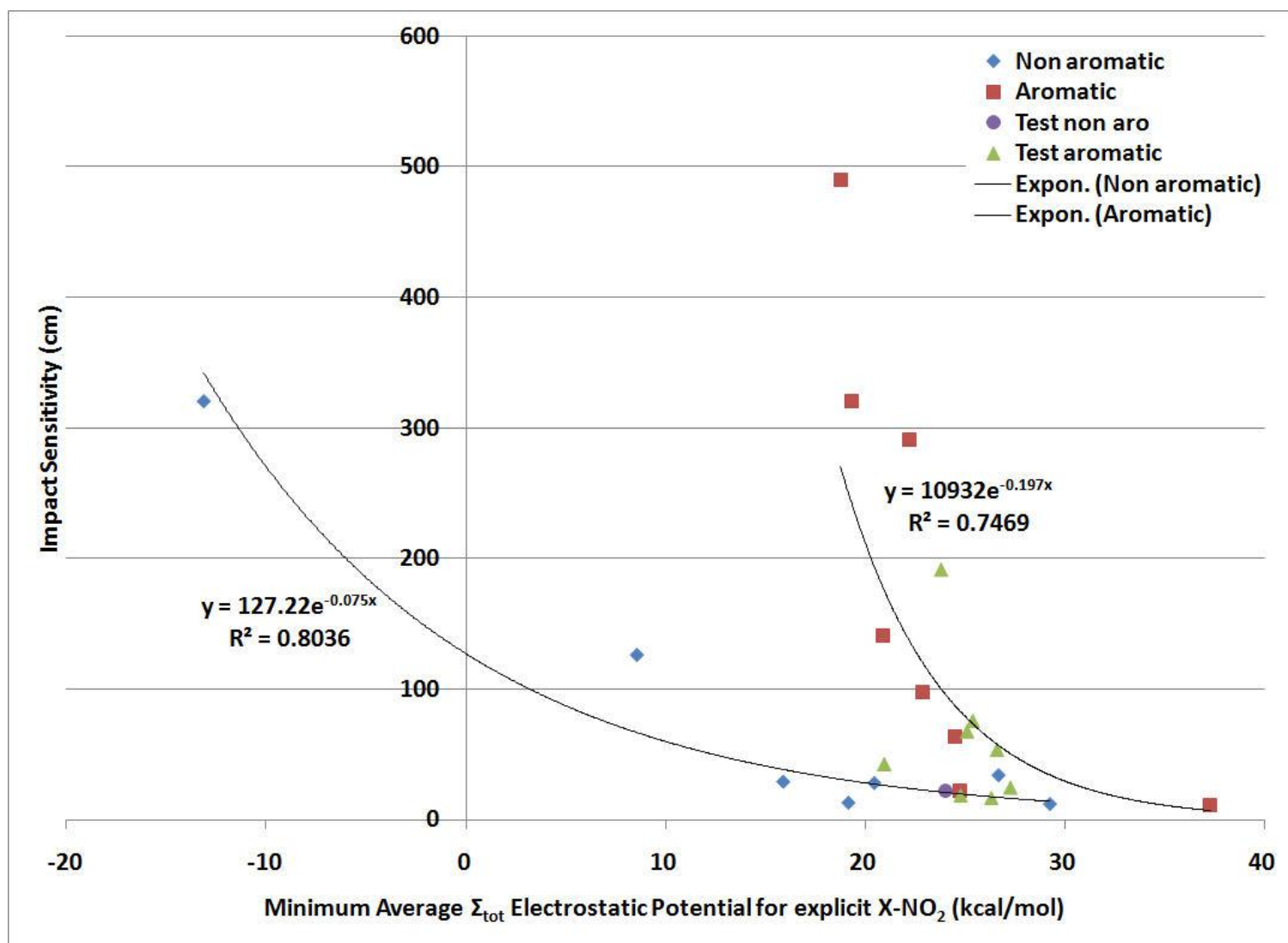


Figure A-133. Impact sensitivity (cm) vs. minimum average Σ_{tot} electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

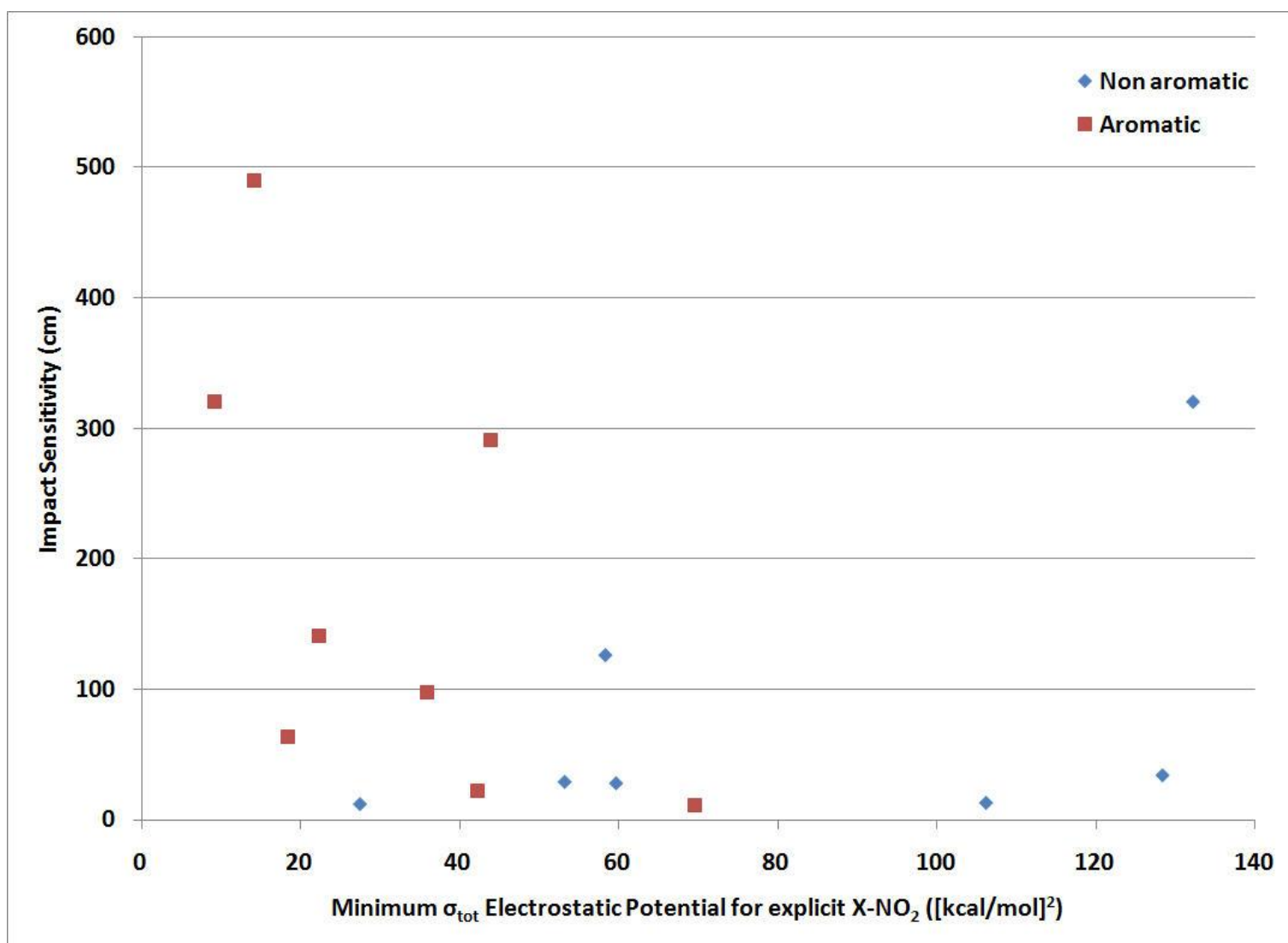


Figure A-134. Impact sensitivity (cm) vs. minimum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for explicit X-N subgroups of the X-NO₂ for nonaromatic and aromatic species for PBE/6-31G**.

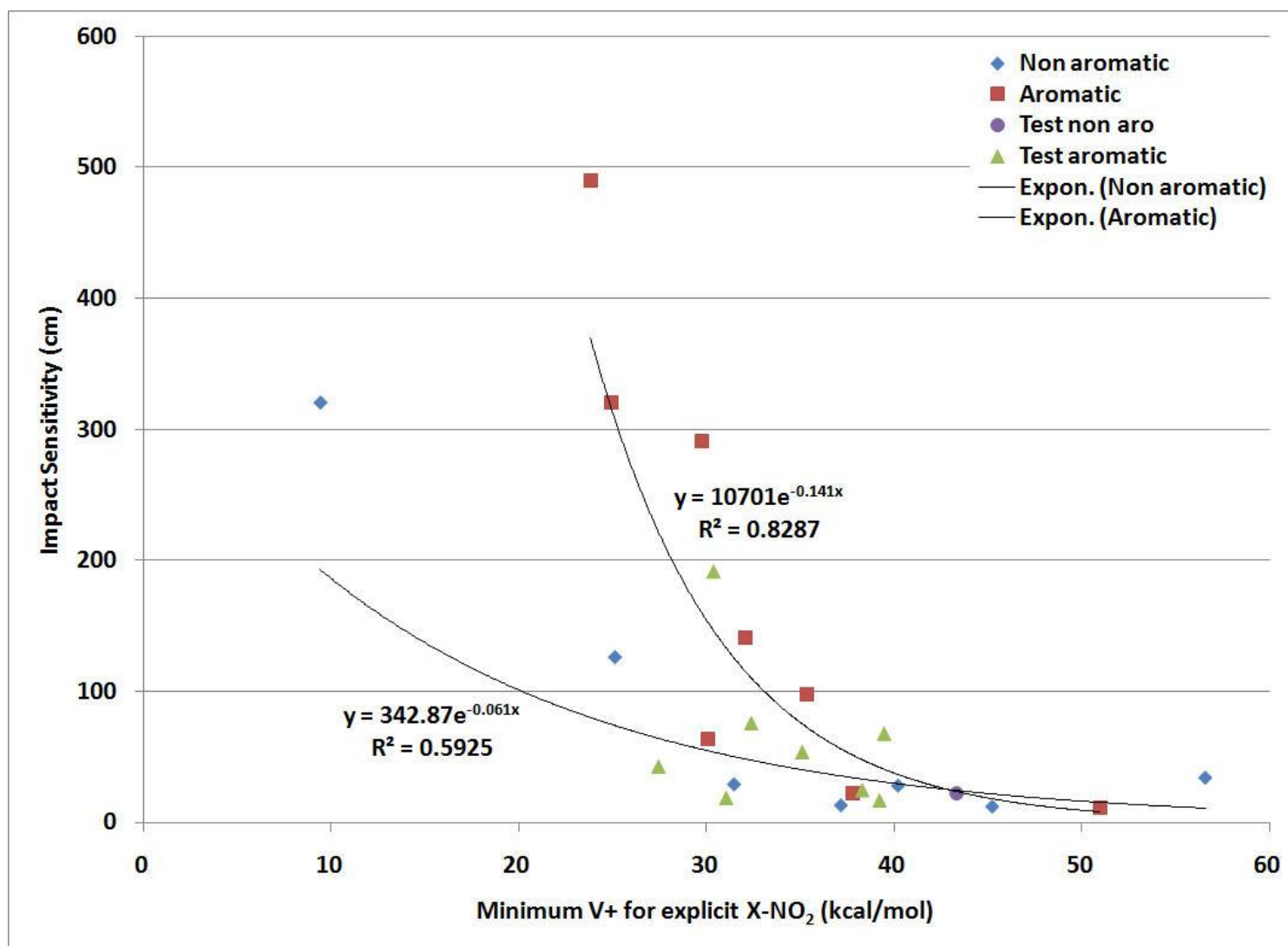


Figure A-135. Impact sensitivity (cm) vs. minimum V+ electrostatic potential (kcal/mol) for explicit X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R² factors included.

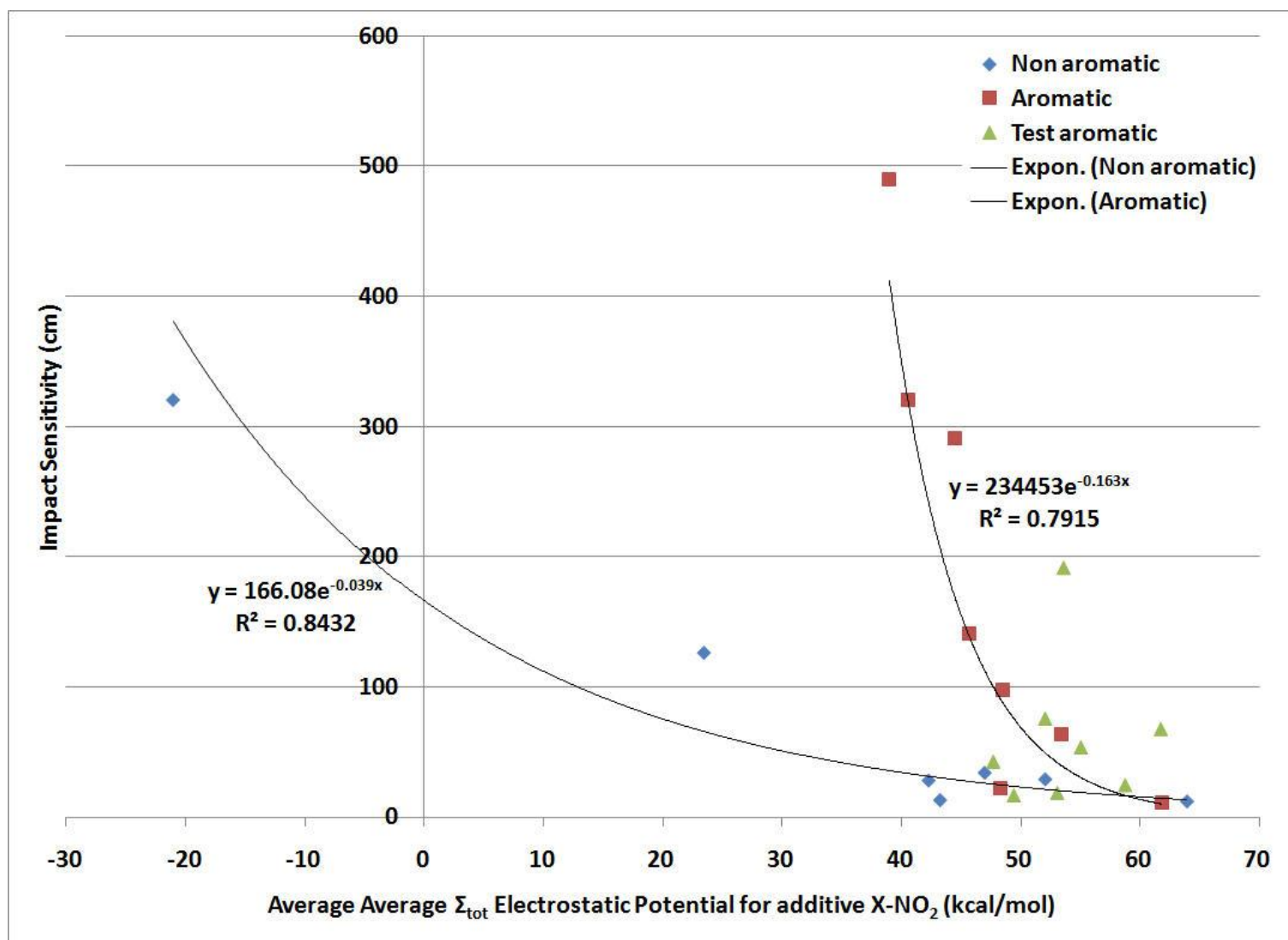


Figure A-136. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fits with associated R^2 factors included.

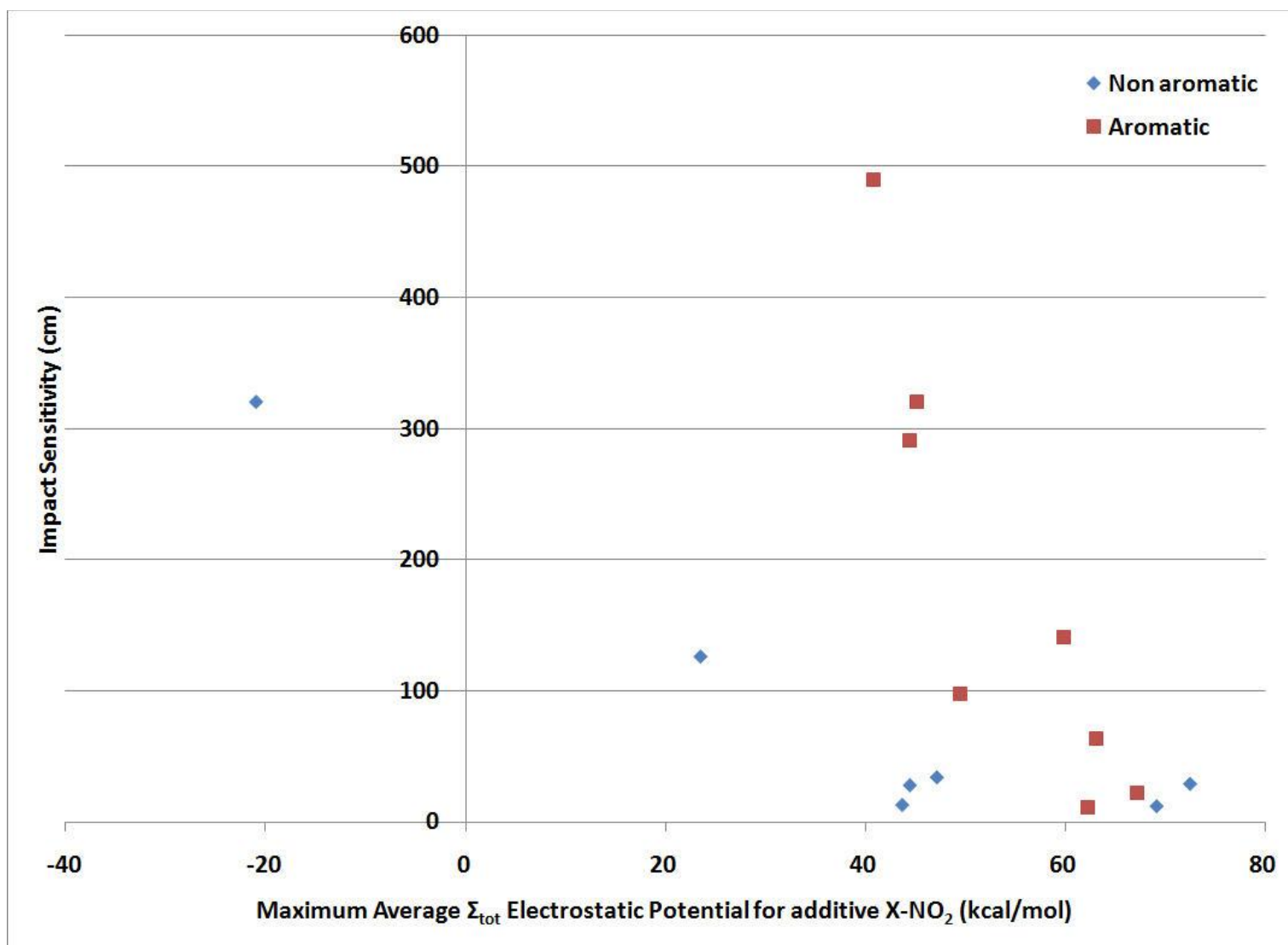


Figure A-137. Impact sensitivity (cm) vs. maximum average Σ_{tot} electrostatic potential (kcal/mol) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for PBE/6-31G**.

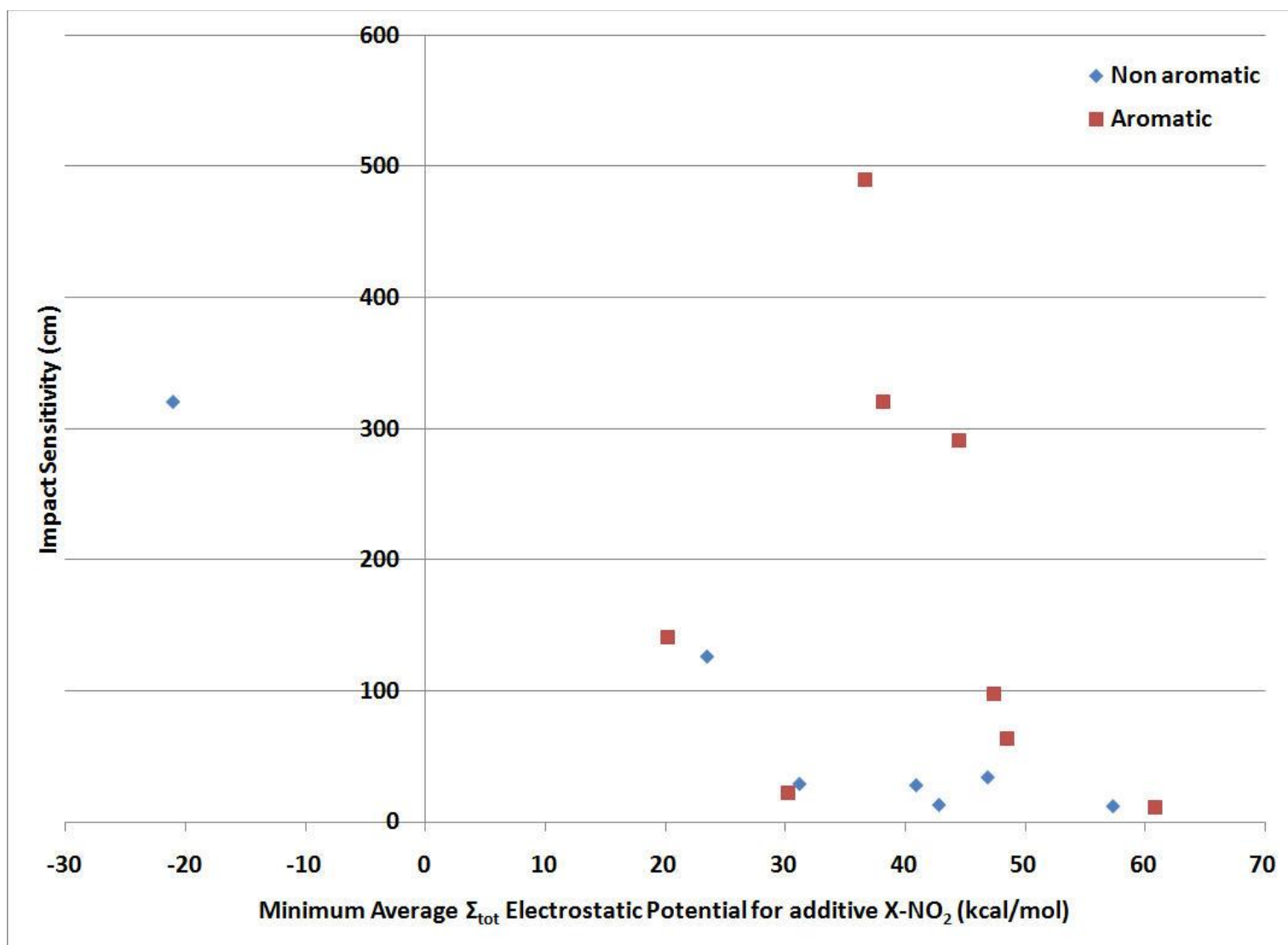


Figure A-138. Impact sensitivity (cm) vs. minimum average Σ_{tot} electrostatic potential (kcal/mol) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for PBE/6-31G**.

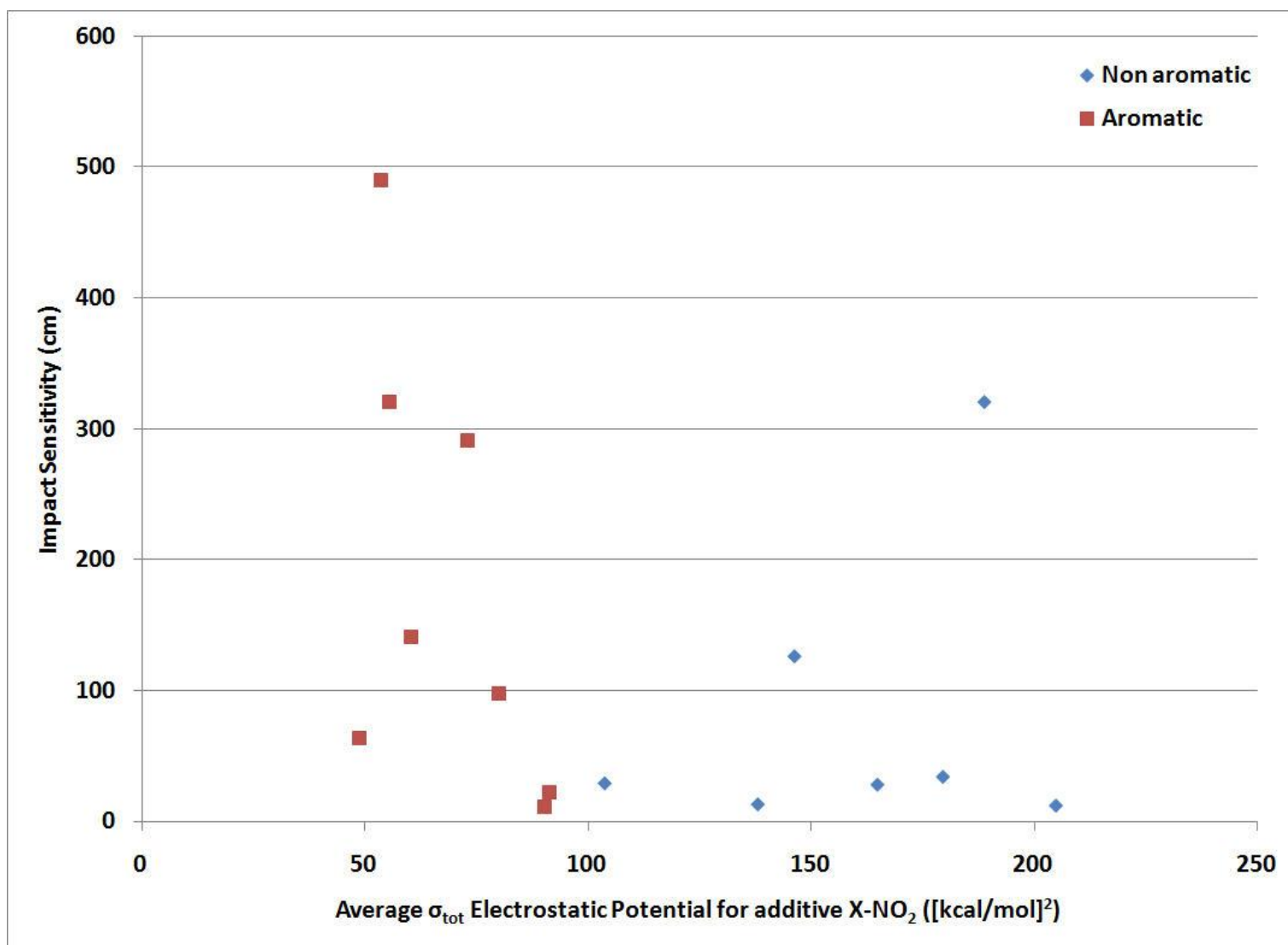


Figure A-139. Impact sensitivity (cm) vs. average σ_{tot}^2 electrostatic potential ([kcal/mol]²) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for PBE/6-31G**.

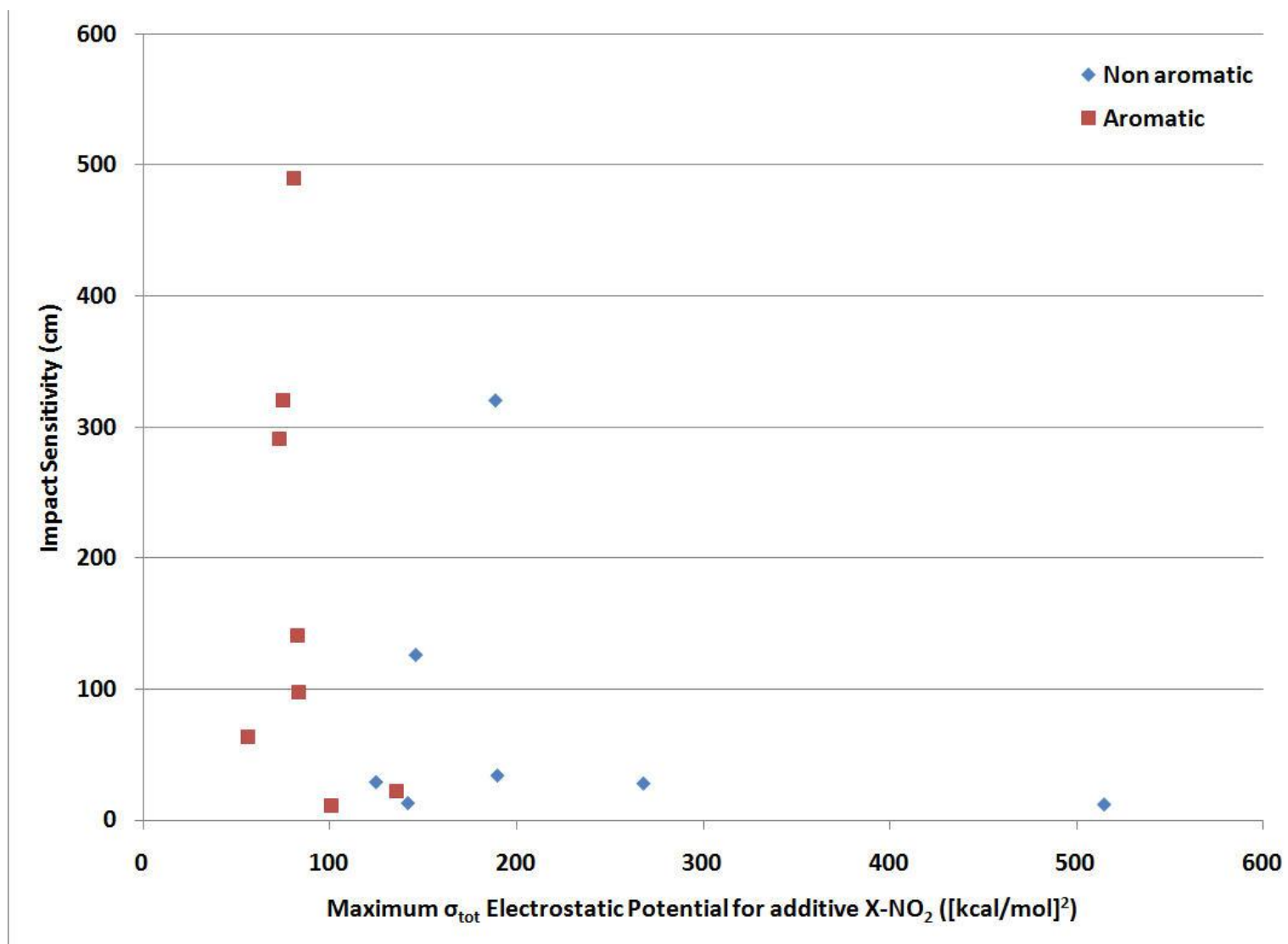


Figure A-140. Impact sensitivity (cm) vs. maximum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for PBE/6-31G**.

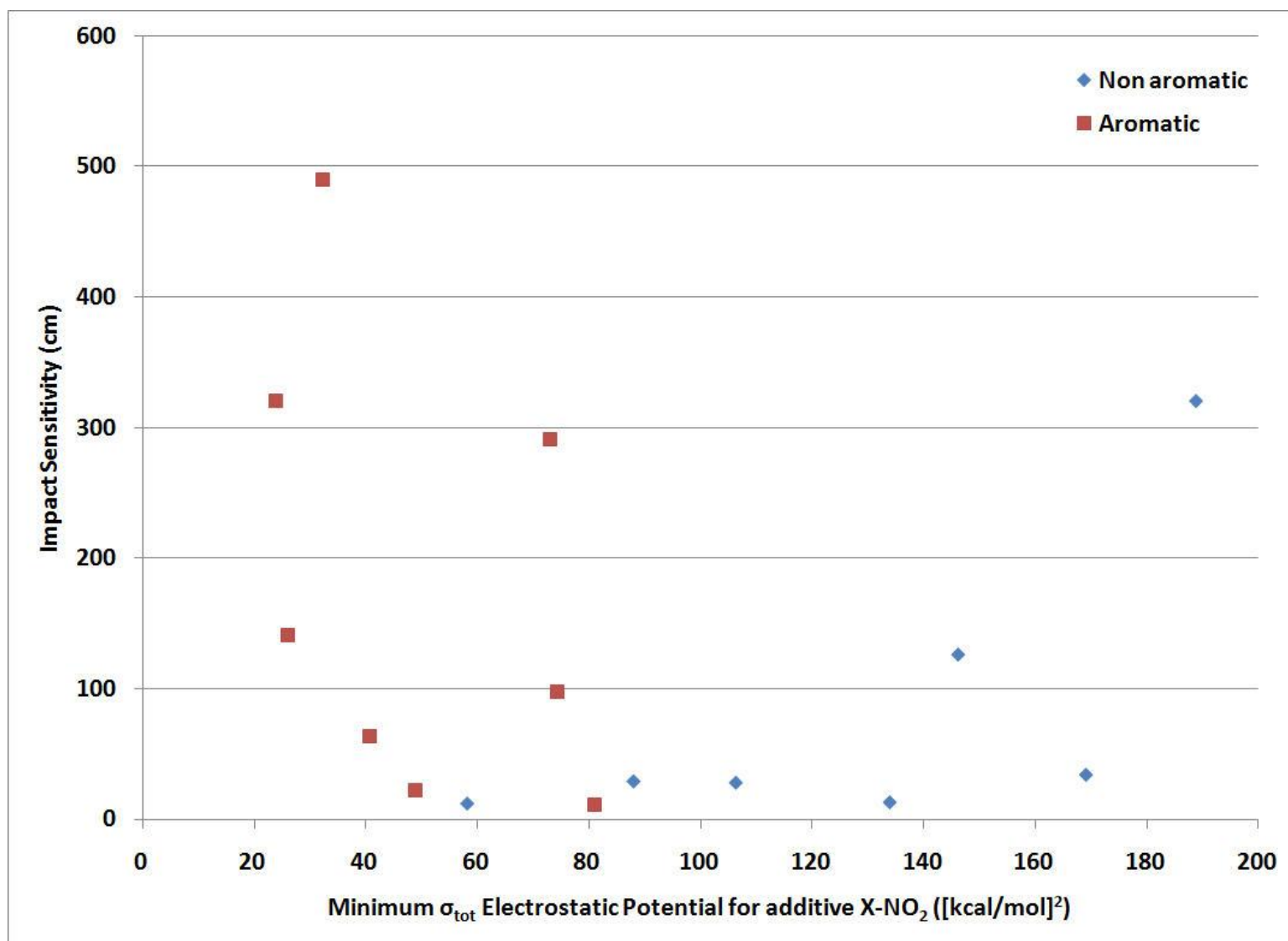


Figure A-141. Impact sensitivity (cm) vs. minimum σ_{tot} electrostatic potential ([kcal/mol]²) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for PBE/6-31G**.

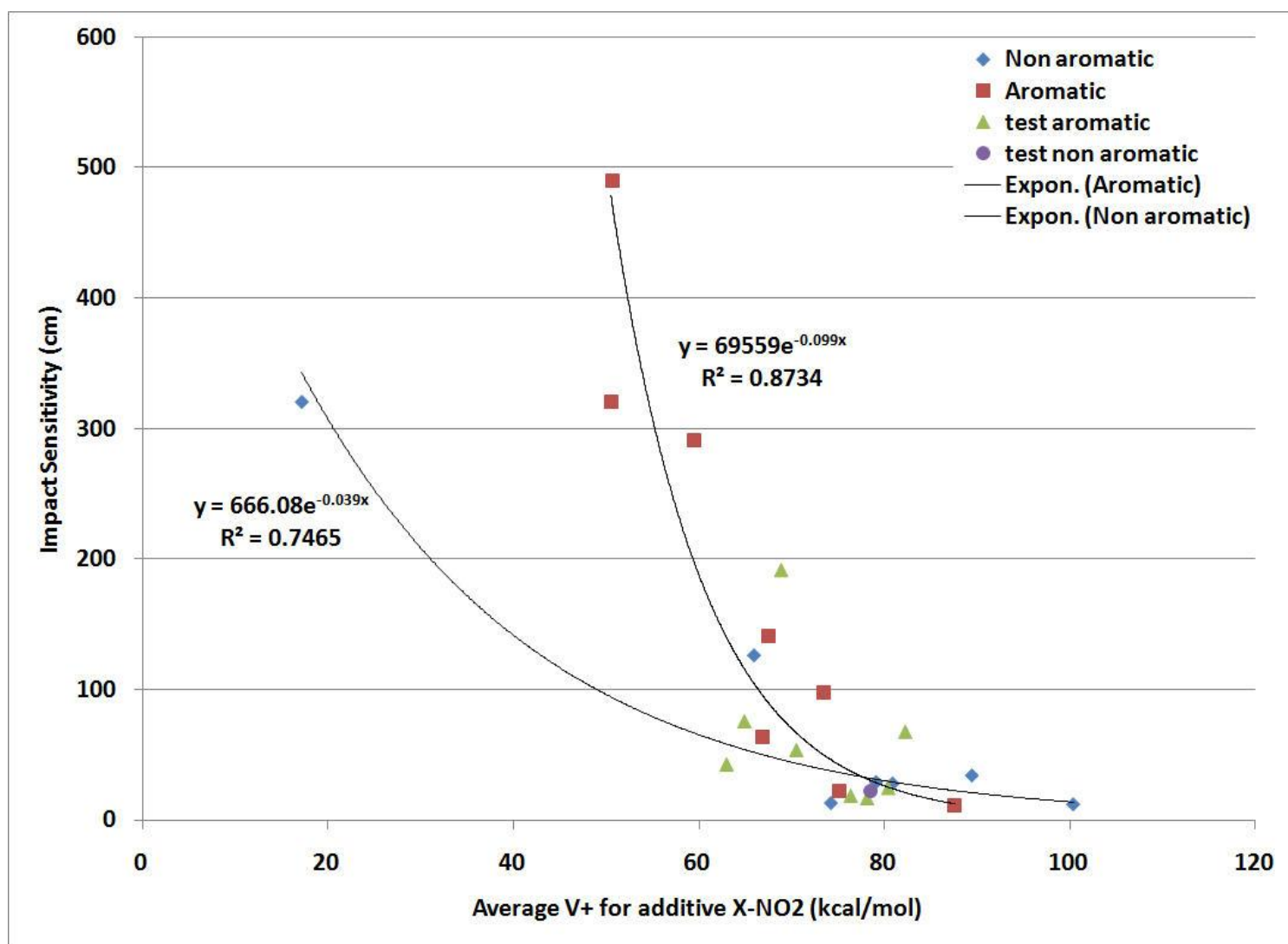


Figure A-142. Impact sensitivity (cm) vs. average V+ electrostatic potential (kcal/mol) for additive X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**. Exponential fit for with associated R² factors included.

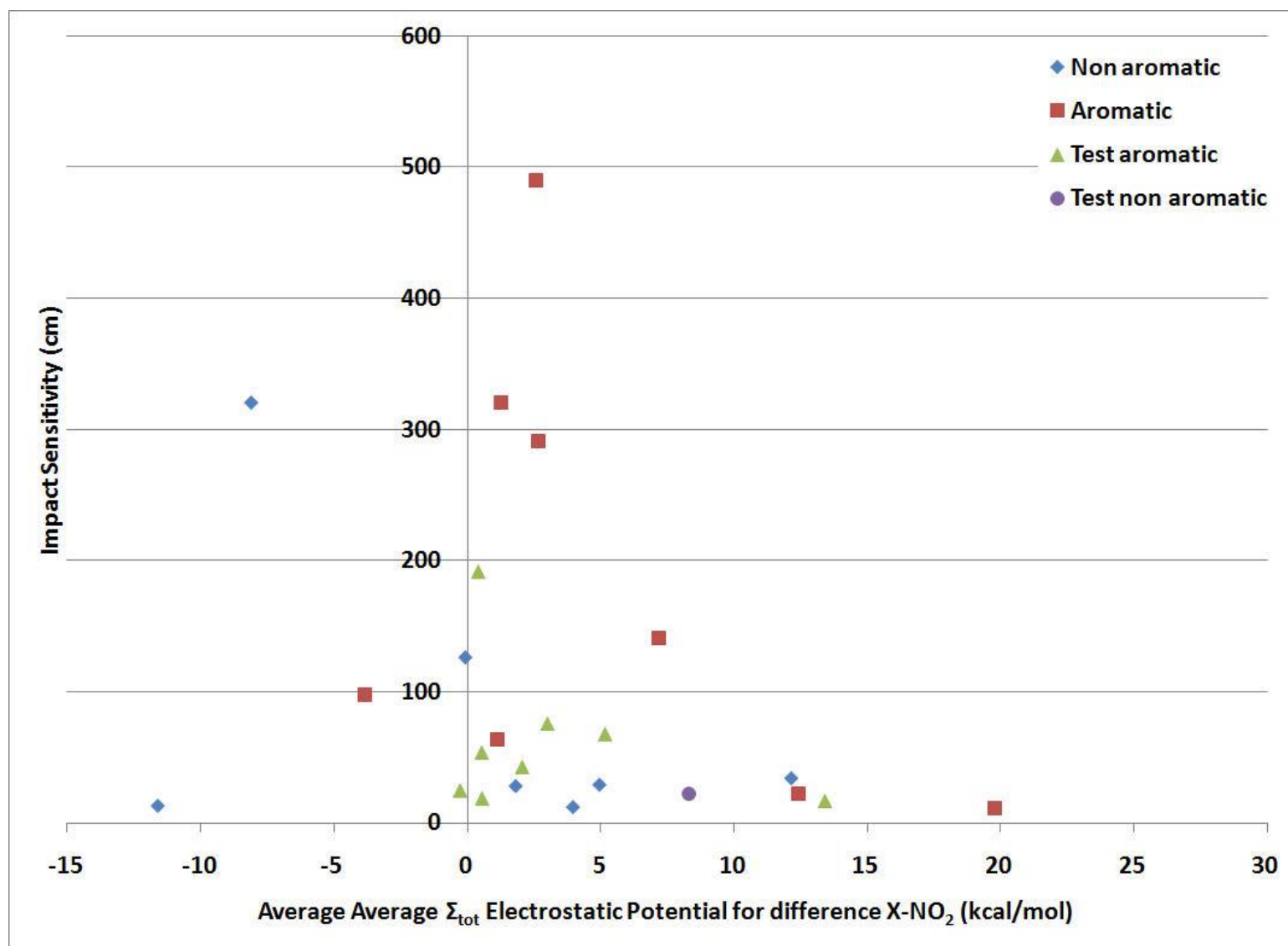


Figure A-143. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for both the training and test sets for PBE/6-31G**.

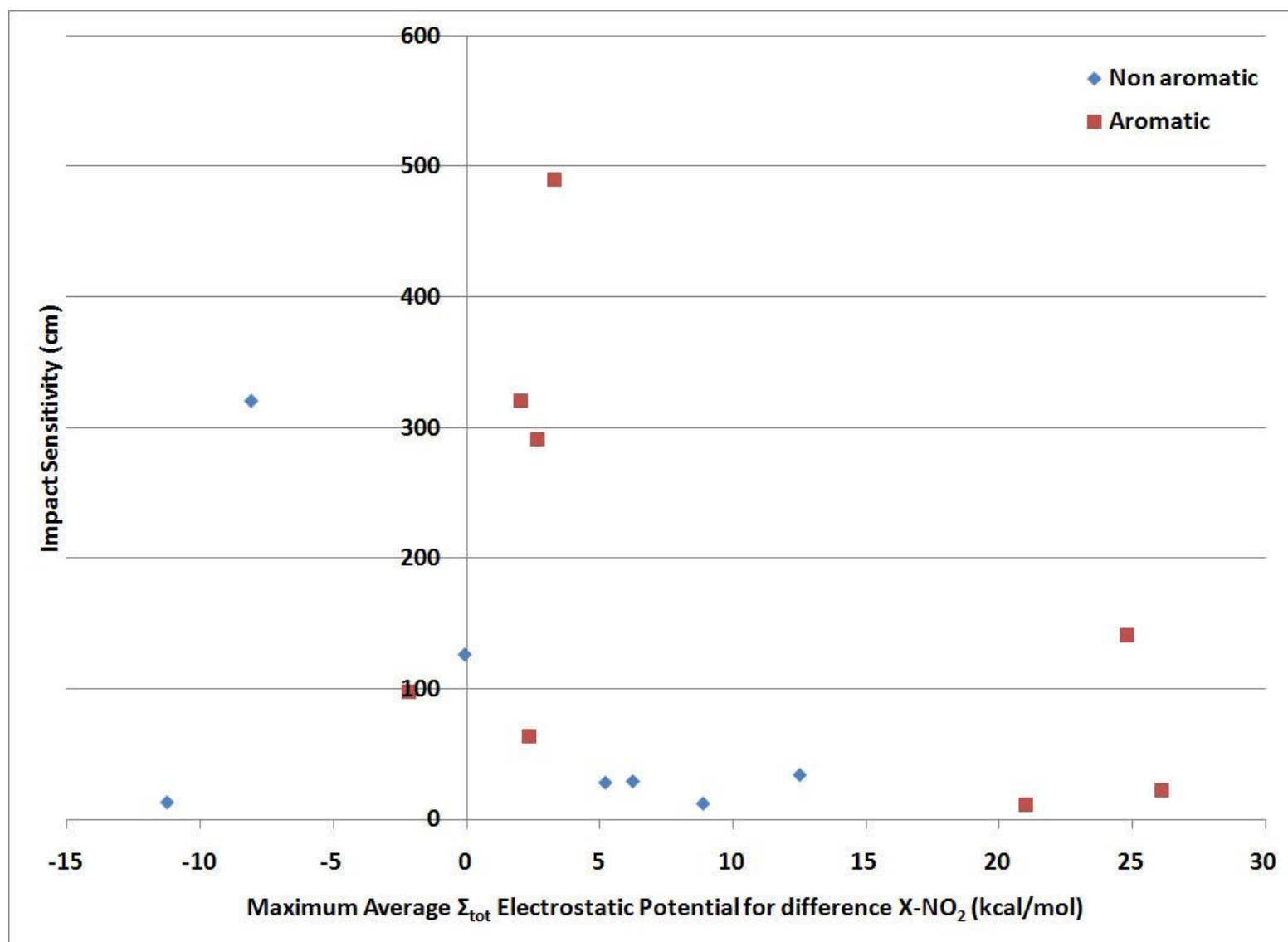


Figure A-144. Impact sensitivity (cm) vs. maximum average Σ_{tot} electrostatic potential (kcal/mol) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

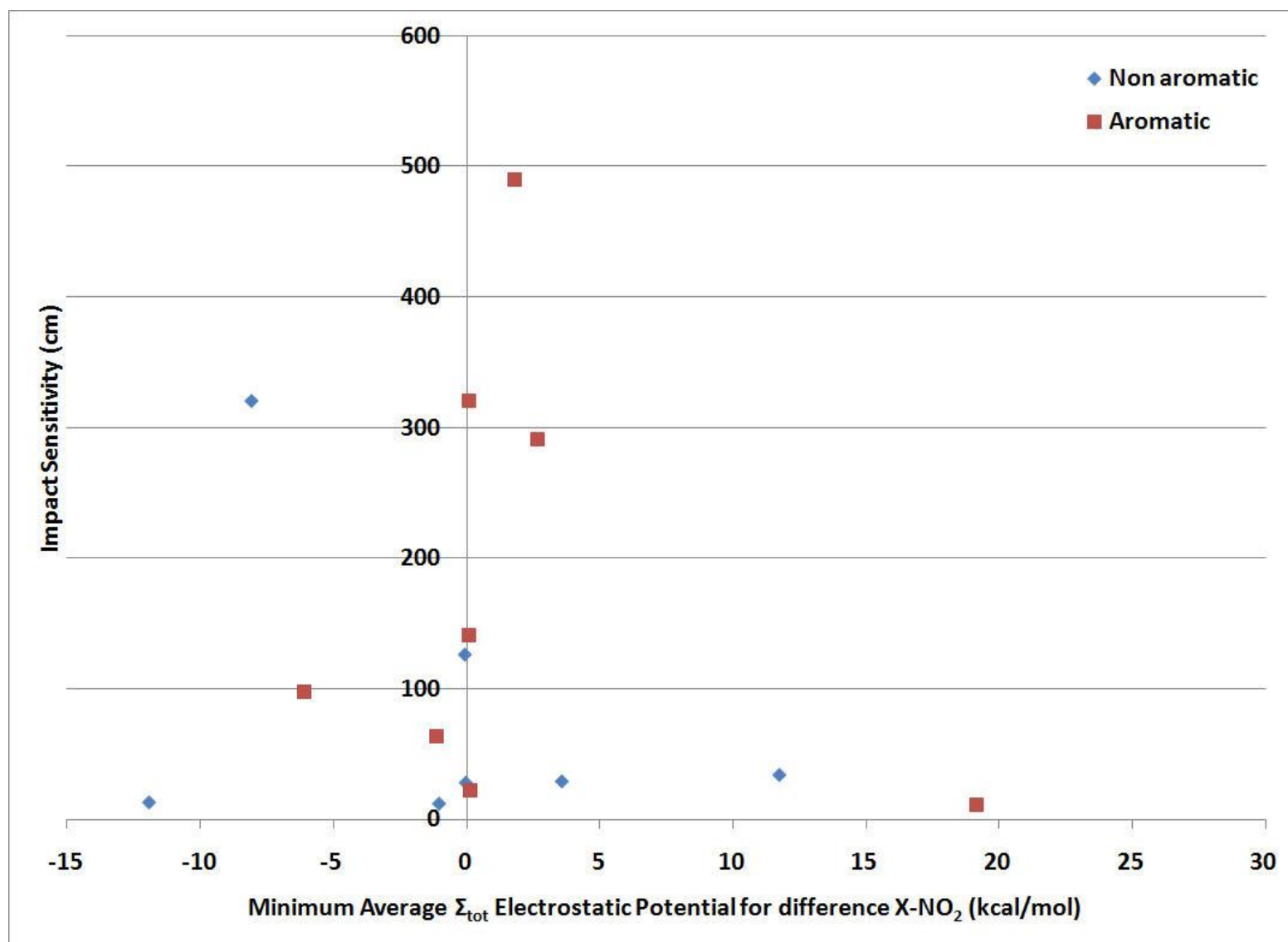


Figure A-145. Impact sensitivity (cm) vs. minimum average Σ_{tot} electrostatic potential (kcal/mol) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

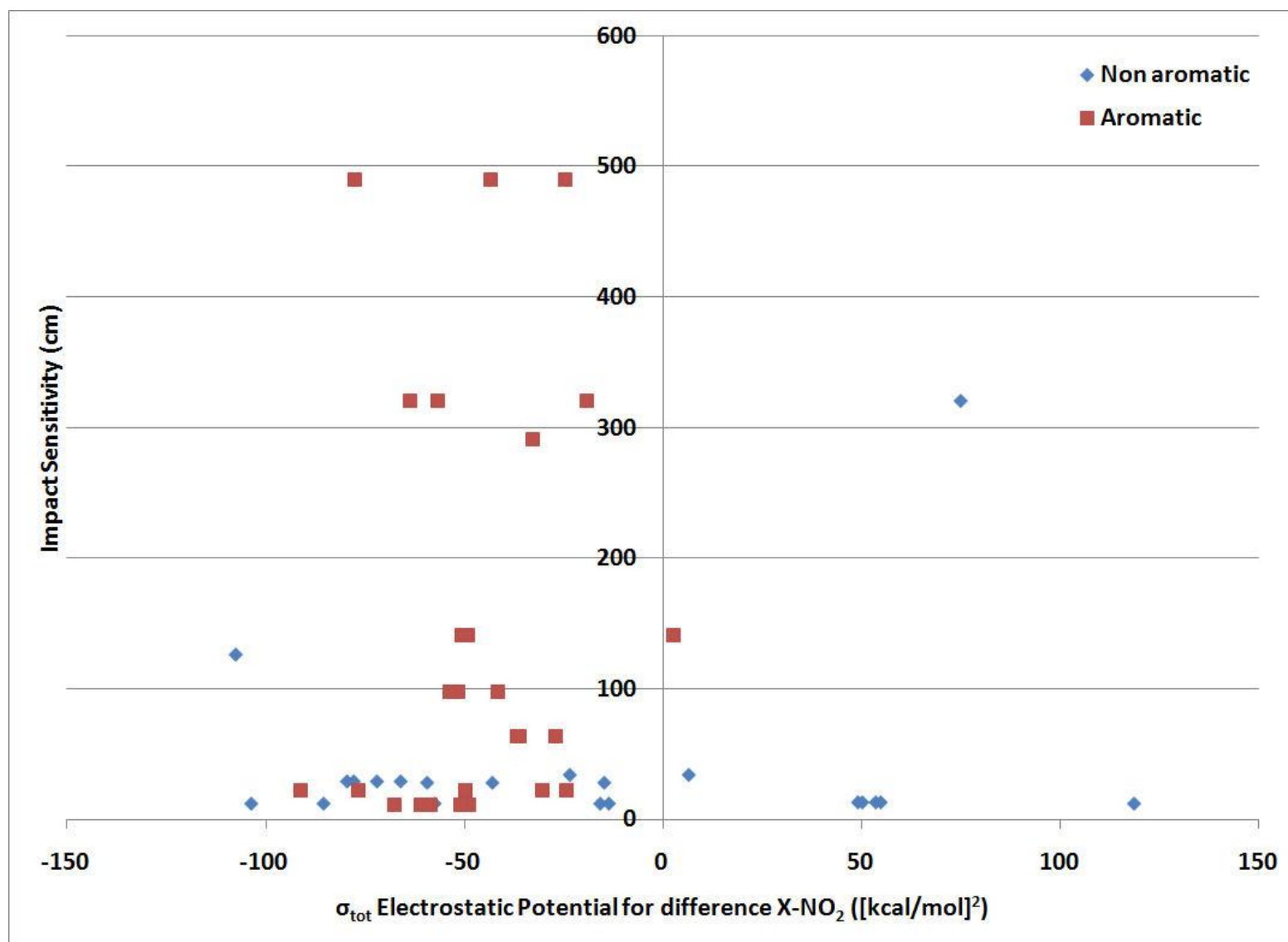


Figure A-146. Impact sensitivity (cm) vs. σ_{tot}^2 electrostatic potential ([kcal/mol]²) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

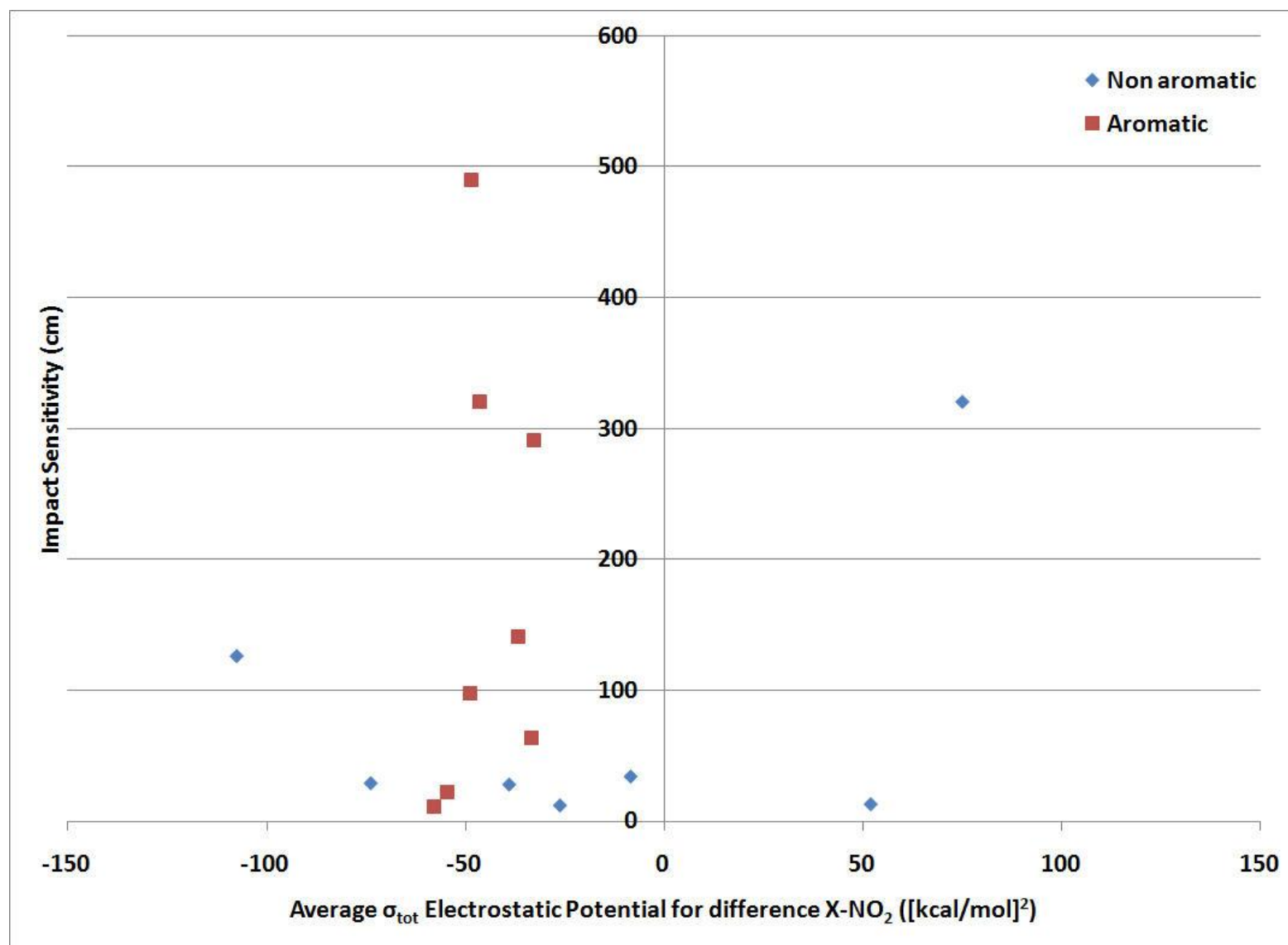


Figure A-147. Impact sensitivity (cm) vs. average σ_{tot}^2 electrostatic potential ([kcal/mol]²) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

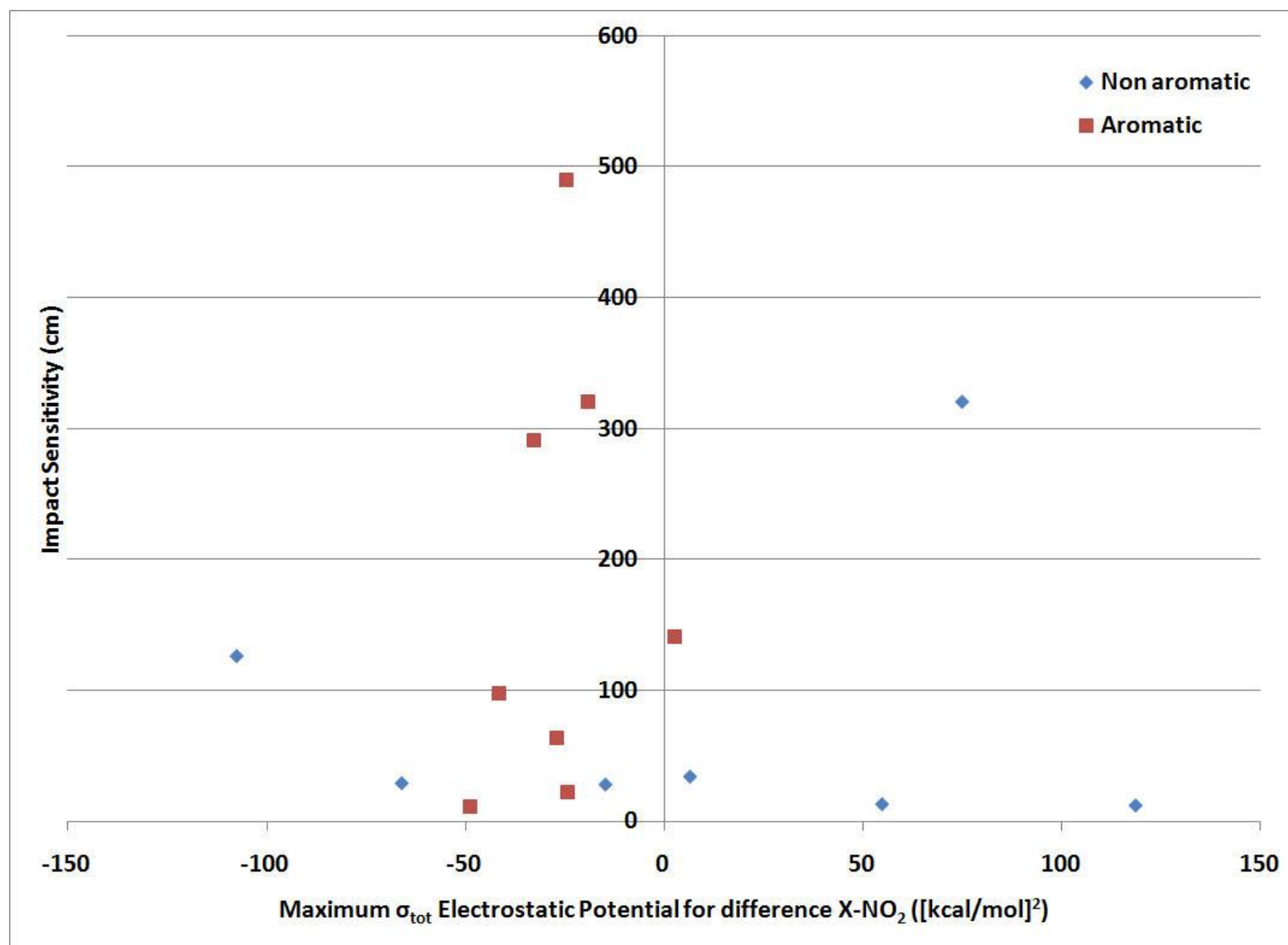


Figure A-148. Impact sensitivity (cm) vs. maximum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

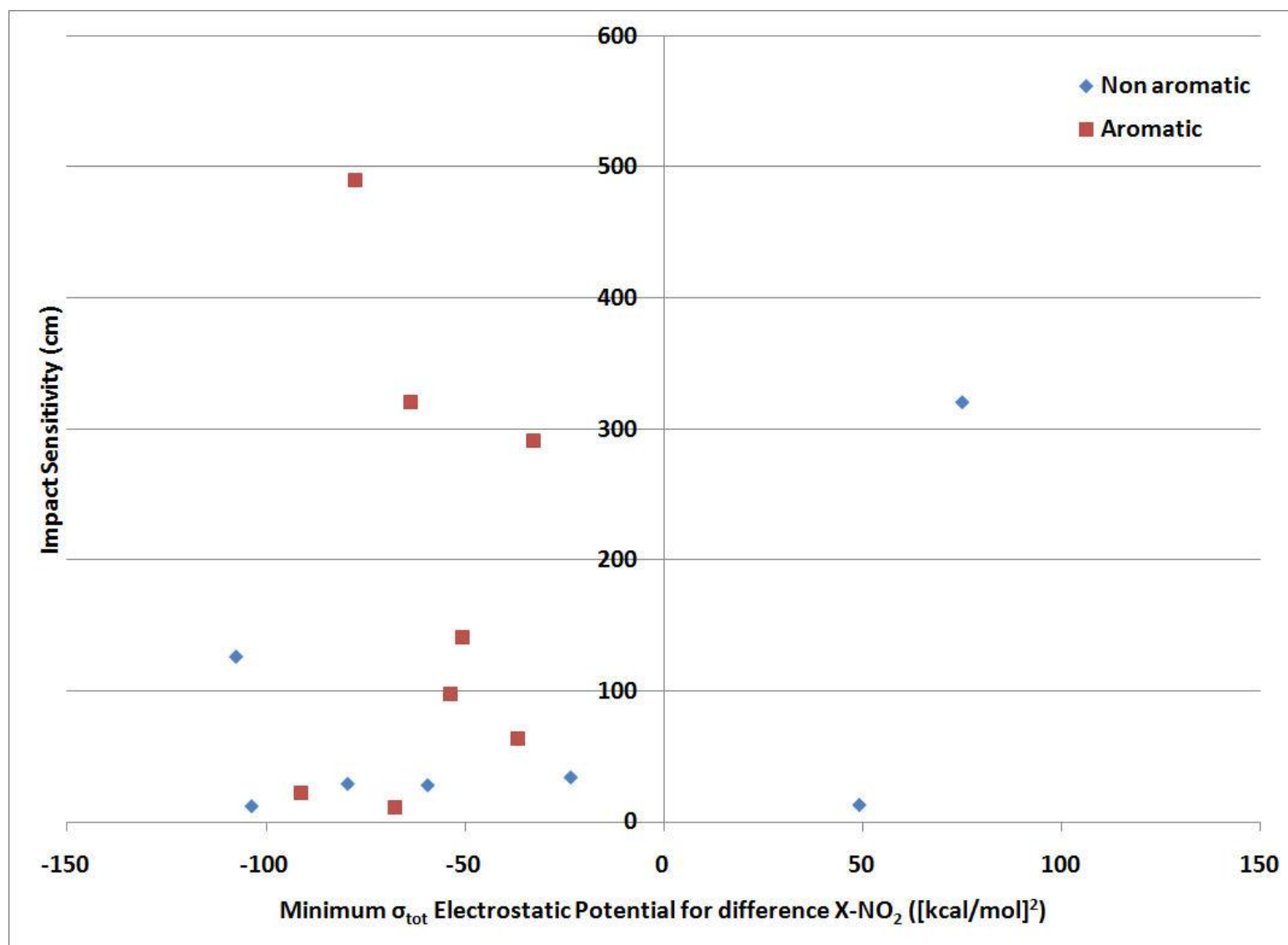


Figure A-149. Impact sensitivity (cm) vs. minimum σ_{tot}^2 electrostatic potential ([kcal/mol]²) for difference X-N subgroups of the X-NO₂ for (1) nonaromatic and (2) aromatic species for the training set for PBE/6-31G**.

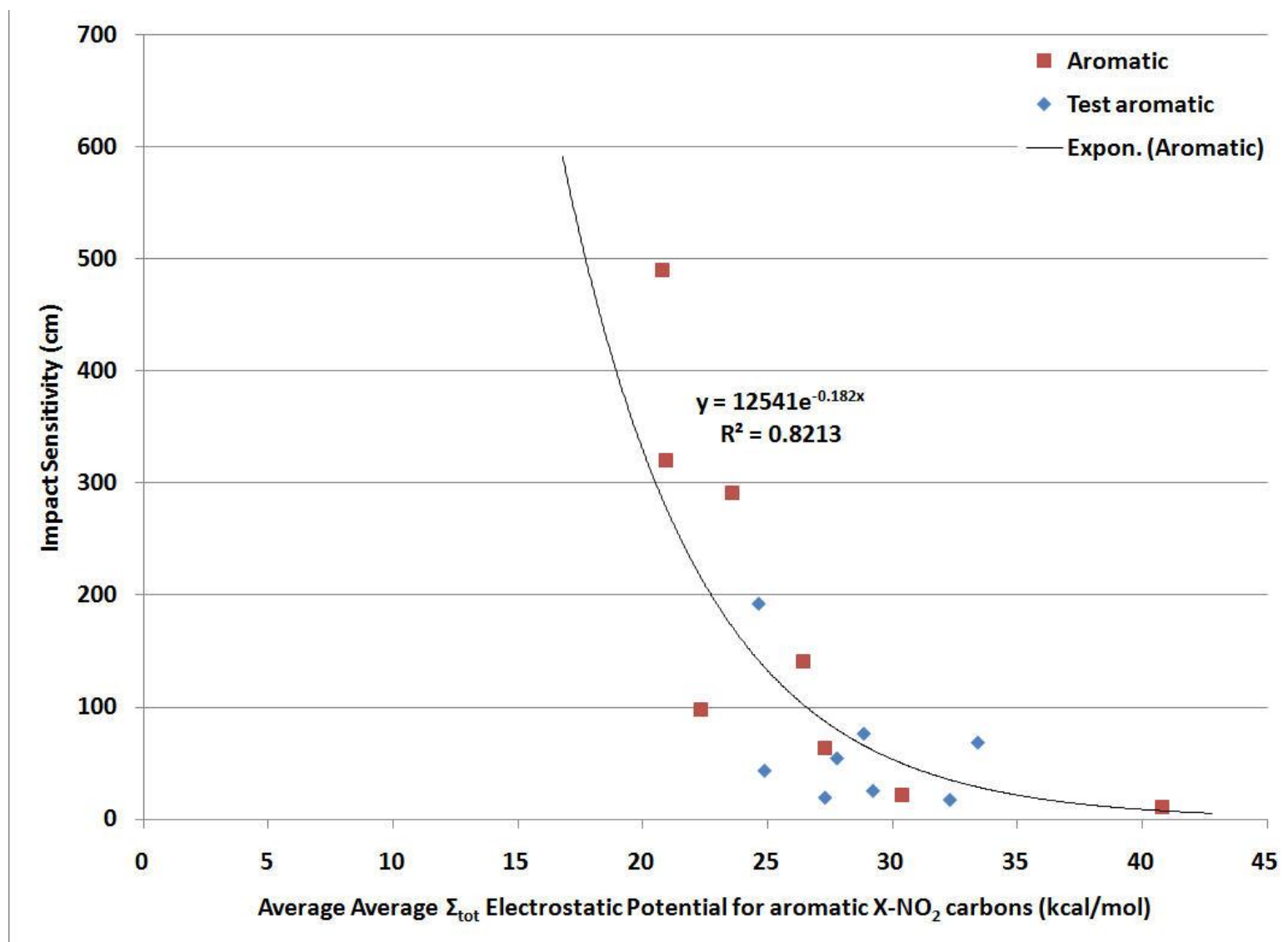


Figure A-150. Impact sensitivity (cm) vs. average average Σ_{tot} electrostatic potential (kcal/mol) for the carbon of the X-NO₂ nitro group for both the training and test sets for PBE/6-31G**. Exponential fit for with associated R^2 factors included.

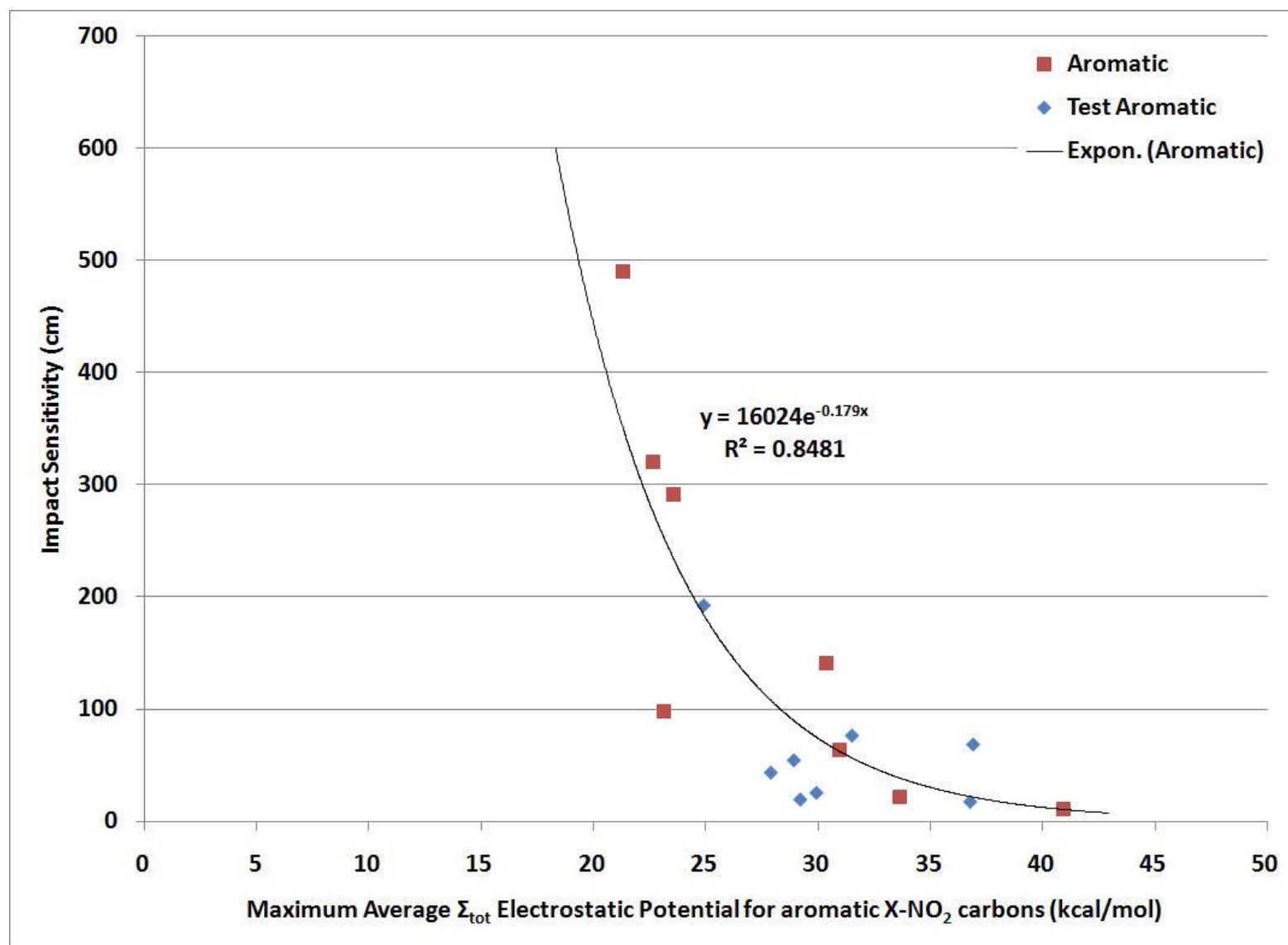


Figure A-151. Impact sensitivity (cm) vs. maximum average Σ_{tot} electrostatic potential (kcal/mol) for the carbon of the X-NO₂ nitro group for both the training and test sets for PBE/6-31G**. Exponential fit for with associated R^2 factors included.

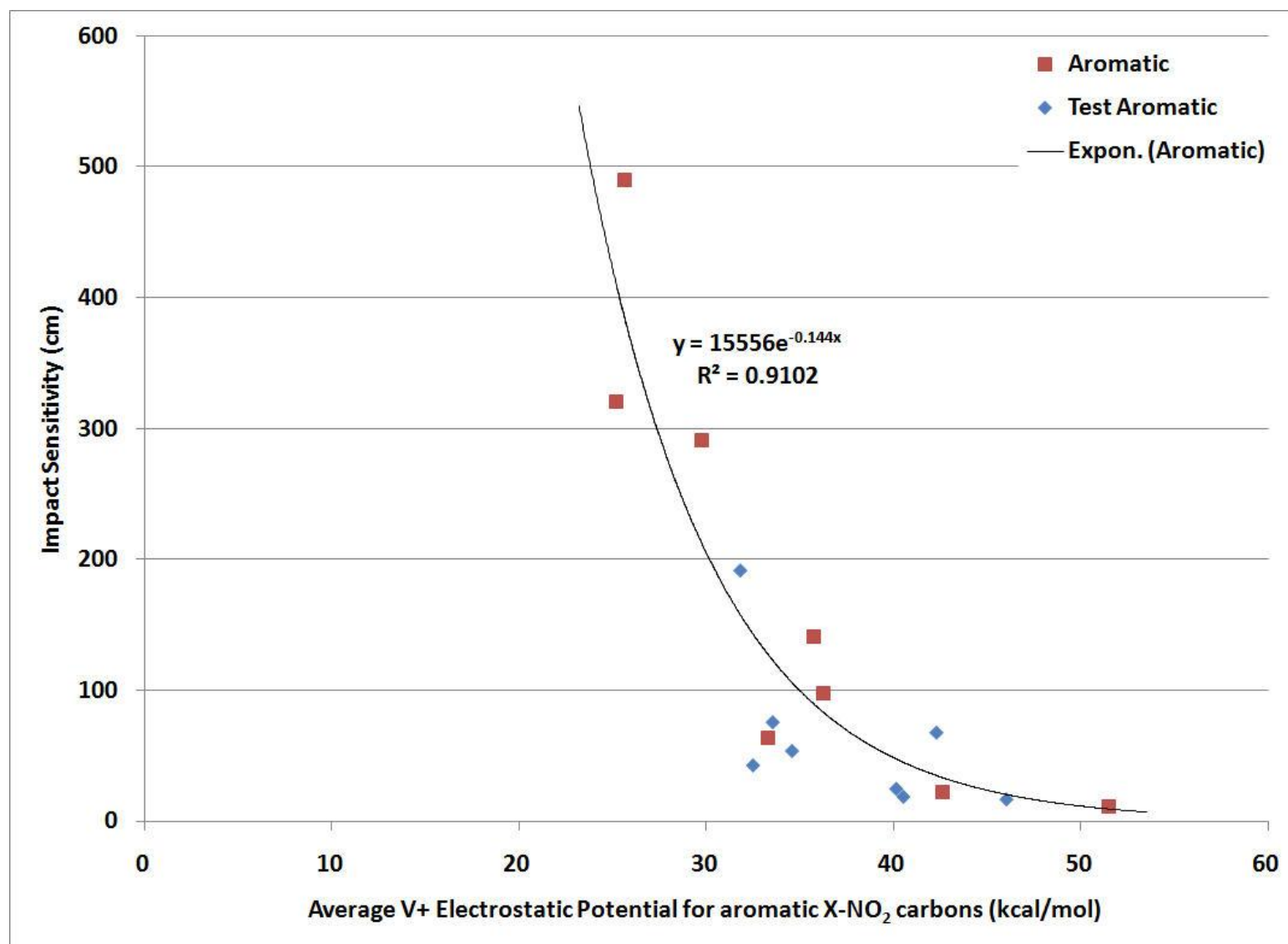


Figure A-152. Impact sensitivity (cm) vs. average V+ electrostatic potential (kcal/mol) for the carbon of the X-NO₂ nitro group for both the training and test sets for PBE/6-31G**. Exponential fit for with associated R² factors included.

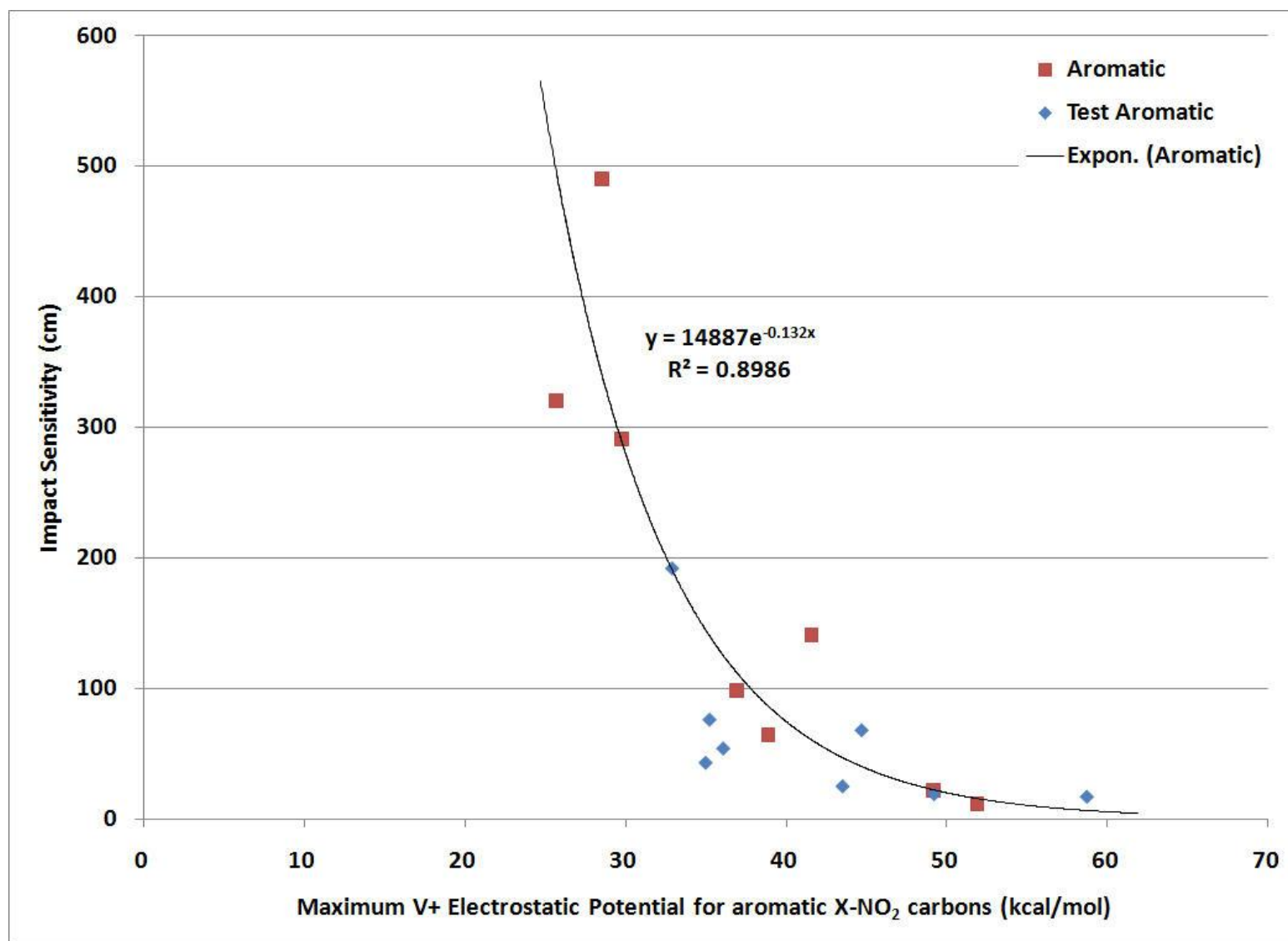


Figure A-153. Impact sensitivity (cm) vs. maximum V+ electrostatic potential (kcal/mol) for the carbon of the X-NO₂ nitro group for both the training and test sets for PBE/6-31G**. Exponential fit for with associated R² factors included.

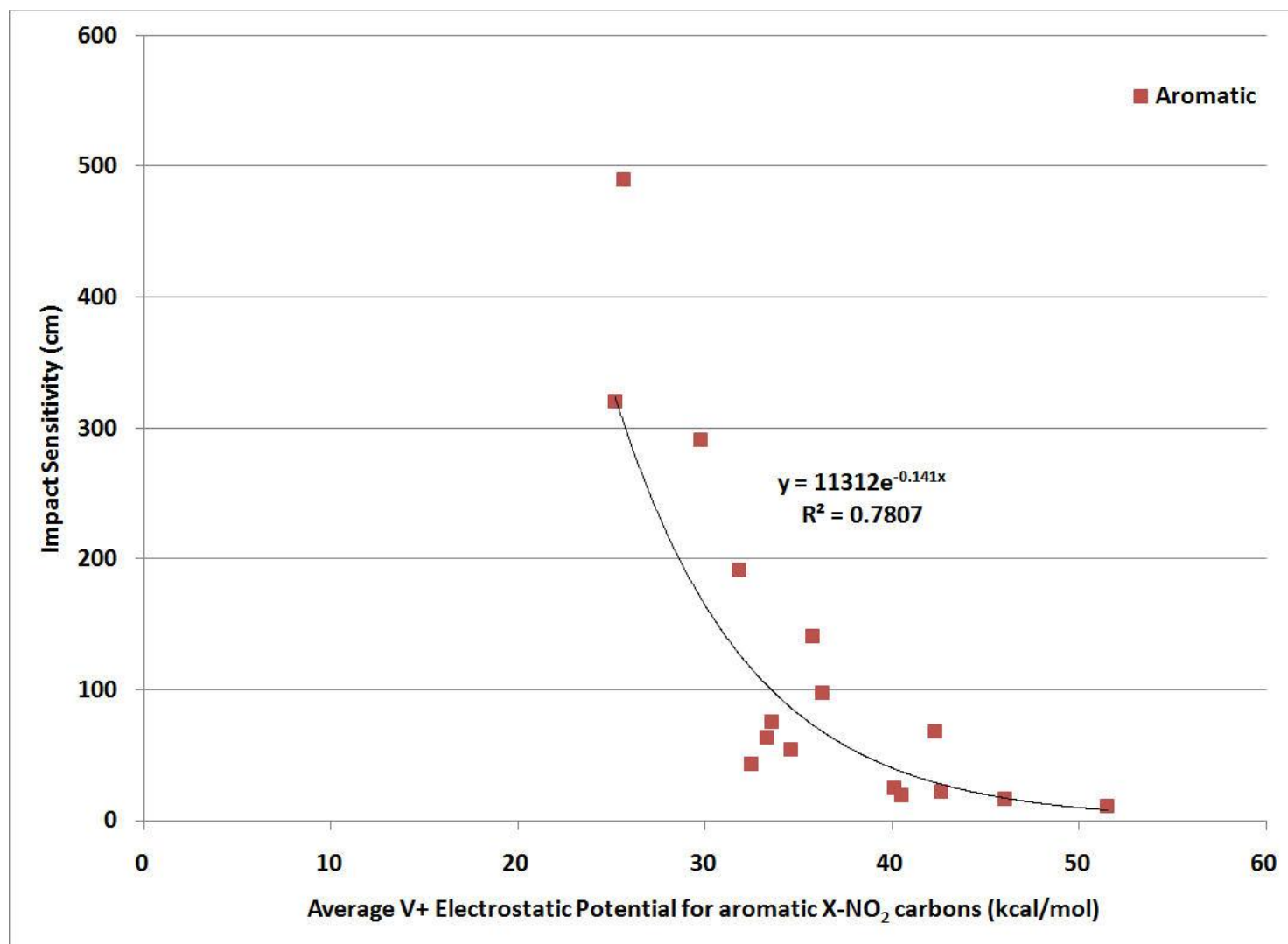


Figure A-154. Impact sensitivity (cm) vs. average V+ electrostatic potential (kcal/mol) for the carbon of the X-NO₂ nitro group for all molecules in the training and test sets for PBE/6-31G** in order to determine if fit improves with more data. Exponential fit for with associated R² factors included.

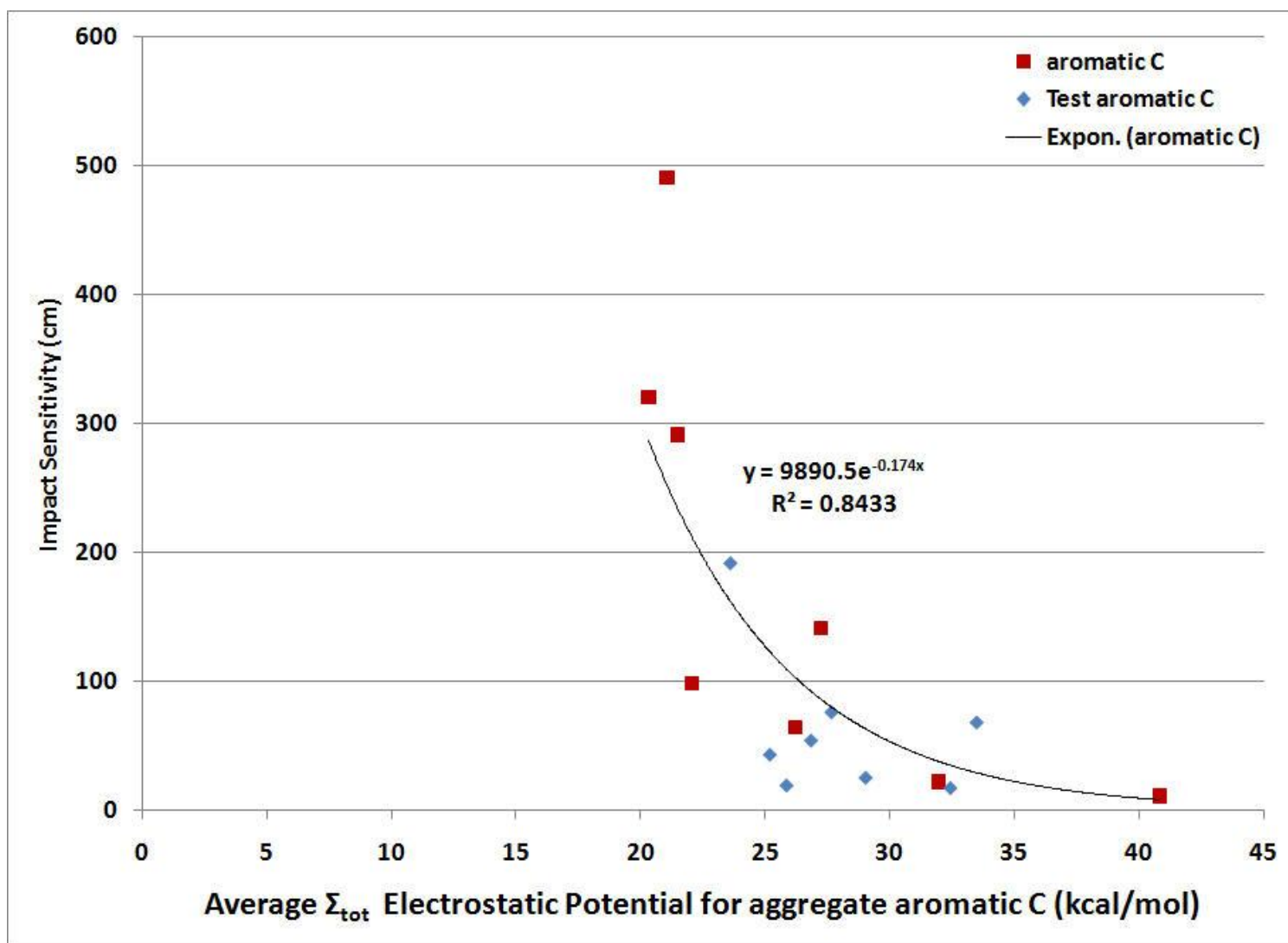


Figure A-155. Impact sensitivity (cm) vs. average Σ_{tot} electrostatic potential (kcal/mol) for the aggregate aromatic carbons for all aromatic molecules in the training and test sets for PBE/6-31G**. Exponential fit for with associated R^2 factors included.

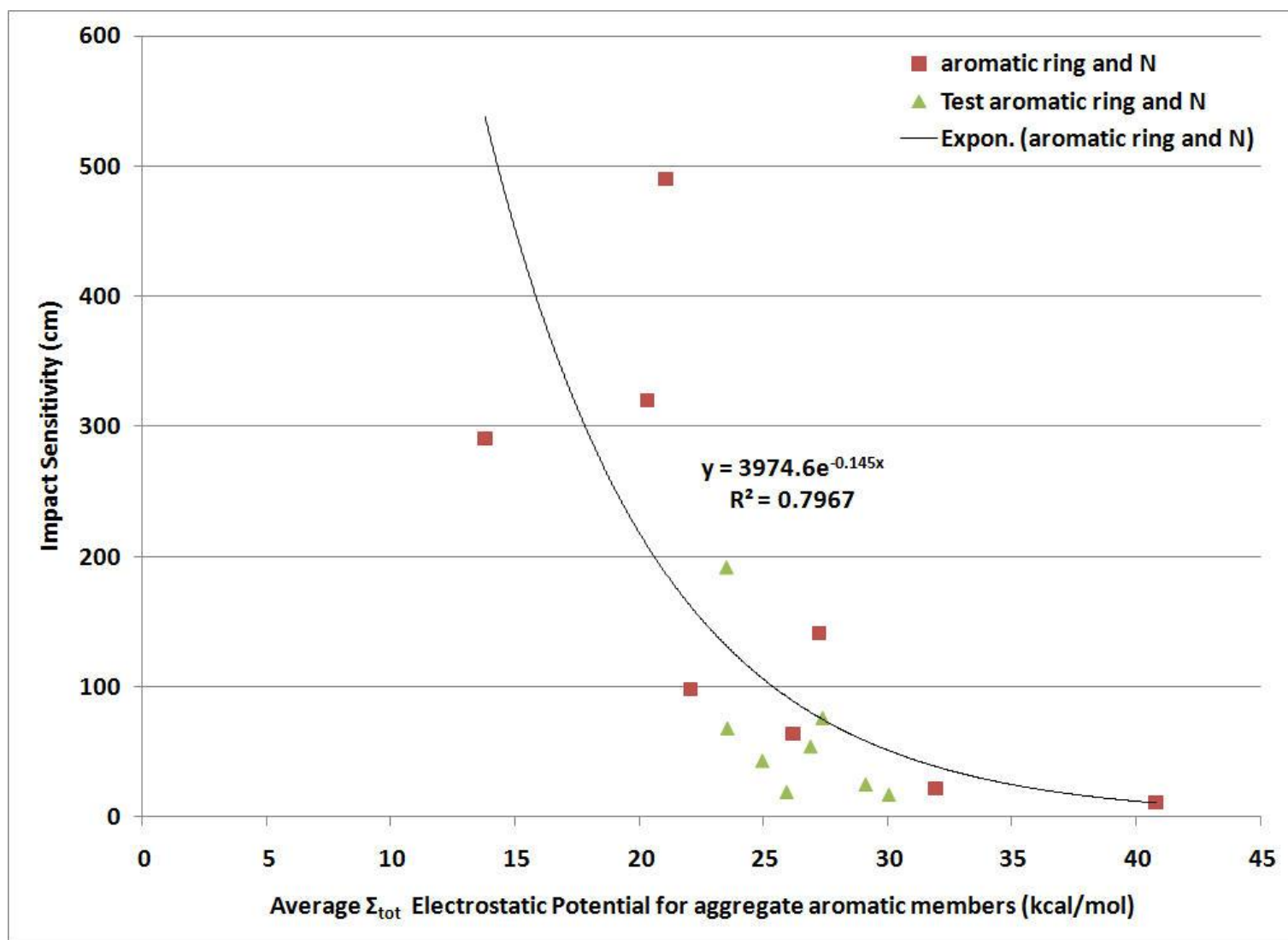


Figure A-156. Impact sensitivity (cm) vs. average Σ_{tot} electrostatic potential (kcal/mol) for the aggregate aromatic members (carbon and nitrogen) for all aromatic molecules in the training and test sets for PBE/6-31G**. Exponential fit for with associated R^2 factors included.

A.4 B3LYP/6-31G* Training Set Data

Table A-1. FOX-7 atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.90143	21.149	0	21.149	27.4784	0	27.4784	0	3.54732
N - amino	2	16.112	30.2913	0	30.2913	157.345	0	157.345	0	10.6374
H - amino	3	5.8596	62.0055	0	62.0055	52.916	0	52.916	0	6.00499
H - amino	4	3.11972	36.0257	0	36.0257	86.4503	0	86.4503	0	7.83227
N - amino	5	16.2672	30.1139	0	30.1139	162.098	0	162.098	0	10.8932
H - amino	6	2.73426	33.0523	0	33.0523	96.6471	0	96.6471	0	8.37684
H - amino	7	6.07142	63.054	0	63.054	60.8881	0	60.8881	0	6.60424
C	8	6.64294	9.54445	-2.17357	9.45375	23.8422	2.50451	26.3468	0.086023	4.16895
N - nitro	9	3.34425	10.2231	-6.50091	5.20057	56.7696	27.5043	84.2739	0.219852	8.37478
O - nitro	10	20.344	3.15658	-29.1745	-28.7604	3.28212	85.0338	88.3159	0.035782	7.61989
O - nitro	11	19.7789	8.71163	-18.6065	-14.5554	42.1693	87.8442	130.013	0.219146	10.7696
N - nitro	12	3.78496	6.12249	-6.46483	1.76796	12.7596	32.6643	45.4239	0.201996	5.81885
O - nitro	13	20.2858	0.263711	-30.8992	-30.8392	0.013305	86.2086	86.2219	0.000154	7.34
O - nitro	14	19.8208	7.23147	-20.2339	-16.0935	21.9808	108.443	130.423	0.140131	11.5692

See figure A-1 for corresponding atom with atom number.

Table A-2. HMX atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.22976	35.7534	0	35.7534	40.0291	0	40.0291	0	5.54337
C	2	1.61168	33.3813	0	33.3813	65.0128	0	65.0128	0	6.52199
H	3	7.26617	38.0613	0	38.0613	36.458	0	36.458	0	5.02326
H	4	6.21413	29.9721	0	29.9721	61.0841	0	61.0841	0	6.4626
H	5	7.20738	27.5014	0	27.5014	34.7576	0	34.7576	0	4.85709
H	6	7.44781	35.8804	0	35.8804	66.4063	0	66.4063	0	6.63529
N - nitro	7	2.40869	15.0506	-5.52357	12.842	44.3042	48.4628	92.767	0.249498	7.44439
N - nitramine	8	3.45288	15.265	0	15.265	32.8998	0	32.8998	0	4.6032
N - nitramine	9	2.54446	37.24	0	37.24	6.61716	0	6.61716	0	1.92888
N - nitro	10	2.59798	32.9821	0	32.9821	74.2161	0	74.2161	0	6.46122
O - nitro	11	19.9858	6.91529	-16.0491	-12.9262	21.7218	47.1516	68.8734	0.215918	8.30095
O - nitro	12	20.7205	8.34618	-13.4938	-8.7052	37.4166	46.6137	84.0303	0.247005	9.14537
O - nitro	13	19.7343	11.3195	-8.97992	-1.76515	82.0577	23.1047	105.162	0.171435	9.38491
O - nitro	14	18.1013	13.6576	-11.9561	-4.31622	99.2316	23.7201	122.952	0.155703	11.043
N - nitramine	15	2.54018	37.3196	0	37.3196	7.10841	0	7.10841	0	2.01408
C	16	1.76288	33.4941	0	33.4941	66.1198	0	66.1198	0	6.44082
C	17	2.25333	35.0039	0	35.0039	42.7814	0	42.7814	0	5.71881
N - nitro	18	2.70531	31.8121	-5.68377	31.2865	85.2821	14.5253	99.8073	0.124353	7.50204
H	19	7.24872	27.2459	0	27.2459	35.4731	0	35.4731	0	4.87993
H	20	7.31616	36.0329	0	36.0329	65.1283	0	65.1283	0	6.59162
N - nitramine	21	3.47811	15.5889	0	15.5889	39.4294	0	39.4294	0	4.8274
H	22	7.2104	37.9891	0	37.9891	35.5469	0	35.5469	0	4.97139
H	23	6.19097	29.8914	0	29.8914	65.3624	0	65.3624	0	6.60258
O - nitro	24	19.602	11.2991	-8.97143	-1.82131	79.2811	23.48	102.761	0.176283	9.34771
O - nitro	25	18.0006	13.6999	-12.0398	-4.27673	96.0428	23.4085	119.451	0.157564	11.1465
N - nitro	26	2.3948	15.0618	-6.18558	12.4059	45.8179	45.5397	91.3576	0.249998	7.95802
O - nitro	27	20.045	6.82956	-15.9681	-12.9161	20.6334	46.9984	67.6318	0.212008	8.22917
O - nitro	28	20.6815	8.58802	-13.4341	-8.66171	39.6026	46.7952	86.3978	0.248267	9.15839

See figure A-2 for corresponding atom with atom number.

Table A-3. PETN atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.973351	29.8667	0	29.8667	48.3969	0	48.3969	0	5.93742
O - nitro	3	20.9062	10.4966	-6.35265	1.31816	66.0157	12.9069	78.9225	0.136794	8.42094
O - nitro	4	23.8737	8.12477	-9.36753	-5.39655	35.6803	15.1453	50.8256	0.20919	6.84913
O - nitrate	5	9.24505	15.1418	-0.80183	14.6571	97.3969	0.355827	97.7527	0.003627	8.43241
N - nitro	6	3.64419	27.2432	-4.48858	27.0081	37.9155	3.04758	40.9631	0.068863	5.11867
H	7	6.21711	28.6883	0	28.6883	27.8608	0	27.8608	0	4.12841
H	8	7.48494	28.5192	0	28.5192	21.5182	0	21.5182	0	3.66184
C	9	1.01708	28.6956	0	28.6956	53.6123	0	53.6123	0	6.37284
C	10	0.951943	28.7515	0	28.7515	55.8315	0	55.8315	0	6.53442
C	11	0.860056	28.1761	0	28.1761	51.9395	0	51.9395	0	6.30756
O - nitro	12	20.8826	10.6986	-6.31804	1.36141	68.1298	12.9964	81.1262	0.134536	8.4876
O - nitro	13	20.939	10.6044	-6.32125	1.37884	68.8352	12.7517	81.5869	0.131867	8.46052
O - nitro	14	20.8942	10.577	-6.30697	1.31333	66.4976	12.9174	79.415	0.1362	8.41972
O - nitro	15	23.833	8.30502	-9.36006	-5.40836	35.6875	15.3467	51.0342	0.210285	6.87105
O - nitro	16	23.8487	8.06375	-9.34364	-5.42671	34.9262	15.1676	50.0938	0.211106	6.80814
O - nitro	17	23.8017	8.196	-9.33694	-5.41977	34.6308	15.1012	49.7319	0.211447	6.81503
O - nitrate	18	9.2388	15.2005	-0.86977	14.7661	100.037	0.270811	100.308	0.002693	8.54952
O - nitrate	19	9.17597	15.0193	-0.91582	14.5552	96.4693	0.381376	96.8506	0.003922	8.40267
O - nitrate	20	9.28424	15.2129	-0.68653	14.7557	99.6467	0.201674	99.8483	0.002016	8.5399
N - nitro	21	3.62882	26.9309	-2.65029	26.4877	41.4495	4.72807	46.1776	0.091905	5.49068
N - nitro	22	3.61855	27.1431	-0.64006	27.0398	39.9717	0	39.9717	0	5.12925
N - nitro	23	3.69384	27.0081	-2.29339	26.5803	42.8719	5.28459	48.1565	0.097695	5.49256
H	24	6.26075	28.7787	0	28.7787	27.9178	0	27.9178	0	4.15069
H	25	6.31999	28.7518	0	28.7518	28.6163	0	28.6163	0	4.1899
H	26	6.35663	28.7313	0	28.7313	28.9127	0	28.9127	0	4.20109
H	27	7.46085	28.5772	0	28.5772	20.6853	0	20.6853	0	3.58977
H	28	7.5804	28.6191	0	28.6191	21.8483	0	21.8483	0	3.69423
H	29	7.57335	28.5512	0	28.5512	22.0831	0	22.0831	0	3.70568

See figure A-3 for corresponding atom with atom number.

Table A-4. EDNA atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.50214	31.9809	0	31.9809	57.249	0	57.249	0	5.819
H	2	8.58945	32.3802	0	32.3802	35.8024	0	35.8024	0	4.53592
H	3	7.37389	27.0685	0	27.0685	35.8083	0	35.8083	0	4.40907
H	4	5.53685	48.1822	0	48.1822	61.6289	0	61.6289	0	6.56806
N - nitramine	5	9.31728	28.3365	0	28.3365	98.6248	0	98.6248	0	7.88978
N - nitro	6	3.4007	16.6267	-8.16048	14.8974	47.7326	57.994	105.727	0.247645	7.00605
O - nitro	7	23.9956	9.00879	-19.3662	-15.2531	42.465	62.4953	104.96	0.240895	10.0777
O - nitro	8	21.0157	8.25446	-16.5717	-12.4644	35.7672	66.0603	101.827	0.227874	9.76265
C	9	2.57585	31.4219	0	31.4219	47.0273	0	47.0273	0	4.96758
H	10	8.44872	32.4668	0	32.4668	36.2595	0	36.2595	0	4.54198
H	11	7.26259	27.0098	0	27.0098	35.8362	0	35.8362	0	4.38552
N - nitramine	12	9.43822	28.4267	0	28.4267	100.375	0	100.375	0	7.97108
H	13	5.49556	48.4293	0	48.4293	65.0363	0	65.0363	0	6.70174
N - nitro	14	3.27238	16.9101	-7.57179	15.2969	45.0287	19.9096	64.9383	0.212593	6.69528
O - nitro	15	24.1201	9.05166	-19.257	-15.3599	38.2351	64.0162	102.251	0.234107	9.97572
O - nitro	16	20.9365	7.77755	-16.5397	-12.2724	32.6281	65.2671	97.8952	0.22221	9.78883

See figure A-4 for corresponding atom with atom number.

Table A-5. NQ atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.1288	3.85864	-26.1867	-24.6768	8.37101	149.608	157.979	0.05018	11.308
O - nitro	2	23.6084	0	-39.3902	-39.3902	0	49.4944	49.4944	0	5.39083
N - amino	3	16.9156	23.9201	0	23.9201	168.797	0	168.797	0	11.0309
N - amino	4	16.8882	20.7973	-0.46263	20.7551	155.798	0.282615	156.081	0.001807	10.7246
N - nitramine	5	15.6934	3.5946	-20.5052	-17.4696	5.43819	150.58	156.018	0.033641	11.9847
N - nitro	6	3.63554	2.17412	-10.0593	-8.68338	3.48763	46.9006	50.3883	0.064424	5.89146
C	7	2.6782	12.0623	0	12.0623	32.6752	0	32.6752	0	4.2039
H - amino	8	5.46852	38.1192	0	38.1192	94.9289	0	94.9289	0	8.11501
H - amino	9	6.93018	58.32	0	58.32	66.502	0	66.502	0	6.88254
H - amino	10	6.56807	57.1007	0	57.1007	80.6394	0	80.6394	0	7.65799
H - amino	11	2.74512	23.0719	0	23.0719	81.2145	0	81.2145	0	7.66805

See figure A-5 for corresponding atom with atom number.

Table A-6. RDX atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.45168	28.8637	0	28.8637	15.8398	0	15.8398	0	2.42817
C	2	2.70601	29.7884	0	29.7884	5.71472	0	5.71472	0	1.79582
C	3	2.34931	30.4889	0	30.4889	15.3328	0	15.3328	0	2.375
H	4	9.28893	39.2948	0	39.2948	31.8783	0	31.8783	0	4.85992
H	5	4.87019	21.1576	-2.84689	20.612	48.4359	2.91891	51.3549	0.053607	6.29176
H	6	5.58386	25.2052	-3.46009	25.1501	38.3207	0	38.3207	0	4.91886
H	7	9.29597	39.6851	0	39.6851	27.0743	0	27.0743	0	4.4646
H	8	9.52332	39.0121	0	39.0121	26.9371	0	26.9371	0	4.40824
H	9	4.98455	22.3859	-2.98279	21.914	52.3243	4.02549	56.3498	0.066334	6.32728
N - nitramine	10	4.06821	23.3655	0	23.3655	128.997	0	128.997	0	10.4141
N - nitramine	11	6.02802	18.7074	0	18.7074	38.138	0	38.138	0	4.90119
N - nitramine	12	6.01144	19.0961	0	19.0961	35.2063	0	35.2063	0	4.72272
N - nitro	13	3.35512	19.6861	-5.7977	18.9462	98.4931	25.1225	123.616	0.161928	9.19316
N - nitro	14	2.83699	20.4173	-7.9823	19.8894	56.6761	18.8391	75.5153	0.187237	5.94519
N - nitro	15	2.96216	20.7589	-9.48412	19.6511	53.099	44.0663	97.1653	0.247839	6.18085
O - nitro	16	21.2708	9.57326	-15.9104	-11.6855	56.6834	46.98	103.663	0.24781	9.33138
O - nitro	17	21.3868	8.58685	-16.2774	-12.5866	49.6368	51.6251	101.262	0.249904	9.0821
O - nitro	18	19.0874	7.54099	-15.9419	-12.3103	24.2013	41.9286	66.1299	0.232035	8.59091
O - nitro	19	20.6421	8.54978	-14.4405	-10.0568	34.6899	42.3976	77.0875	0.247501	9.03307
O - nitro	20	18.9582	9.14579	-15.5301	-11.2232	40.6579	40.4853	81.1432	0.249999	9.17343
O - nitro	21	20.7948	7.93369	-14.0316	-9.51821	31.8207	38.1472	69.9679	0.247956	8.82911

See figure A-6 for corresponding atom with atom number.

Table A-7. CL20 atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.6445	11.1258	-8.78463	-1.29007	66.1391	21.296	87.4351	0.18424	9.3875
O - nitro	2	18.8643	10.862	-9.64101	-3.30249	58.2053	17.5535	75.7587	0.178016	8.97625
O - nitro	3	19.8153	10.6817	-7.82431	-0.09173	60.4217	19.4379	79.8596	0.184157	9.00332
O - nitro	4	17.4912	10.8698	-8.71428	-1.99678	65.1662	16.2092	81.3754	0.159513	8.89811
O - nitro	5	19.9424	11.6232	-7.76589	-0.20159	82.6839	16.7147	99.3986	0.139881	9.22745
O - nitro	6	19.5695	12.5273	-9.29661	-3.01371	106.875	17.1835	124.058	0.119326	9.17856
O - nitro	7	20.0701	13.65	-8.91759	-1.56471	132.797	14.9583	147.755	0.090988	9.95564
O - nitro	8	20.562	9.89162	-8.00283	-2.324	79.2588	16.5195	95.7782	0.142728	7.91984
O - nitro	9	21.4527	12.652	-7.41942	1.70394	100.543	15.5723	116.115	0.116125	10.05
O - nitro	10	19.9414	12.9228	-8.66764	-1.25899	113.486	15.9227	129.409	0.107903	9.76978
O - nitro	11	20.4048	8.64404	-7.74235	-3.37965	55.061	14.3136	69.3746	0.163754	6.78415
O - nitro	12	21.3881	13.1924	-6.43392	2.22259	122.2	12.3986	134.598	0.08363	9.81344
N - nitramine	13	5.01433	27.2349	0	27.2349	27.8791	0	27.8791	0	4.30086
N - nitramine	14	5.37799	27.0561	0	27.0561	30.9699	0	30.9699	0	4.54243
N - nitramine	15	3.3236	37.3358	0	37.3358	27.97	0	27.97	0	4.52029
N - nitramine	16	1.14448	33.409	0	33.409	306.457	0	306.457	0	15.1028
N - nitramine	17	2.07566	38.0343	0	38.0343	46.896	0	46.896	0	5.5027
N - nitramine	18	1.57451	30.2972	0	30.2972	128.087	0	128.087	0	7.03222
N - nitro	19	2.00913	25.5593	-8.0361	24.829	33.3026	16.367	49.6695	0.220936	5.21844
N - nitro	20	2.00609	26.7415	-7.3519	25.9894	25.9072	4.78224	30.6894	0.131545	4.84165
N - nitro	21	1.95402	28.1461	-3.93428	27.3699	121.625	0.580672	122.206	0.004729	9.75145
N - nitro	22	3.16299	32.3665	0	32.3665	214.104	0	214.104	0	12.8024
N - nitro	23	3.25057	29.8773	-9.76468	29.7057	88.8804	0	88.8804	0	8.00391
N - nitro	24	3.15186	33.3311	-5.48067	33.1067	204.769	0	204.769	0	12.3894
C	25	1.05559	51.5368	0	51.5368	32.3129	0	32.3129	0	4.2922
C	26	1.20759	50.6006	0	50.6006	27.9529	0	27.9529	0	4.38628
C	27	0.580999	36.5851	0	36.5851	10.7276	0	10.7276	0	2.41557
C	28	0.427561	34.0617	0	34.0617	44.4823	0	44.4823	0	5.70632
C	29	1.0423	52.1494	0	52.1494	71.4665	0	71.4665	0	6.07868

Table A-7. CL20 atom specific Politzer parameters using B3LYP/6-31G* (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	30	1.07034	55.4067	0	55.4067	35.9488	0	35.9488	0	4.25203
H	31	5.55513	43.3397	0	43.3397	82.5788	0	82.5788	0	7.29947
H	32	5.99654	44.3348	0	44.3348	56.5274	0	56.5274	0	6.03714
H	33	6.2256	36.8998	0	36.8998	12.4296	0	12.4296	0	2.74695
H	34	3.60268	30.8867	0	30.8867	49.2548	0	49.2548	0	5.78106
H	35	3.87401	39.8653	0	39.8653	110.846	0	110.846	0	8.74172
H	36	4.1894	43.4018	0	43.4018	85.6528	0	85.6528	0	7.38048

See figure A-7 for corresponding atom with atom number.

Table A-8. HNB atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.14893	44.1343	0	44.1343	19.0656	0	19.0656	0	3.36067
C	2	4.23515	44.3573	0	44.3573	17.842	0	17.842	0	3.25586
C	3	4.20832	44.0643	0	44.0643	17.856	0	17.856	0	3.28329
N - nitro	4	0.850367	21.2388	0	21.2388	92.1069	0	92.1069	0	8.11136
N - nitro	5	0.900335	23.2867	0	23.2867	81.6118	0	81.6118	0	7.90075
N - nitro	6	0.8501	22.2341	-6.62211	21.776	106.463	0	106.463	0	9.64451
O - nitro	7	20.2473	10.8064	-6.30217	-0.23717	78.8509	12.6985	91.5494	0.119467	7.83149
O - nitro	8	19.654	10.4279	-3.93928	5.47078	84.5733	5.50812	90.0815	0.057407	7.93225
O - nitro	9	20.0921	9.33951	-4.15347	3.32603	70.5742	7.74051	78.3147	0.08907	7.24344
O - nitro	10	20.0179	9.88794	-4.22369	4.31756	80.5977	6.95242	87.5501	0.073105	7.72253
O - nitro	11	19.7715	9.50311	-5.38418	1.9408	75.9189	11.3917	87.3107	0.11345	7.62672
O - nitro	12	20.4264	10.9689	-6.3662	-0.11362	88.4379	12.8771	101.315	0.110945	7.99503
C	13	4.16218	44.3778	0	44.3778	18.6543	0	18.6543	0	3.32952
C	14	4.17426	44.1835	0	44.1835	18.373	0	18.373	0	3.28626
C	15	4.3637	44.1366	0	44.1366	18.6047	0	18.6047	0	3.2909
N - nitro	16	0.860106	21.714	0	21.714	102.739	0	102.739	0	9.02055
N - nitro	17	0.868842	21.3716	0	21.3716	104.337	0	104.337	0	9.02956
N - nitro	18	0.852827	21.7716	-0.93855	20.7071	81.8798	0.000308	81.8801	3.76E-06	7.74882
O - nitro	19	20.212	10.7735	-6.31538	-0.31444	80.655	12.5807	93.2358	0.116727	7.79128
O - nitro	20	19.6484	10.4116	-3.8961	5.35812	84.1931	5.62484	89.818	0.058703	7.87966
O - nitro	21	19.7582	9.70741	-5.42878	2.13385	79.7858	11.3643	91.15	0.109132	7.78262
O - nitro	22	20.4009	11.1856	-6.32163	-0.17406	87.8665	13.1343	101.001	0.113131	7.97922
O - nitro	23	20.1989	9.33367	-4.20568	3.43841	72.5871	7.68123	80.2684	0.086537	7.31844
O - nitro	24	19.9547	9.83138	-4.20736	4.21977	77.7284	6.99956	84.7279	0.075787	7.66328

See figure A-8 for corresponding atom with atom number.

Table A-9. TATB atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ^2_+ ([kcal/mol] ²)	σ^2_- ([kcal/mol] ²)	σ^2_{total} ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.82838	20.097	0	20.097	6.30183	0	6.30183	0	1.97878
C	2	3.69986	21.0286	0	21.0286	2.695	0	2.695	0	1.22022
C	3	6.93822	18.634	0	18.634	4.27535	0	4.27535	0	1.61203
C	4	3.8635	20.3645	0	20.3645	1.82742	0	1.82742	0	0.990579
C	5	6.77723	19.7646	0	19.7646	3.09685	0	3.09685	0	1.40805
C	6	3.82579	21.4243	0	21.4243	4.72989	0	4.72989	0	1.83253
H - amino	7	2.25364	26.1359	0	26.1359	39.0294	0	39.0294	0	5.32635
H - amino	8	2.33373	27.131	0	27.131	42.6134	0	42.6134	0	5.44655
H - amino	9	2.27425	26.3793	0	26.3793	53.1078	0	53.1078	0	6.15385
H - amino	10	3.10124	31.7763	0	31.7763	47.07	0	47.07	0	5.76844
H - amino	11	2.28266	26.8035	0	26.8035	42.4989	0	42.4989	0	5.52301
H - amino	12	2.72465	30.3005	0	30.3005	35.7608	0	35.7608	0	4.67092
N - nitro	13	3.93538	18.1848	-2.70519	17.8355	28.1239	3.16571	31.2896	0.090938	4.41213
N - amino	14	15.0614	18.3654	0	18.3654	69.33	0	69.33	0	6.69646
N - nitro	15	3.99579	15.8383	-4.91756	15.0643	24.4152	18.9081	43.3233	0.24596	4.71283
N - amino	16	14.7312	17.7033	0	17.7033	62.1288	0	62.1288	0	6.24225
N - nitro	17	3.97011	17.6503	-4.2502	17.072	22.1989	18.178	40.3769	0.247521	4.32773
N - amino	18	15.1674	18.3188	0	18.3188	85.7	0	85.7	0	7.68939
O - nitro	19	19.0477	9.47571	-13.9889	-7.86592	49.3456	57.9618	107.307	0.248388	10.4649
O - nitro	20	19.2968	8.21613	-14.2924	-8.63868	29.1249	58.2648	87.3897	0.222203	10.1188
O - nitro	21	19.2676	7.63059	-15.8644	-10.8724	30.5332	71.9348	102.468	0.209187	10.4057
O - nitro	22	19.6186	7.02175	-15.9605	-11.3234	22.4	68.1122	90.5123	0.186234	10.0744
O - nitro	23	18.77	9.17863	-14.1327	-7.02788	35.8156	57.6055	93.4212	0.236399	10.9063
O - nitro	24	19.4113	8.03783	-14.6048	-8.90564	27.1538	63.1201	90.274	0.210317	10.3398

See figure A-9 for corresponding atom with atom number.

Table A-10. PNA atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.07015	39.3766	0	39.3766	5.69277	0	5.69277	0	1.625
C	2	5.47816	34.9633	0	34.9633	21.6209	0	21.6209	0	3.69487
C	3	3.64206	30.2468	0	30.2468	20.7315	0	20.7315	0	3.58265
C	4	4.93769	29.3804	0	29.3804	13.1802	0	13.1802	0	2.7011
N - amino	5	15.6271	36.7887	0	36.7887	56.7805	0	56.7805	0	6.26488
H - amino	6	2.83672	47.9652	0	47.9652	35.7076	0	35.7076	0	4.97803
N - nitro	7	3.00393	33.5886	0	33.5886	116.902	0	116.902	0	9.25427
N - nitro	8	0.32023	11.6904	-4.02146	4.85916	96.7466	15.7473	112.494	0.120388	9.64275
N - nitro	9	2.11705	17.8864	-1.67495	17.1928	47.1705	0.253595	47.4241	0.005319	6.28193
O - nitro	10	20.2586	14.1808	-5.3947	7.86659	113.394	9.05301	122.447	0.068468	10.5357
O - nitro	11	18.5129	11.7477	-7.42948	-1.50253	83.2544	11.6832	94.9376	0.107917	8.24013
O - nitro	12	20.469	9.28007	-10.23	-7.01912	45.8027	23.8985	69.7011	0.22531	6.68675
O - nitro	13	19.598	9.12624	-10.6382	-7.75774	44.7496	22.4277	67.1773	0.222397	6.35224
O - nitro	14	18.9174	8.9733	-11.2	-7.38555	44.4771	21.5525	66.0296	0.219865	7.25793
C	15	5.37822	35.0465	0	35.0465	21.0789	0	21.0789	0	3.62853
C	16	3.70034	29.9286	0	29.9286	20.9075	0	20.9075	0	3.6364
H - amino	17	2.81291	47.8167	0	47.8167	39.9102	0	39.9102	0	5.14421
N - nitro	18	3.02278	33.7089	0	33.7089	110.366	0	110.366	0	8.94279
N - nitro	19	0.27137	9.13407	-4.41181	5.07031	89.9339	10.394	100.328	0.092867	8.74809
O - nitro	20	20.1433	14.0033	-5.43099	7.75904	109.886	9.12071	119.007	0.070766	10.4169
O - nitro	21	18.5998	12.0437	-7.37042	-1.37689	83.1422	11.8182	94.9604	0.108965	8.33467
O - nitro	22	20.4489	8.91716	-10.2174	-7.00362	44.4752	23.8696	68.3449	0.227275	6.65234
O - nitro	23	19.5954	8.89057	-10.6942	-7.99784	43.1324	22.1883	65.3207	0.224298	6.1786
O - nitro	24	18.8637	8.8098	-11.2893	-7.44543	44.5739	21.3793	65.9532	0.21908	7.26926

See figure A-10 for corresponding atom with atom number.

Table A-11. TNT atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.8719	8.04196	-9.94795	-5.28188	37.3531	27.695	65.0481	0.244489	7.71301
O - nitro	2	22.2275	9.6641	-10.6049	-4.67873	48.2242	26.4945	74.7187	0.228856	8.86431
O - nitro	3	22.3041	8.92212	-11.8664	-6.75721	36.9602	34.4017	71.3619	0.249679	8.80536
O - nitro	4	22.3082	9.13174	-11.7214	-6.68662	48.4255	30.9359	79.3614	0.237858	8.61405
O - nitro	5	22.8681	10.1139	-10.3135	-4.7042	55.9647	22.9882	78.9529	0.206387	8.65734
O - nitro	6	20.9736	7.86552	-9.86021	-5.42451	37.7405	22.5936	60.3342	0.234243	7.41202
N - nitro	7	3.26306	27.3121	-4.4754	27.1229	38.4922	0	38.4922	0	5.12592
N - nitro	8	3.80442	25.0038	-8.24045	24.3219	38.5224	27.458	65.9805	0.24297	5.60373
N - nitro	9	2.04249	26.7383	-4.38922	25.7553	59.6701	4.74926	64.4193	0.068289	7.1325
C	10	5.34349	23.5768	0	23.5768	14.5084	0	14.5084	0	2.95766
C	11	7.29688	21.9313	0	21.9313	18.7747	0	18.7747	0	3.28534
C	12	5.49058	23.1859	0	23.1859	13.147	0	13.147	0	2.77257
C	13	7.0206	21.6874	0	21.6874	50.5332	0	50.5332	0	6.30486
C	14	4.83901	21.7364	0	21.7364	18.5058	0	18.5058	0	3.29966
C	15	4.69267	23.9987	0	23.9987	21.1985	0	21.1985	0	4.01154
C	16	4.15352	20.7756	0	20.7756	44.1266	0	44.1266	0	5.22915
H	17	6.8761	24.1062	0	24.1062	19.082	0	19.082	0	3.47545
H	18	7.45844	28.8907	0	28.8907	45.2253	0	45.2253	0	5.69406
H	19	8.02274	23.6448	0	23.6448	20.2688	0	20.2688	0	3.36727
H	20	9.32859	16.5735	0	16.5735	12.0135	0	12.0135	0	2.77108
H	21	7.75196	22.7818	0	22.7818	25.2726	0	25.2726	0	3.88776

See figure A-11 for corresponding atom with atom number.

A.5 B3LYP/6-31G** Training Set Data

Table A-12. FOX-7 atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number ^a	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.82177	24.5924	0	24.5924	18.4628	0	18.4628	0	3.36963
N - amino	2	16.3528	31.3528	0	31.3528	132.961	0	132.961	0	9.63419
H - amino	3	6.07973	61.3686	0	61.3686	58.7832	0	58.7832	0	6.39196
H - amino	4	3.24397	36.4432	0	36.4432	88.2992	0	88.2992	0	7.93302
N - amino	5	16.4664	31.405	0	31.405	137.755	0	137.755	0	9.99995
H - amino	6	2.75515	33.7783	0	33.7783	85.8139	0	85.8139	0	7.8723
H - amino	7	6.27586	62.1673	0	62.1673	64.4287	0	64.4287	0	6.81649
C	8	6.34747	13.367	0	13.367	22.9471	0	22.9471	0	3.97392
N - nitro	9	3.0078	12.3921	-6.12935	8.55786	62.9851	34.0694	97.0545	0.227809	8.51492
O - nitro	10	21.3815	4.08124	-27.7777	-26.9589	8.0025	77.1102	85.1127	0.085182	7.76838
O - nitro	11	20.8174	8.50553	-17.7717	-13.1274	43.6334	85.3137	128.947	0.22388	10.9543
N - nitro	12	3.64822	8.6346	-6.91321	5.28116	19.0727	53.5132	72.5859	0.193717	6.19274
O - nitro	13	21.3339	2.09133	-29.5245	-29.1801	1.34976	81.2579	82.6077	0.016073	7.48152
O - nitro	14	20.9107	7.7129	-19.5537	-14.5365	27.5476	102.416	129.964	0.167035	11.8303

See figure A-1 for corresponding atom with atom number.

Table A-13. HMX atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.10725	38.0448	0	38.0448	43.896	0	43.896	0	5.86676
C	2	1.47325	36.0609	0	36.0609	79.1811	0	79.1811	0	7.4923
H	3	7.24045	40.6353	0	40.6353	34.7521	0	34.7521	0	4.92263
H	4	6.34817	31.4691	0	31.4691	63.3629	0	63.3629	0	6.39445
H	5	7.4262	29.4271	0	29.4271	37.1885	0	37.1885	0	4.97059
H	6	7.3348	38.4543	0	38.4543	65.0129	0	65.0129	0	6.57778
N - nitro	7	2.1551	16.4879	-7.14975	14.4823	66.6768	24.18	90.8568	0.195306	8.67262
N - nitramine	8	3.1955	18.4601	0	18.4601	24.6075	0	24.6075	0	4.00814
N - nitramine	9	2.4579	41.0938	0	41.0938	6.72487	0	6.72487	0	1.94567
N - nitro	10	2.49593	35.2124	-7.54141	34.9954	92.9803	0	92.9803	0	7.53112
O - nitro	11	20.9793	7.92801	-15.5522	-11.9574	28.3064	48.3055	76.6119	0.232964	8.73276
O - nitro	12	21.625	9.00146	-13.2173	-7.74254	42.6333	48.1712	90.8045	0.24907	9.61362
O - nitro	13	20.4397	11.8484	-8.63663	-0.43165	87.6181	23.7799	111.398	0.1679	9.84377
O - nitro	14	18.5905	14.2982	-11.4465	-3.23089	111.896	21.9116	133.808	0.136939	11.3752
N - nitramine	15	2.43918	41.0795	0	41.0795	6.13123	0	6.13123	0	1.94381
C	16	1.53712	36.0299	0	36.0299	75.5497	0	75.5497	0	7.20078
C	17	2.06174	37.3719	0	37.3719	43.1444	0	43.1444	0	5.7918
N - nitro	18	2.37892	35.6254	-3.35467	35.2129	85.8744	4.70859	90.583	0.049279	7.33704
H	19	7.27704	29.4274	0	29.4274	33.9533	0	33.9533	0	4.76754
H	20	7.42523	38.604	0	38.604	64.4214	0	64.4214	0	6.57107
N - nitramine	21	3.3125	18.8923	0	18.8923	30.4806	0	30.4806	0	4.40813
H	22	7.28765	40.5912	0	40.5912	34.7994	0	34.7994	0	4.92164
H	23	6.35851	31.5403	0	31.5403	60.2137	0	60.2137	0	6.35683
O - nitro	24	20.4874	11.7986	-8.79635	-0.35736	89.4293	23.1057	112.535	0.163164	9.96623
O - nitro	25	18.5858	13.7642	-11.426	-3.36297	107.259	21.2986	128.558	0.138225	11.1365
N - nitro	26	2.03983	17.2279	-7.44255	15.1851	57.3135	45.8181	103.132	0.246894	8.2237
O - nitro	27	21.016	7.35514	-15.5947	-12.0377	25.2114	47.8183	73.0297	0.226043	8.65479
O - nitro	28	21.6727	8.85894	-13.2702	-7.8418	40.2596	47.7749	88.0345	0.248178	9.5746

See figure A-2 for corresponding atom with atom number.

Table A-14. PETN atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.871068	30.1456	0	30.1456	51.6395	0	51.6395	0	6.25241
O - nitro	3	21.6633	11.1717	-6.08496	2.46618	75.0029	12.6669	87.6698	0.123608	8.82451
O - nitro	4	25.0257	8.50389	-8.77522	-4.73381	39.9832	14.1703	54.1534	0.193198	6.80437
O - nitrate	5	9.21635	16.9682	-0.53202	16.7986	107.997	0.171273	108.168	0.001581	8.73782
N - nitro	6	3.3669	29.1527	-5.39784	28.8785	50.4713	1.65966	52.131	0.030823	5.94723
H	7	6.3271	30.8578	0	30.8578	29.3637	0	29.3637	0	4.29901
H	8	7.51784	30.8842	0	30.8842	21.5854	0	21.5854	0	3.66949
C	9	0.880605	30.4265	0	30.4265	52.3692	0	52.3692	0	6.38224
C	10	0.790156	29.8462	0	29.8462	50.0826	0	50.0826	0	6.17723
C	11	0.732989	30.0084	0	30.0084	42.1019	0	42.1019	0	5.50058
O - nitro	12	21.7003	11.2034	-6.05883	2.48931	75.6535	12.7333	88.3868	0.123309	8.83145
O - nitro	13	21.6676	10.9681	-6.10976	2.43505	74.4924	12.4671	86.9595	0.122813	8.75316
O - nitro	14	21.8031	11.1463	-6.07736	2.55213	75.2741	12.5691	87.8432	0.122612	8.83077
O - nitro	15	24.9352	8.57153	-8.81018	-4.71299	40.5095	14.1227	54.6322	0.191681	6.85275
O - nitro	16	25.122	8.69411	-8.82068	-4.66941	41.5526	14.0823	55.6349	0.18905	6.90767
O - nitro	17	25.079	8.64039	-8.81191	-4.68094	40.9827	14.1215	55.1042	0.190595	6.88457
O - nitrate	18	9.26795	17.1034	-0.68748	16.9022	110.671	0.108377	110.779	0.000977	8.87272
O - nitrate	19	9.14731	17.0785	-0.40725	16.7653	107.277	0.184643	107.461	0.001715	8.74611
O - nitrate	20	9.22434	17.1984	-0.54327	16.9717	109.389	0.110346	109.5	0.001007	8.83476
N - nitro	21	3.38766	28.9669	-3.9348	28.7037	51.4085	10.1038	61.5124	0.137276	5.95291
N - nitro	22	3.30186	29.4955	0	29.4955	44.8653	0	44.8653	0	5.41469
N - nitro	23	3.27678	29.3574	-8.41992	29.2019	46.848	0	46.848	0	5.67097
H	24	6.29203	30.8012	0	30.8012	29.0509	0	29.0509	0	4.27577
H	25	6.35544	30.8513	0	30.8513	30.2228	0	30.2228	0	4.3439
H	26	6.3177	30.9501	0	30.9501	28.8296	0	28.8296	0	4.27273
H	27	7.51295	30.7672	0	30.7672	22.6811	0	22.6811	0	3.74723
H	28	7.58533	30.9138	0	30.9138	21.9509	0	21.9509	0	3.68692
H	29	7.63361	30.7373	0	30.7373	23.3316	0	23.3316	0	3.80422

See figure A-3 for corresponding atom with atom number.

Table A-15. EDNA atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.39525	34.3506	0	34.3506	51.4504	0	51.4504	0	5.3826
H	2	8.69212	34.5698	0	34.5698	32.261	0	32.261	0	4.25097
H	3	7.4341	29.2511	0	29.2511	32.2283	0	32.2283	0	4.12737
H	4	5.42174	48.2946	0	48.2946	81.265	0	81.265	0	7.56561
N - nitramine	5	9.39721	30.5927	0	30.5927	92.5757	0	92.5757	0	7.58593
N - nitro	6	3.16012	19.6523	-5.94361	18.3671	61.651	31.2848	92.9358	0.22331	7.37697
O - nitro	7	25.5552	8.99596	-18.5202	-14.4664	36.0083	60.8592	96.8675	0.233546	9.90977
O - nitro	8	22.0772	8.71443	-15.7568	-10.7075	40.7073	63.6646	104.372	0.237905	10.2061
C	9	2.25025	34.2171	0	34.2171	44.5255	0	44.5255	0	4.95298
H	10	8.68947	34.6562	0	34.6562	34.961	0	34.961	0	4.3789
H	11	7.52846	29.2624	0	29.2624	32.0405	0	32.0405	0	4.09986
N - nitramine	12	9.49295	30.5479	0	30.5479	91.3461	0	91.3461	0	7.53681
H	13	5.43751	48.4347	0	48.4347	81.3554	0	81.3554	0	7.60464
N - nitro	14	3.11287	20.1493	-8.28166	18.7736	54.3159	50.5965	104.912	0.249686	7.07544
O - nitro	15	25.6157	8.87185	-18.5785	-14.4828	37.8988	60.0079	97.9067	0.237251	9.91151
O - nitro	16	21.9795	9.22931	-15.6552	-10.733	40.6219	64.949	105.571	0.236725	10.2284

See figure A-4 for corresponding atom with atom number.

Table A-16. NQ atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	21.2304	4.59615	-24.8437	-22.83	13.4353	146.115	159.55	0.077117	11.5487
O - nitro	2	25.187	0	-37.714	-37.714	0	51.0145	51.0145	0	5.46248
N - amino	3	17.2283	24.8615	0	24.8615	137.513	0	137.513	0	9.85367
N - amino	4	17.1685	22.2289	0	22.2289	134.596	0	134.596	0	9.89705
N - nitramine	5	16.2652	4.71205	-18.9352	-14.3972	8.71798	132.096	140.814	0.058079	11.9319
N - nitro	6	3.37466	2.90201	-9.13642	-5.99323	4.72773	56.718	61.4457	0.071022	6.49371
C	7	2.47261	15.5498	0	15.5498	33.2173	0	33.2173	0	4.27007
H - amino	8	5.70453	37.7443	0	37.7443	103.377	0	103.377	0	8.46492
H - amino	9	7.20981	57.345	0	57.345	75.3864	0	75.3864	0	7.37109
H - amino	10	6.87621	56.2057	0	56.2057	84.3833	0	84.3833	0	7.87099
H - amino	11	2.6931	23.8331	-0.10228	23.7624	78.0717	0	78.0717	0	7.56358

See figure A-5 for corresponding atom with atom number.

Table A-17. RDX atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.20372	31.1944	0	31.1944	18.187	0	18.187	0	2.80937
C	2	2.46173	31.9963	0	31.9963	9.79272	0	9.79272	0	1.71184
C	3	2.13272	32.3717	0	32.3717	15.3266	0	15.3266	0	2.44977
H	4	9.47319	41.6045	0	41.6045	34.6908	0	34.6908	0	5.08085
H	5	5.00754	22.141	-3.01438	21.5315	45.0373	3.90489	48.9422	0.07342	6.05368
H	6	5.7238	26.2655	0	26.2655	32.6476	0	32.6476	0	4.49081
H	7	9.50805	41.9432	0	41.9432	28.2663	0	28.2663	0	4.60897
H	8	9.59823	41.4187	0	41.4187	29.4026	0	29.4026	0	4.63175
H	9	5.06259	23.3456	-3.27654	23.1002	47.5992	1.35404	48.9532	0.026895	5.80039
N - nitramine	10	3.75951	26.5457	0	26.5457	138.771	0	138.771	0	10.8885
N - nitramine	11	6.09917	21.4126	0	21.4126	37.1517	0	37.1517	0	4.8575
N - nitramine	12	6.06321	21.8749	0	21.8749	34.4134	0	34.4134	0	4.65887
N - nitro	13	3.20025	22.3976	-6.83107	21.3223	108.745	46.3191	155.064	0.209482	9.73179
N - nitro	14	2.59596	22.8788	-6.87445	21.9072	66.8218	53.7207	120.543	0.247047	6.73969
N - nitro	15	2.80996	23.175	-8.83149	22.1748	71.4756	30.0669	101.542	0.208425	7.01765
O - nitro	16	22.2	10.1703	-15.4823	-10.7653	65.2625	47.0851	112.348	0.243456	9.67969
O - nitro	17	22.3775	9.54795	-16.0403	-11.8783	57.0728	51.2614	108.334	0.249281	9.45259
O - nitro	18	19.7166	7.87827	-15.4532	-11.452	28.8226	42.2259	71.0486	0.241103	8.85525
O - nitro	19	21.4191	9.10186	-14.2085	-9.39097	37.5717	42.8129	80.3847	0.248937	9.3477
O - nitro	20	19.6053	9.43905	-15.1473	-10.6136	47.3298	39.4756	86.8055	0.247953	9.27226
O - nitro	21	21.4749	8.32319	-13.7303	-9.13303	34.0025	38.9411	72.9437	0.248854	8.88783

See figure A-6 for corresponding atom with atom number.

Table A-18. CL20 atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.0251	11.4373	-8.1179	-0.3513	72.7531	18.9118	91.6649	0.163749	9.3671
O - nitro	2	19.5267	11.7828	-8.75172	-1.53951	69.6719	15.2854	84.9573	0.147548	9.4006
O - nitro	3	20.3858	11.1041	-7.31523	1.08509	71.1876	16.8958	88.0833	0.155022	9.17891
O - nitro	4	17.8329	11.5743	-7.74673	-0.57515	75.6065	15.2082	90.8147	0.13942	9.02422
O - nitro	5	20.6222	12.066	-7.40757	0.865056	89.1469	16.0427	105.19	0.129252	9.53804
O - nitro	6	19.8996	12.2872	-8.82811	-2.13617	103.839	15.572	119.411	0.113401	9.24477
O - nitro	7	20.7272	14.2229	-8.54283	-0.88636	144.97	14.225	159.195	0.081371	10.179
O - nitro	8	20.9355	9.93499	-7.70848	-1.75819	84.4373	16.9624	101.4	0.139299	7.97844
O - nitro	9	22.2638	13.3992	-7.11563	2.49672	109.032	16.3972	125.429	0.113639	10.3805
O - nitro	10	20.5972	13.3543	-8.18626	-0.36807	116.126	16.0361	132.162	0.106614	9.9628
O - nitro	11	20.6855	9.16046	-7.44669	-2.99237	62.5984	14.3202	76.9186	0.151513	6.82938
O - nitro	12	22.1707	13.6435	-6.24877	3.03147	135.275	12.7201	147.995	0.078562	10.1682
N - nitramine	13	4.93297	31.5158	0	31.5158	25.859	0	25.859	0	4.06167
N - nitramine	14	5.24399	31.3007	0	31.3007	28.6879	0	28.6879	0	4.25536
N - nitramine	15	3.2793	40.2493	0	40.2493	28.3436	0	28.3436	0	4.52032
N - nitramine	16	0.952927	38.0073	0	38.0073	359.445	0	359.445	0	17.0255
N - nitramine	17	1.92621	41.5708	0	41.5708	39.348	0	39.348	0	5.00649
N - nitramine	18	1.5474	33.7786	0	33.7786	132.078	0	132.078	0	6.99845
N - nitro	19	1.86702	28.8763	0	28.8763	43.5556	0	43.5556	0	4.94224
N - nitro	20	1.84453	29.3363	0	29.3363	50.5061	0	50.5061	0	5.197
N - nitro	21	1.84477	30.3272	-7.00222	29.0174	139.817	13.65	153.468	0.081033	10.8795
N - nitro	22	2.89805	36.3253	0	36.3253	236.031	0	236.031	0	13.4907
N - nitro	23	2.93851	32.057	-8.5288	31.6705	107.029	1.95027	108.979	0.017576	8.71904
N - nitro	24	3.0126	35.3017	-5.5522	35.0511	237.253	0	237.253	0	12.8804
C	25	0.813401	55.2628	0	55.2628	23.9254	0	23.9254	0	3.3987
C	26	1.05366	53.252	0	53.252	34.1841	0	34.1841	0	4.76737
C	27	0.457938	39.0292	0	39.0292	8.21341	0	8.21341	0	2.25778
C	28	0.285441	37.4131	0	37.4131	31.8231	0	31.8231	0	4.5785

See figure A-7 for corresponding atom with atom number.

Table A-18. CL20 atom specific Politzer parameters using B3LYP/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	29	0.912986	55.4303	0	55.4303	70.6886	0	70.6886	0	6.22758
C	30	0.924783	58.0937	0	58.0937	31.313	0	31.313	0	4.88183
H	31	5.77699	45.4477	0	45.4477	80.6931	0	80.6931	0	7.17582
H	32	6.25425	46.6539	0	46.6539	53.1825	0	53.1825	0	5.81854
H	33	6.34408	38.7797	0	38.7797	15.845	0	15.845	0	3.1689
H	34	3.63514	32.8064	0	32.8064	45.0638	0	45.0638	0	5.54457
H	35	3.83136	41.9975	0	41.9975	86.2542	0	86.2542	0	7.66315
H	36	4.43815	44.775	0	44.775	82.5069	0	82.5069	0	7.18278

See figure A-7 for corresponding atom with atom number.

Table A-19. HNB atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.91595	46.3007	0	46.3007	21.0685	0	21.0685	0	3.59328
C	2	4.01251	46.1053	0	46.1053	19.9099	0	19.9099	0	3.43535
C	3	3.89221	46.0421	0	46.0421	20.7824	0	20.7824	0	3.59003
N - nitro	4	0.706133	21.9777	-1.10755	21.4968	97.674	0	97.674	0	8.71401
N - nitro	5	0.702257	25.2181	-2.31237	24.6783	102.9	0	102.9	0	9.32762
N - nitro	6	0.609493	23.4092	0	23.4092	118.477	0	118.477	0	9.89784
O - nitro	7	20.9679	10.4786	-5.81158	0.491105	82.9554	11.4104	94.3658	0.106296	7.73968
O - nitro	8	19.9471	10.503	-3.53762	6.32984	81.0108	4.08055	85.0914	0.045655	7.70505
O - nitro	9	20.7956	8.917	-3.99442	4.10993	70.0667	6.29901	76.3657	0.075681	7.09969
O - nitro	10	20.4976	9.65812	-3.87595	5.0163	74.4126	5.48698	79.8996	0.063957	7.43977
O - nitro	11	20.3858	9.45315	-4.92967	3.20239	78.7215	9.44257	88.164	0.095631	7.62002
O - nitro	12	21.0974	10.6041	-5.49252	0.795394	85.8855	11.6434	97.5289	0.105132	7.68842
C	13	3.87758	46.0648	0	46.0648	19.0143	0	19.0143	0	3.38847
C	14	3.95631	45.8046	0	45.8046	19.7476	0	19.7476	0	3.47557
C	15	4.02845	45.9016	0	45.9016	17.5814	0	17.5814	0	3.24945
N - nitro	16	0.648215	21.3831	0	21.3831	103.649	0	103.649	0	8.50244
N - nitro	17	0.742839	23.6829	0	23.6829	103.407	0	103.407	0	9.43581
N - nitro	18	0.662175	22.8574	-0.31721	21.8712	79.1574	0.005718	79.1632	7.22E-05	7.68825
O - nitro	19	20.9267	10.4435	-5.77063	0.496664	80.8942	11.5664	92.4607	0.109447	7.7005
O - nitro	20	20.1506	10.6181	-3.58343	6.453	84.0547	4.01979	88.0744	0.043558	7.82898
O - nitro	21	20.298	9.00177	-4.87444	2.82911	71.9586	9.55126	81.5098	0.103448	7.29398
O - nitro	22	21.0401	10.6382	-5.53321	0.808299	85.5867	11.5595	97.1462	0.104832	7.73159
O - nitro	23	20.7968	8.93502	-3.92114	4.13238	68.026	6.4763	74.5023	0.079371	7.04687
O - nitro	24	20.516	9.712	-3.98233	5.14413	76.8773	5.40814	82.2855	0.061405	7.54966

See figure A-8 for corresponding atom with atom number.

Table A-20. TATB atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.80055	23.5753	0	23.5753	4.2263	0	4.2263	0	1.60442
C	2	3.63684	24.3763	0	24.3763	1.79886	0	1.79886	0	0.953843
C	3	6.77441	22.2025	0	22.2025	2.73514	0	2.73514	0	1.29305
C	4	3.7772	23.7164	0	23.7164	1.24014	0	1.24014	0	0.837891
C	5	6.58696	23.3256	0	23.3256	1.86327	0	1.86327	0	1.10457
C	6	3.78539	24.7211	0	24.7211	2.81375	0	2.81375	0	1.31639
H - amino	7	2.16188	26.5194	0	26.5194	44.6938	0	44.6938	0	5.68357
H - amino	8	2.31467	27.5731	0	27.5731	43.6687	0	43.6687	0	5.53012
H - amino	9	2.19187	26.5665	0	26.5665	58.2088	0	58.2088	0	6.38888
H - amino	10	3.21232	30.9813	0	30.9813	52.5276	0	52.5276	0	6.05616
H - amino	11	2.30374	26.9398	0	26.9398	46.2253	0	46.2253	0	5.78203
H - amino	12	2.89449	30.1885	0	30.1885	36.1127	0	36.1127	0	4.70789
N - nitro	13	3.69768	21.3822	-3.23063	21.1087	29.7517	1.77826	31.5299	0.053218	4.42746
N - amino	14	15.4112	19.9147	0	19.9147	58.704	0	58.704	0	6.10697
N - nitro	15	3.79005	19.2871	-8.79768	18.0748	26.2555	59.0138	85.2693	0.213103	5.32847
N - amino	16	15.0994	19.029	0	19.029	51.8484	0	51.8484	0	5.67846
N - nitro	17	3.90802	20.5474	-7.58872	20.0555	27.3099	27.4893	54.7992	0.249997	4.60024
N - amino	18	15.2355	19.7217	0	19.7217	71.2238	0	71.2238	0	7.0031
O - nitro	19	19.8826	9.57317	-13.6892	-7.1545	49.8004	56.4062	106.207	0.249033	10.5725
O - nitro	20	20.2212	8.88316	-14.0269	-7.66581	34.8576	56.8121	91.6697	0.23566	10.4756
O - nitro	21	20.2422	8.46294	-15.5439	-9.86189	34.4139	69.9606	104.374	0.221003	10.7517
O - nitro	22	20.5441	7.61788	-15.6601	-10.4712	26.1319	67.9504	94.0822	0.200607	10.3982
O - nitro	23	19.5878	9.68446	-13.7277	-6.18396	41.3443	55.6044	96.9487	0.244591	11.066
O - nitro	24	20.3258	8.40717	-14.3266	-8.15355	31.3783	60.3459	91.7241	0.225066	10.4686

See figure A-9 for corresponding atom with atom number.

Table A-21. PNA atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.08328	42.1706	0	42.1706	6.43703	0	6.43703	0	1.76438
C	2	5.18688	37.5802	0	37.5802	25.463	0	25.463	0	3.93186
C	3	3.45234	32.1003	0	32.1003	22.1736	0	22.1736	0	3.80388
C	4	4.57443	31.7793	0	31.7793	12.3498	0	12.3498	0	2.64211
N - amino	5	16.0517	38.251	0	38.251	50.1493	0	50.1493	0	5.80994
H - amino	6	2.753	47.8689	0	47.8689	40.4804	0	40.4804	0	5.31108
N - nitro	7	2.73145	35.989	-2.92608	35.7925	128.887	0	128.887	0	9.84375
N - nitro	8	0.234	7.36822	-5.53802	3.57226	82.1394	33.5717	115.711	0.205956	6.84005
N - nitro	9	1.90051	19.1054	-2.03024	18.3048	47.8545	2.06133	49.9159	0.039591	6.33884
O - nitro	10	21.0089	14.4537	-5.3868	8.41937	113.818	8.43234	122.25	0.064219	10.6362
O - nitro	11	19.1991	12.0267	-6.78379	-0.54162	90.7282	11.7229	102.451	0.101332	8.35056
O - nitro	12	21.0819	9.46964	-9.38289	-5.68907	51.667	21.932	73.599	0.209193	6.83846
O - nitro	13	20.2918	9.29857	-9.6763	-6.63709	52.4008	20.3408	72.7415	0.201437	6.2673
O - nitro	14	19.4993	9.48783	-10.5186	-6.51142	48.0102	20.6771	68.6873	0.210412	7.29354
C	15	5.18721	37.5591	0	37.5591	24.6354	0	24.6354	0	3.88478
C	16	3.47138	32.1249	0	32.1249	22.1747	0	22.1747	0	3.79071
H - amino	17	2.77321	47.9277	0	47.9277	39.0263	0	39.0263	0	5.1968
N - nitro	18	2.60869	35.7804	0	35.7804	134.672	0	134.672	0	10.0057
N - nitro	19	0.229684	5.07035	-3.8145	1.89719	42.1507	20.5905	62.7412	0.220478	4.73499
O - nitro	20	20.9846	14.52	-5.30974	8.43405	113.944	8.63437	122.578	0.065478	10.6327
O - nitro	21	19.2165	12.2558	-6.82664	-0.52276	95.0811	11.5758	106.657	0.096754	8.44965
O - nitro	22	21.0814	9.47446	-9.34943	-5.70651	52.201	22.1299	74.3309	0.209083	6.81426
O - nitro	23	20.184	9.20734	-9.67323	-6.69279	52.3622	20.4071	72.7693	0.201791	6.21566
O - nitro	24	19.5302	9.52848	-10.4733	-6.50531	48.948	20.8164	69.7644	0.20935	7.27142

See figure A-10 for corresponding atom with atom number.

Table A-22. TNT atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.7121	8.49626	-9.58682	-4.13569	45.4728	28.5685	74.0414	0.236969	8.11297
O - nitro	2	23.1033	10.2192	-10.1697	-4.01791	54.535	27.6088	82.1439	0.223138	9.00789
O - nitro	3	23.4109	9.30278	-11.5838	-6.02599	42.6363	34.716	77.3523	0.247379	9.04357
O - nitro	4	23.3247	9.87081	-11.3198	-5.73939	54.7127	31.5235	86.2362	0.231923	8.96387
O - nitro	5	23.8747	10.2019	-9.86801	-3.86244	60.5618	21.588	82.1498	0.193731	8.72892
O - nitro	6	21.9501	8.4378	-9.22973	-4.15879	44.0745	22.0383	66.1128	0.222226	7.70365
N - nitro	7	3.24867	28.9006	-9.28087	27.771	58.4513	31.6329	90.0842	0.227843	7.03038
N - nitro	8	3.54912	27.4636	-2.20836	26.815	45.1658	6.95856	52.1244	0.115677	5.90258
N - nitro	9	1.79253	28.6491	-6.21987	28.229	71.3388	0	71.3388	0	7.03267
C	10	5.21715	25.3866	0	25.3866	16.2912	0	16.2912	0	3.0374
C	11	7.17809	23.6308	0	23.6308	20.9578	0	20.9578	0	3.38462
C	12	5.41616	24.9038	0	24.9038	15.4807	0	15.4807	0	2.91693
C	13	6.81314	23.4	0	23.4	48.2239	0	48.2239	0	6.0428
C	14	4.56648	23.4113	0	23.4113	17.7178	0	17.7178	0	3.18676
C	15	4.6406	26.1266	0	26.1266	21.403	0	21.403	0	3.93872
C	16	3.70782	23.3098	0	23.3098	39.09	0	39.09	0	4.73802
H	17	6.99601	25.4996	0	25.4996	22.2945	0	22.2945	0	3.80736
H	18	7.77584	30.4861	0	30.4861	50.6337	0	50.6337	0	5.95152
H	19	8.26568	25.5301	0	25.5301	21.3183	0	21.3183	0	3.21486
H	20	9.50324	17.9815	0	17.9815	13.6559	0	13.6559	0	2.99619
H	21	7.90003	24.8237	0	24.8237	21.5693	0	21.5693	0	3.45128

See figure A-11 for corresponding atom with atom number.

A.6 PBE/6-31G* Training Set Data

Table A-23. FOX-7 atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.10049	17.9198	0	17.9198	18.8431	0	18.8431	0	3.3505
N - amino	2	16.0264	29.1447	0	29.1447	165.245	0	165.245	0	10.9268
H - amino	3	5.87179	60.9191	0	60.9191	50.1882	0	50.1882	0	5.85591
H - amino	4	3.13297	35.134	0	35.134	84.531	0	84.531	0	7.71709
N - amino	5	16.1221	28.8891	0	28.8891	166.725	0	166.725	0	11.0947
H - amino	6	2.75022	32.2605	0	32.2605	91.2594	0	91.2594	0	8.11384
H - amino	7	6.09525	61.7957	0	61.7957	57.4	0	57.4	0	6.41416
C	8	6.51004	7.37512	-1.95856	7.19761	19.7674	1.25873	21.0261	0.056281	3.82562
N - nitro	9	3.47109	8.95675	-6.68549	3.29484	47.8355	31.6784	79.5139	0.239678	8.01589
O - nitro	10	20.284	2.40538	-28.2391	-27.9043	1.98928	76.3575	78.3468	0.024746	7.15055
O - nitro	11	19.6603	8.79134	-17.8114	-14.0761	39.954	80.5065	120.46	0.221667	10.2213
N - nitro	12	3.85552	4.92162	-6.26667	0.262307	9.40933	30.5995	40.0089	0.179871	5.44045
O - nitro	13	20.2358	0	-29.8924	-29.8924	0	76.659	76.659	0	6.85426
O - nitro	14	19.7749	6.76728	-19.3647	-15.4971	20.2761	99.8412	120.117	0.140308	11.0002

See figure A-1 for corresponding atom with atom number.

Table A-24. HMX atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.32378	32.9396	0	32.9396	42.3347	0	42.3347	0	5.67239
C	2	1.68924	31.375	0	31.375	56.3109	0	56.3109	0	5.98769
H	3	7.23016	36.301	0	36.301	31.8585	0	31.8585	0	4.69644
H	4	6.20035	28.6321	0	28.6321	57.5048	0	57.5048	0	6.26876
H	5	7.17732	26.3862	0	26.3862	31.779	0	31.779	0	4.66971
H	6	7.43274	34.2036	0	34.2036	60.1529	0	60.1529	0	6.30829
N - nitro	7	2.47588	13.6839	-5.48779	11.6	38.4777	41.0258	79.5035	0.249743	6.95399
N - nitramine	8	3.42078	13.9465	0	13.9465	30.0235	0	30.0235	0	4.38806
N - nitramine	9	2.4773	34.7031	0	34.7031	5.21498	0	5.21498	0	1.74933
N - nitro	10	2.67259	30.5082	0	30.5082	66.8445	0	66.8445	0	6.11844
O - nitro	11	19.8968	6.34705	-15.2245	-12.3673	18.2126	42.2818	60.4944	0.210424	7.76686
O - nitro	12	20.6396	7.87548	-12.785	-8.33169	33.3012	42.2978	75.5991	0.24646	8.61734
O - nitro	13	19.6786	10.6746	-8.52532	-1.73949	72.7283	20.7333	93.4616	0.172626	8.8574
O - nitro	14	18.0417	12.8337	-11.3619	-4.23806	86.8448	21.4345	108.279	0.158769	10.3834
N - nitramine	15	2.50557	34.7865	0	34.7865	6.117	0	6.117	0	1.86087
C	16	1.80091	31.0186	0	31.0186	63.0525	0	63.0525	0	6.27941
C	17	2.2641	32.8523	0	32.8523	39.2206	0	39.2206	0	5.48407
N - nitro	18	2.72376	29.732	-5.62771	29.2386	73.6629	13.4542	87.117	0.130587	6.94655
H	19	7.21179	26.2123	0	26.2123	32.0671	0	32.0671	0	4.68468
H	20	7.3143	34.4228	0	34.4228	57.3321	0	57.3321	0	6.1887
N - nitramine	21	3.3951	14.1042	0	14.1042	33.5806	0	33.5806	0	4.45188
H	22	7.20933	36.2405	0	36.2405	32.6328	0	32.6328	0	4.7399
H	23	6.23671	28.501	0	28.501	61.686	0	61.686	0	6.46267
O - nitro	24	19.5455	10.7298	-8.47375	-1.78897	69.9026	21.2344	91.137	0.178708	8.81324
O - nitro	25	17.9535	12.8438	-11.4646	-4.16466	84.6658	20.9376	105.603	0.158957	10.5105
N - nitro	26	2.45382	13.8635	-4.27457	11.7296	39.704	14.3493	54.0533	0.194994	7.02356
O - nitro	27	19.9742	6.27312	-15.1857	-12.3664	17.409	42.2366	59.6457	0.206684	7.73456
O - nitro	28	20.6361	8.00391	-12.7482	-8.28873	33.968	42.3523	76.3203	0.246983	8.62628

See figure A-2 for corresponding atom with atom number.

Table A-25. PETN atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.98498	27.2614	0	27.2614	39.0122	0	39.0122	0	5.31148
O - nitro	3	20.7969	9.82047	-5.87918	1.25188	57.8905	11.2379	69.1284	0.136138	7.84523
O - nitro	4	23.7897	7.61016	-8.79763	-5.10744	30.6086	13.348	43.9566	0.211452	6.40697
O - nitrate	5	9.12924	13.8441	-0.75443	13.3931	81.9553	0.319364	82.2747	0.003867	7.76081
N - nitro	6	3.81821	25.1703	-4.2655	24.9608	33.0924	2.76419	35.8566	0.071147	4.76954
H	7	6.22246	27.0051	0	27.0051	24.868	0	24.868	0	3.9055
H	8	7.46007	26.9447	0	26.9447	19.3518	0	19.3518	0	3.48226
C	9	1.00424	26.3043	0	26.3043	45.9641	0	45.9641	0	5.87659
C	10	0.97041	26.5093	0	26.5093	46.5366	0	46.5366	0	5.98998
C	11	0.995112	25.9561	0	25.9561	44.2797	0	44.2797	0	5.75957
O - nitro	12	20.7713	9.91383	-5.89094	1.2434	58.0319	11.2877	69.3196	0.13632	7.88422
O - nitro	13	20.8477	9.9266	-5.85202	1.26138	58.9203	11.2162	70.1365	0.134345	7.86645
O - nitro	14	20.7995	9.88191	-5.84395	1.1934	56.8972	11.3373	68.2345	0.138546	7.82368
O - nitro	15	23.7489	7.73437	-8.78874	-5.09707	30.805	13.391	44.1961	0.211188	6.42709
O - nitro	16	23.7985	7.65717	-8.7795	-5.09238	30.7273	13.3349	44.0622	0.211048	6.41367
O - nitro	17	23.7923	7.64164	-8.77393	-5.12487	30.1138	13.2464	43.3602	0.212169	6.37294
O - nitrate	18	9.20857	14.0479	-0.81639	13.6436	85.4572	0.248067	85.7052	0.002886	7.90254
O - nitrate	19	9.09263	13.8108	-0.86446	13.3813	81.154	0.340888	81.4949	0.004165	7.72557
O - nitrate	20	9.15262	13.9977	-0.64532	13.5726	83.3662	0.177801	83.544	0.002124	7.82604
N - nitro	21	3.77447	24.8643	-3.60755	24.2498	35.4601	5.13754	40.5976	0.110533	5.24894
N - nitro	22	3.69611	25.1843	-0.59049	25.0902	34.4945	0	34.4945	0	4.69927
N - nitro	23	3.74262	25.1094	-1.4075	24.918	33.932	1.08115	35.0132	0.029925	4.75577
H	24	6.26835	27.0908	0	27.0908	24.1731	0	24.1731	0	3.87341
H	25	6.32996	27.0429	0	27.0429	25.1021	0	25.1021	0	3.9356
H	26	6.33318	27.0259	0	27.0259	25.2538	0	25.2538	0	3.94088
H	27	7.44717	27.0028	0	27.0028	18.4636	0	18.4636	0	3.40629
H	28	7.58651	27.0413	0	27.0413	19.1957	0	19.1957	0	3.46423
H	29	7.5277	27.0135	0	27.0135	19.4553	0	19.4553	0	3.48973

See figure A-3 for corresponding atom with atom number.

Table A-26. EDNA atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.66498	29.8808	0	29.8808	52.0243	0	52.0243	0	5.48071
H	2	8.55133	31.0158	0	31.0158	34.1582	0	34.1582	0	4.50343
H	3	7.29847	25.7438	0	25.7438	32.3728	0	32.3728	0	4.21023
H	4	5.51812	47.1206	0	47.1206	56.7021	0	56.7021	0	6.30145
N - nitramine	5	9.26989	27.1562	0	27.1562	96.0199	0	96.0199	0	7.78915
N - nitro	6	3.4129	15.4123	-6.00679	13.6823	39.4889	28.3933	67.8822	0.243321	6.47979
O - nitro	7	23.9818	8.70761	-18.5521	-14.5775	41.2455	57.4582	98.7037	0.243255	9.68082
O - nitro	8	20.967	7.69445	-15.8978	-12.0838	30.7381	61.1052	91.8433	0.222669	9.25956
C	9	2.65933	29.7197	0	29.7197	46.2751	0	46.2751	0	4.98736
H	10	8.42198	31.1388	0	31.1388	35.0928	0	35.0928	0	4.5452
H	11	7.2376	25.705	0	25.705	33.1421	0	33.1421	0	4.23349
N - nitramine	12	9.31576	27.042	0	27.042	92.7882	0	92.7882	0	7.68445
H	13	5.51735	47.2521	0	47.2521	58.5244	0	58.5244	0	6.36531
N - nitro	14	3.3894	15.3754	-6.93824	13.7816	39.2671	20.5004	59.7675	0.225352	6.32214
O - nitro	15	24.005	8.53501	-18.4426	-14.7644	35.5081	58.852	94.36	0.234699	9.49682
O - nitro	16	20.8882	7.16016	-15.8852	-11.9515	27.6803	60.492	88.1723	0.215379	9.26402

See figure A-4 for corresponding atom with atom number.

Table A-27. NQ atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.0701	3.62965	-25.1664	-23.9208	8.30086	138.342	146.643	0.053402	10.7184
O - nitro	2	23.5677	0	-38.1198	-38.1198	0	44.4451	44.4451	0	5.10675
N - amino	3	16.7578	23.0396	0	23.0396	171.87	0	171.87	0	11.1662
N - amino	4	16.7284	19.8127	-0.7574	19.689	156.849	0.41841	157.267	0.002653	10.8521
N - nitramine	5	15.5379	2.8921	-19.9662	-17.8595	4.12753	143.649	147.777	0.027151	11.286
N - nitro	6	3.68565	1.83094	-10.1249	-9.43008	2.07433	43.005	45.0793	0.043898	5.37516
C	7	2.92972	9.51012	-0.26063	9.42103	30.8236	0.016526	30.8401	0.000536	4.07268
H - amino	8	5.52053	37.4787	0	37.4787	95.1277	0	95.1277	0	8.11743
H - amino	9	6.93801	57.3544	0	57.3544	62.6142	0	62.6142	0	6.67559
H - amino	10	6.61878	55.8479	0	55.8479	76.7114	0	76.7114	0	7.48182
H - amino	11	2.8048	21.9722	-0.25477	21.9083	79.1986	0	79.1986	0	7.65004

See figure A-5 for corresponding atom with atom number.

Table A-28. RDX atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.53959	27.2625	0	27.2625	15.2111	0	15.2111	0	2.44265
C	2	2.83725	28.0702	0	28.0702	10.3211	0	10.3211	0	2.06529
C	3	2.42195	28.5012	0	28.5012	13.4568	0	13.4568	0	2.24038
H	4	9.25737	37.4668	0	37.4668	29.1323	0	29.1323	0	4.6568
H	5	4.88613	20.0752	-3.11144	19.5482	45.6906	3.48219	49.1728	0.065801	6.10532
H	6	5.57739	23.9852	-3.75627	23.9317	35.7891	0	35.7891	0	4.74241
H	7	9.23668	37.9175	0	37.9175	25.2541	0	25.2541	0	4.32947
H	8	9.47473	37.2202	0	37.2202	24.1677	0	24.1677	0	4.19172
H	9	4.9411	21.2962	-3.98415	20.8922	47.8236	3.99623	51.8199	0.071171	6.02265
N - nitramine	10	4.0675	21.4195	0	21.4195	121.702	0	121.702	0	10.0962
N - nitramine	11	5.95797	17.2771	0	17.2771	32.9523	0	32.9523	0	4.5742
N - nitramine	12	5.96246	17.7296	0	17.7296	31.9733	0	31.9733	0	4.47812
N - nitro	13	3.44368	17.6866	-4.42752	16.989	85.2519	18.1479	103.4	0.144707	8.50709
N - nitro	14	2.93678	18.5056	-6.54419	17.961	43.5742	20.06	63.6342	0.215864	5.27948
N - nitro	15	3.06776	19.0287	-8.92413	18.0479	41.2784	37.9347	79.2131	0.249555	5.4946
O - nitro	16	21.184	8.85585	-15.1623	-11.2925	47.8236	42.4391	90.2627	0.24911	8.73464
O - nitro	17	21.2511	8.04063	-15.4193	-12.1766	41.3431	46.9883	88.3314	0.248979	8.42691
O - nitro	18	19.0274	6.89398	-15.1157	-11.7346	20.9361	37.0573	57.9934	0.230681	8.04743
O - nitro	19	20.5345	7.92652	-13.6522	-9.61405	28.7972	37.8151	66.6123	0.245418	8.44828
O - nitro	20	18.8193	8.36393	-14.6475	-10.7323	32.1419	36.5059	68.6478	0.24899	8.54242
O - nitro	21	20.7314	7.33652	-13.2407	-9.07289	27.3257	33.8626	61.1883	0.247147	8.249

See figure A-6 for corresponding atom with atom number.

Table A-29. CL20 atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.5319	10.2206	-8.31426	-1.5086	55.744	19.2765	75.0206	0.190927	8.67667
O - nitro	2	18.7943	10.2591	-9.18677	-3.36263	50.1626	16.3824	66.545	0.185578	8.42224
O - nitro	3	19.7271	9.81497	-7.43389	-0.29083	51.7247	17.4294	69.1541	0.188515	8.37207
O - nitro	4	17.4561	10.1094	-8.29335	-2.0403	57.1663	14.6649	71.8311	0.162477	8.33639
O - nitro	5	19.8358	10.9456	-7.149	-0.04592	73.6152	14.4485	88.0637	0.13715	8.62957
O - nitro	6	19.4284	11.404	-8.67011	-2.79832	92.5018	14.4956	106.997	0.117123	8.50265
O - nitro	7	20.0506	12.7494	-8.35434	-1.45661	114.256	13.0993	127.356	0.092277	9.3257
O - nitro	8	20.5185	9.21445	-7.44262	-2.1738	68.0938	14.3312	82.4249	0.143639	7.3606
O - nitro	9	21.3778	11.8286	-6.84431	1.64831	86.1221	13.6477	99.7697	0.11808	9.34955
O - nitro	10	19.8787	12.1198	-8.04452	-1.15113	97.5971	13.8232	111.42	0.108672	9.10867
O - nitro	11	20.3231	7.83598	-7.1795	-3.21156	44.8706	12.182	57.0526	0.16793	6.20112
O - nitro	12	21.3206	12.1982	-5.9359	2.17002	102.613	10.5446	113.158	0.084501	9.11367
N - nitramine	13	4.99373	25.1372	0	25.1372	24.8809	0	24.8809	0	4.08455
N - nitramine	14	5.33875	25.0069	0	25.0069	27.1574	0	27.1574	0	4.28213
N - nitramine	15	3.27032	34.1423	0	34.1423	23.1335	0	23.1335	0	4.10311
N - nitramine	16	1.06839	28.9656	0	28.9656	227.418	0	227.418	0	12.2782
N - nitramine	17	2.02035	34.7275	0	34.7275	40.6408	0	40.6408	0	5.17035
N - nitramine	18	1.57985	27.8597	0	27.8597	121.122	0	121.122	0	6.99323
N - nitro	19	2.1177	23.224	-7.98673	22.5783	33.6834	15.2219	48.9053	0.214375	5.14158
N - nitro	20	2.03608	24.8461	-7.33266	24.1414	23.4627	4.29541	27.7581	0.130798	4.58238
N - nitro	21	2.03014	26.0027	-3.56279	25.3151	107.762	0.5175	108.279	0.004756	9.25474
N - nitro	22	3.15932	29.9185	0	29.9185	178.253	0	178.253	0	11.7285
N - nitro	23	3.27506	27.6097	0	27.6097	76.866	0	76.866	0	7.30653
N - nitro	24	3.24451	30.7986	-5.14181	30.5955	169.431	0	169.431	0	11.2634
C	25	1.06216	47.4265	0	47.4265	27.5052	0	27.5052	0	4.01977
C	26	1.27737	46.1921	0	46.1921	28.3985	0	28.3985	0	4.47209
C	27	0.614418	34.0273	0	34.0273	9.82036	0	9.82036	0	2.34031
C	28	0.412063	32.8407	0	32.8407	30.4457	0	30.4457	0	4.67092

See figure A-7 for corresponding atom with atom number.

Figure A-29. CL20 atom specific Politzer parameters using PBE/6-31G* (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	29	1.08571	48.2409	0	48.2409	59.1224	0	59.1224	0	5.53348
C	30	1.13166	50.9629	0	50.9629	29.0574	0	29.0574	0	3.62733
H	31	5.55672	40.8221	0	40.8221	73.8145	0	73.8145	0	6.90219
H	32	6.00719	41.8528	0	41.8528	51.3471	0	51.3471	0	5.75115
H	33	6.19856	34.7813	0	34.7813	11.9505	0	11.9505	0	2.71413
H	34	3.58745	28.621	0	28.621	45.0575	0	45.0575	0	5.47164
H	35	3.83755	37.4341	0	37.4341	99.1044	0	99.1044	0	8.18828
H	36	4.18348	40.6241	0	40.6241	77.7105	0	77.7105	0	6.97571

See figure A-7 for corresponding atom with atom number.

Table A-30. HNB atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.20308	37.9932	0	37.9932	14.4475	0	14.4475	0	2.89884
C	2	4.2641	38.0007	0	38.0007	13.0911	0	13.0911	0	2.76171
C	3	4.21499	37.8754	0	37.8754	13.0168	0	13.0168	0	2.79629
N - nitro	4	0.852592	19.253	0	19.253	61.0278	0	61.0278	0	6.44004
N - nitro	5	0.953352	20.8153	0	20.8153	47.2892	0	47.2892	0	5.77141
N - nitro	6	0.855616	20.3138	-1.53363	19.9777	74.0514	0	74.0514	0	8.05058
O - nitro	7	20.2032	9.50921	-5.48986	-0.03277	58.3704	10.3533	68.7237	0.127955	6.94333
O - nitro	8	19.6342	9.29052	-3.46942	5.18678	64.1561	4.17975	68.3358	0.057424	7.04814
O - nitro	9	19.9569	8.12117	-3.65538	3.19987	52.5696	6.11334	58.683	0.093323	6.39528
O - nitro	10	19.9684	8.78204	-3.7102	4.05736	60.9315	5.64263	66.5741	0.077573	6.86233
O - nitro	11	19.7275	8.3616	-4.83178	1.68832	55.6357	9.54992	65.1856	0.12504	6.75673
O - nitro	12	20.3607	9.61343	-5.68481	-0.28481	62.7369	10.9507	73.6876	0.126525	6.99112
C	13	4.09897	38.0866	0	38.0866	13.2728	0	13.2728	0	2.79296
C	14	4.16621	37.9054	0	37.9054	13.6941	0	13.6941	0	2.82269
C	15	4.37588	37.8793	0	37.8793	13.548	0	13.548	0	2.78982
N - nitro	16	0.890557	19.3294	0	19.3294	69.1093	0	69.1093	0	7.05897
N - nitro	17	0.931045	19.3904	0	19.3904	70.2813	0	70.2813	0	7.41434
N - nitro	18	0.9124	19.6307	-0.47879	19.3306	57.0005	0	57.0005	0	6.13972
O - nitro	19	20.166	9.41965	-5.48894	-0.08576	60.4157	10.2576	70.6733	0.124075	6.89018
O - nitro	20	19.57	9.16254	-3.4852	5.04488	63.6192	4.10709	67.7263	0.056965	6.98643
O - nitro	21	19.6888	8.50065	-4.87776	1.85498	58.6099	9.53216	68.142	0.120318	6.87958
O - nitro	22	20.3099	9.51339	-5.7452	-0.32984	63.7261	10.8143	74.5404	0.124032	6.99059
O - nitro	23	20.122	8.27876	-3.65232	3.35377	54.5066	6.13544	60.642	0.090938	6.50656
O - nitro	24	19.888	8.63678	-3.70058	3.91402	58.1643	5.66839	63.8327	0.080915	6.76157

See figure A-8 for corresponding atom with atom number.

Table A-31. TATB atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.70507	17.2558	0	17.2558	5.8177	0	5.8177	0	1.8864
C	2	3.98949	17.6704	0	17.6704	2.22082	0	2.22082	0	1.13511
C	3	6.62977	15.7088	0	15.7088	3.41257	0	3.41257	0	1.42842
C	4	3.9925	17.0148	0	17.0148	1.17416	0	1.17416	0	0.794421
C	5	6.67657	16.8173	0	16.8173	2.64014	0	2.64014	0	1.34507
C	6	3.93386	17.979	0	17.979	4.4425	0	4.4425	0	1.7664
H - amino	7	2.27351	25.7881	0	25.7881	37.3557	0	37.3557	0	5.19582
H - amino	8	2.42832	26.4584	0	26.4584	44.1346	0	44.1346	0	5.49631
H - amino	9	2.29888	25.9268	0	25.9268	51.8965	0	51.8965	0	6.10404
H - amino	10	3.22938	30.6409	0	30.6409	45.7983	0	45.7983	0	5.63583
H - amino	11	2.35678	26.2226	0	26.2226	41.5626	0	41.5626	0	5.48257
H - amino	12	2.80143	29.386	0	29.386	35.2822	0	35.2822	0	4.74307
N - nitro	13	4.04981	16.254	-2.56425	15.9465	22.4749	2.80166	25.2766	0.098555	3.93298
N - amino	14	14.8736	17.6893	0	17.6893	71.7466	0	71.7466	0	6.82239
N - nitro	15	4.12682	14.2283	-3.74767	13.4112	17.6937	16.6989	34.3927	0.249791	4.16903
N - amino	16	14.5447	16.8763	0	16.8763	65.0261	0	65.0261	0	6.43608
N - nitro	17	4.13404	15.7228	-4.01125	15.159	17.6164	14.1364	31.7528	0.246997	3.90971
N - amino	18	15.0187	17.5651	0	17.5651	85.9575	0	85.9575	0	7.6947
O - nitro	19	18.8993	8.52764	-13.1282	-7.56214	39.9106	52.1018	92.0124	0.245611	9.694
O - nitro	20	19.2253	7.77351	-13.4331	-7.99071	25.7044	52.6257	78.3302	0.220469	9.60701
O - nitro	21	19.2019	7.13852	-14.9803	-10.2433	26.5452	65.2934	91.8385	0.205497	9.85688
O - nitro	22	19.5109	6.59054	-15.0728	-10.676	19.0339	61.6277	80.6616	0.180289	9.53736
O - nitro	23	18.6855	8.48714	-13.2766	-6.63864	31.2676	51.7448	83.0124	0.234788	10.2132
O - nitro	24	19.2737	7.32553	-13.8122	-8.34993	24.0126	56.2438	80.2564	0.209679	9.7487

See figure A-9 for corresponding atom with atom number.

Table A-32. PNA atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.16643	34.0978	0	34.0978	5.54824	0	5.54824	0	1.55146
C	2	5.40905	29.9977	0	29.9977	18.2358	0	18.2358	0	3.31175
C	3	3.66538	25.284	0	25.284	15.9665	0	15.9665	0	3.13313
C	4	4.88956	24.8946	0	24.8946	9.05398	0	9.05398	0	2.1821
N - amino	5	15.5799	34.9093	0	34.9093	61.2951	0	61.2951	0	6.55824
H - amino	6	2.82395	46.5276	0	46.5276	36.5107	0	36.5107	0	5.05024
N - nitro	7	3.10462	30.4519	-4.36998	30.2985	97.1171	0	97.1171	0	8.61779
N - nitro	8	0.312076	9.35101	-2.82348	4.92392	64.2865	11.5576	75.8442	0.129165	7.85195
N - nitro	9	2.21634	16.205	-1.18085	15.6136	31.872	0.245826	32.1178	0.007595	5.1402
O - nitro	10	20.1917	13.2877	-5.11981	7.31279	99.5582	8.60365	108.162	0.073217	9.86558
O - nitro	11	18.4363	10.6271	-6.95828	-1.72097	66.2074	10.6962	76.9036	0.119741	7.44315
O - nitro	12	20.4184	7.85922	-9.1353	-6.48881	31.3931	19.5324	50.9255	0.236439	5.78688
O - nitro	13	19.5594	7.66604	-9.53527	-7.13868	31.4805	18.1344	49.6149	0.231911	5.50032
O - nitro	14	18.8281	7.9942	-10.1894	-6.82726	32.9856	18.7083	51.6939	0.23093	6.54452
C	15	5.35479	30.0958	0	30.0958	17.4265	0	17.4265	0	3.23972
C	16	3.75574	25.0458	0	25.0458	16.0283	0	16.0283	0	3.19259
H - amino	17	2.83612	46.2024	0	46.2024	41.2913	0	41.2913	0	5.28033
N - nitro	18	3.03785	30.7369	-0.02134	30.5945	89.6995	0	89.6995	0	8.31387
N - nitro	19	0.256429	6.90286	-3.25677	2.71948	46.5138	8.09631	54.6101	0.126277	5.73543
O - nitro	20	20.0688	13.0419	-5.20031	7.18157	96.9811	8.41492	105.396	0.073466	9.7469
O - nitro	21	18.5559	10.7118	-6.95326	-1.60781	66.7905	10.5225	77.313	0.117579	7.52424
O - nitro	22	20.3875	7.66057	-9.0935	-6.41521	31.4166	19.6681	51.0847	0.236777	5.79822
O - nitro	23	19.541	7.3841	-9.57584	-7.34295	29.7413	17.9349	47.6762	0.234669	5.34069
O - nitro	24	18.775	7.69375	-10.2403	-6.86988	31.9787	18.2208	50.1995	0.231222	6.50113

See figure A-10 for corresponding atom with atom number.

Table A-33. TNT atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.7548	7.32329	-9.12761	-4.71273	32.1411	23.6424	55.7835	0.244197	7.12649
O - nitro	2	22.167	8.98422	-9.8493	-4.36677	41.7396	22.706	64.4456	0.228193	8.21797
O - nitro	3	22.2154	8.12632	-11.1484	-6.53698	31.2872	30.2948	61.5821	0.249935	8.11088
O - nitro	4	22.2134	8.45921	-10.9685	-6.4272	40.2621	27.3843	67.6464	0.24094	7.9535
O - nitro	5	22.6341	9.0398	-9.46628	-4.29325	47.5097	18.4684	65.9781	0.201564	7.88484
O - nitro	6	20.8542	7.16947	-8.91396	-4.72637	32.8475	18.0642	50.9117	0.228921	6.78397
N - nitro	7	3.33468	25.0221	-9.43617	24.6143	31.0161	30.6287	61.6448	0.24999	4.82045
N - nitro	8	3.87041	22.8505	-9.37386	22.0368	29.7848	31.0081	60.7929	0.249899	5.15423
N - nitro	9	2.19509	25.4611	-3.44168	24.6026	43.9711	4.27712	48.2482	0.08079	6.03449
C	10	5.32651	20.484	0	20.484	13.4583	0	13.4583	0	2.81463
C	11	7.31312	18.8786	0	18.8786	17.541	0	17.541	0	3.19629
C	12	5.38221	20.12	0	20.12	12.3361	0	12.3361	0	2.66494
C	13	7.15169	18.7475	0	18.7475	47.4577	0	47.4577	0	6.08
C	14	4.71821	18.7188	0	18.7188	17.2749	0	17.2749	0	3.14878
C	15	4.78661	20.8018	0	20.8018	18.8524	0	18.8524	0	3.72116
C	16	4.29799	19.325	0	19.325	32.8716	0	32.8716	0	4.51252
H	17	6.90587	22.0866	0	22.0866	18.1696	0	18.1696	0	3.40891
H	18	7.46801	26.9478	0	26.9478	41.9144	0	41.9144	0	5.42944
H	19	8.00253	22.7224	0	22.7224	15.5656	0	15.5656	0	2.94192
H	20	9.27976	16.2248	0	16.2248	12.1735	0	12.1735	0	2.78405
H	21	7.72638	22.0317	0	22.0317	22.041	0	22.041	0	3.63143

See figure A-11 for corresponding atom with atom number.

A.7 PBE/6-31G** Training Set Data

Table A-34. FOX-7 atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	3.08797	22.008	0	22.008	20.5216	0	20.5216	0	3.46114	42.3738	8.99786
N - amino	2	16.2059	30.3942	0	30.3942	133.994	0	133.994	0	9.748	68.5378	7.70456
H - amino	3	6.1334	60.5534	0	60.5534	57.561	0	57.561	0	6.32836	76.3397	44.2463
H - amino	4	3.277	35.4167	0	35.4167	91.608	0	91.608	0	8.03735	49.9479	7.24271
N - amino	5	16.283	30.4986	0	30.4986	140.31	0	140.31	0	10.1316	74.235	11.1057
H - amino	6	2.80176	33.0238	0	33.0238	86.1614	0	86.1614	0	7.89305	47.2182	10.1914
H - amino	7	6.30246	61.1717	0	61.1717	61.283	0	61.283	0	6.64417	76.4325	43.9062
C	8	6.12987	11.7374	-0.83145	11.695	19.2819	0.001821	19.2837	9.44E-05	3.67304	25.0182	-0.87412
N - nitro	9	3.07369	11.1252	-5.59186	7.45558	56.1164	18.9305	75.0469	0.18862	8.03335	25.1223	-21.2682
O - nitro	10	21.4247	3.77453	-26.8886	-26.1575	6.25407	70.6508	76.9049	0.074709	7.37478	8.70795	-40.5603
O - nitro	11	20.7531	8.23248	-17.0716	-12.7531	42.3736	79.0623	121.436	0.22718	10.4398	26.0247	-33.1413
N - nitro	12	3.75617	7.7469	-5.67165	4.31	14.5931	37.2555	51.8486	0.202238	5.66295	15.7837	-30.8277
O - nitro	13	21.3102	1.34802	-28.5457	-28.2734	0.87663	73.781	74.6577	0.011604	7.07476	2.77924	-40.5804
O - nitro	14	20.8875	7.36666	-18.7742	-14.0092	26.4756	95.8663	122.342	0.169575	11.3606	23.3528	-36.6955
NH ₂	2,3,4	25.6163	38.4242	0	38.4242	271.627	0	271.627	0	14.1388	76.3397	7.24271
NH ₂	5,6,7	25.3872	38.3024	0	38.3024	284.911	0	284.911	0	14.3992	76.4325	10.1914
NO ₂	9,10,11	45.2515	8.86879	-22.1769	-17.8831	48.2928	101.47	149.762	0.218481	11.9616	26.0247	-40.5603
NO ₂	12,13,14	45.9538	7.34251	-23.741	-19.2224	22.1136	113.434	135.547	0.136527	12.6047	23.3528	-40.5804

See figure A-1 for corresponding atom with atom number.

Table A-35. HMX atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	2.14135	36.0932	0	36.0932	42.9376	0	42.9376	0	5.78655	46.7331	20.9055
C	2	1.54093	34.4694	0	34.4694	70.2873	0	70.2873	0	7.09932	46.6472	13.7908
H	3	7.22805	39.135	0	39.135	30.5413	0	30.5413	0	4.61492	50.6488	23.0472
H	4	6.33796	30.6232	0	30.6232	57.9359	0	57.9359	0	6.18785	41.8003	2.87023
H	5	7.38939	28.5004	0	28.5004	35.4065	0	35.4065	0	4.87987	39.3492	13.0905
H	6	7.33524	37.0103	0	37.0103	59.2474	0	59.2474	0	6.2791	50.315	13.8297
N - nitro	7	2.21659	15.7379	-6.02867	13.5612	57.11	30.9556	88.0657	0.22795	8.2461	27.6437	-22.8715
N - nitramine	8	3.14997	17.5937	0	17.5937	22.0054	0	22.0054	0	3.7856	31.4677	7.69201
N - nitramine	9	2.42791	39.2054	0	39.2054	5.06851	0	5.06851	0	1.74413	45.5792	34.0713
N - nitro	10	2.57662	33.4521	-7.28288	33.2514	82.947	0	82.947	0	7.08802	50.7881	-7.28288
O - nitro	11	20.9855	7.4357	-14.8135	-11.3497	25.0881	43.6304	68.7185	0.231798	8.31836	20.7003	-25.0972
O - nitro	12	21.5677	8.48482	-12.5735	-7.3948	38.3295	44.1804	82.5099	0.248743	9.12344	26.9107	-23.6922
O - nitro	13	20.3989	11.2476	-8.17127	-0.36988	78.8697	21.562	100.432	0.1686	9.34127	39.7684	-15.93
O - nitro	14	18.4988	13.304	-10.9337	-3.13531	100.284	19.2276	119.512	0.135001	10.742	43.9426	-17.0714
N - nitramine	15	2.42139	39.2213	0	39.2213	5.8864	0	5.8864	0	1.84149	49.8726	32.5182
C	16	1.65585	34.6088	0	34.6088	68.6761	0	68.6761	0	6.7168	46.3391	11.7564
C	17	2.1612	35.7968	0	35.7968	40.3688	0	40.3688	0	5.59508	46.437	21.7137
N - nitro	18	2.47365	33.5728	-5.18909	32.9795	75.0978	10.3445	85.4423	0.106412	7.18493	50.202	-9.00915
H	19	7.28544	28.5431	0	28.5431	32.2111	0	32.2111	0	4.67558	39.0813	13.8002
H	20	7.32657	37.0022	0	37.0022	60.7724	0	60.7724	0	6.37154	50.1857	13.8234
N - nitramine	21	3.21693	17.9909	0	17.9909	26.4466	0	26.4466	0	4.09356	34.8437	7.36947
H	22	7.23336	39.1342	0	39.1342	31.2866	0	31.2866	0	4.65734	50.6676	23.1074
H	23	6.3629	30.4962	0	30.4962	58.9945	0	58.9945	0	6.31184	41.6509	5.60931
O - nitro	24	20.4432	11.0533	-8.34781	-0.35531	80.0514	20.8827	100.934	0.164089	9.40276	39.737	-15.9682

See figure A-2 for corresponding atom with atom number.

Table A-35. HMX atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
O - nitro	25	18.5249	12.9734	-10.8356	-3.25923	95.7796	19.3909	115.171	0.140019	10.5038	41.2951	-17.0607
N - nitro	26	2.11482	16.5854	-7.94754	14.4116	49.8765	48.5929	98.4694	0.249958	7.92935	25.9582	-22.7604
O - nitro	27	20.9494	7.03266	-14.7753	-11.4072	22.7396	44.0794	66.819	0.224501	8.25022	18.9972	-25.1236
O - nitro	28	21.6134	8.38796	-12.6743	-7.49094	36.6911	43.8487	80.5398	0.248025	9.13127	26.4853	-23.7462
NO ₂	7,11,12	44.7698	9.575	-13.6885	-8.16763	47.3144	45.4481	92.7626	0.249899	9.78659	27.6437	-25.0972
NO ₂	10,13,14	41.4743	15.6002	-9.57029	0.643338	150.193	22.2766	172.47	0.112479	12.1499	50.7881	-17.0714
NO ₂	26,27,28	44.6776	9.49347	-13.7327	-8.27105	46.67	45.2767	91.9467	0.249943	9.75039	26.4853	-25.1236
NO ₂	18,24,25	41.4417	15.2159	-9.63354	0.458257	147.261	21.6661	168.927	0.111807	11.993	50.202	-17.0607

See figure A-2 for corresponding atom with atom number.

Table A-36. PETN atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	Zero surface area for atom										
C	2	0.935798	27.9607	0	27.9607	48.0705	0	48.0705	0	6.04918	38.0848	15.5296
O - nitro	3	21.5986	10.524	-5.6265	2.49339	66.1657	11.2138	77.3794	0.123918	8.29175	34.8858	-11.4878
O - nitro	4	24.9727	8.0761	-8.23221	-4.37486	35.5286	12.3202	47.8488	0.191185	6.43789	22.6443	-14.2388
O - nitrate	5	9.1362	15.894	-0.61609	15.7589	95.158	0.170846	95.3288	0.001789	8.19391	37.1661	-1.20545
N - nitro	6	3.50738	27.5273	-6.31526	27.0106	42.9596	2.17212	45.1318	0.045812	5.69439	37.0802	-8.02961
H	7	6.30875	29.2549	0	29.2549	25.7732	0	25.7732	0	4.0452	38.4607	15.2516
H	8	7.50773	29.4489	0	29.4489	19.0265	0	19.0265	0	3.46493	38.3026	16.6924
C	9	0.926774	28.0531	0	28.0531	48.039	0	48.039	0	6.02624	38.2442	14.9542
C	10	0.807007	27.6554	0	27.6554	45.9282	0	45.9282	0	5.93871	37.9549	15.2817
C	11	0.871611	27.1321	0	27.1321	44.0351	0	44.0351	0	5.75027	37.9643	15.2761
O - nitro	12	21.6509	10.6081	-5.6129	2.48088	67.5373	11.2025	78.7398	0.122031	8.3249	34.9655	-11.4972
O - nitro	13	21.6677	10.4318	-5.63433	2.45389	66.1286	11.0707	77.1992	0.122839	8.2539	34.695	-11.4753
O - nitro	14	21.7146	10.5645	-5.5959	2.5175	66.2589	11.1982	77.4571	0.123672	8.29578	35.0232	-11.4841
O - nitro	15	24.9337	8.10213	-8.25252	-4.3333	36.9322	12.2518	49.184	0.18705	6.48217	23.3044	-14.2489
O - nitro	16	25.083	8.28124	-8.23739	-4.29264	37.1648	12.3961	49.5609	0.187559	6.53245	23.8554	-14.2539
O - nitro	17	25.086	8.26676	-8.25828	-4.26267	37.0678	12.2403	49.3081	0.186618	6.55781	24.1773	-14.2445
O - nitrate	18	9.18371	16.1178	-0.52174	15.8751	95.3812	0.175424	95.5566	0.001832	8.27231	37.185	-1.09375
O - nitrate	19	9.1435	16.1083	-0.40275	15.8129	93.5684	0.188618	93.757	0.002008	8.18621	37.2025	-1.41252
O - nitrate	20	9.11263	16.0865	-0.49354	15.8708	95.0232	0.125283	95.1485	0.001315	8.21947	37.323	-1.27384
N - nitro	21	3.45719	27.2313	-0.67646	27.1231	46.4357	0	46.4357	0	5.50985	37.0469	-0.67646
N - nitro	22	3.36019	27.7519	0	27.7519	40.1681	0	40.1681	0	5.07535	37.0469	4.24447
N - nitro	23	3.34325	27.7852	0	27.7852	40.3189	0	40.3189	0	5.07452	36.8555	2.03627
H	24	6.31214	29.2753	0	29.2753	26.1707	0	26.1707	0	4.0688	38.4632	15.027
H	25	6.30955	29.3464	0	29.3464	25.9799	0	25.9799	0	4.06018	38.4111	15.1581
H	26	6.28832	29.4359	0	29.4359	25.2274	0	25.2274	0	4.01017	38.4375	14.7333
H	27	7.45754	29.3603	0	29.3603	19.6506	0	19.6506	0	3.51512	38.2963	16.7758
H	28	7.6064	29.4328	0	29.4328	19.8264	0	19.8264	0	3.52127	38.2222	16.5142

See figure A-3 for corresponding atom with atom number.

Table A-36. PETN atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
H	29	7.55368	29.4622	0	29.4622	19.78	0	19.78	0	3.5236	38.2668	16.5255
NO ₂	6,3,4	50.0787	13.0004	-7.28985	1.00035	102.661	13.4662	116.127	0.102514	9.83249	37.0802	-14.2388
NO ₂	21,12,15	50.0418	12.9776	-7.28549	1.00342	102.392	13.499	115.891	0.102912	9.82431	37.0469	-14.2489
NO ₂	22,13,16	50.1109	12.9621	-7.29544	0.997982	102.556	13.4812	116.037	0.102682	9.8226	37.0469	-14.2539
NO ₂	23,14,17	50.1438	12.9851	-7.28905	1.02071	101.999	13.502	115.501	0.103234	9.83555	36.8555	-14.2445

See figure A-3 for corresponding atom with atom number.

Table A-37. EDNA atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	2.48194	32.8933	0	32.8933	46.513	0	46.513	0	5.04565	52.8307	24.53
H	2	8.64888	33.4565	0	33.4565	31.7616	0	31.7616	0	4.24019	51.5593	16.0605
H	3	7.4396	28.1865	0	28.1865	30.7556	0	30.7556	0	4.0259	43.8541	11.383
H	4	5.47327	47.3958	0	47.3958	78.7889	0	78.7889	0	7.45673	60.0326	24.5551
N - nitramine	5	9.26452	29.6741	0	29.6741	87.8032	0	87.8032	0	7.38572	56.7476	15.0671
N - nitro	6	3.24695	18.5852	-6.34031	17.1609	54.427	26.8703	81.2973	0.221276	7.13047	32.5539	-17.7271
O - nitro	7	25.5741	8.68621	-17.7399	-13.8111	34.0628	56.0227	90.0855	0.235144	9.52848	23.7424	-29.6919
O - nitro	8	21.9718	8.16434	-15.1057	-10.3477	35.8903	59.5204	95.4107	0.234665	9.73421	28.7964	-28.7556
C	9	2.58009	32.6744	0	32.6744	42.5607	0	42.5607	0	4.798	53.3126	22.7968
H	10	8.58313	33.5076	0	33.5076	33.5853	0	33.5853	0	4.32024	52.0971	16.9082
H	11	7.376	28.1847	0	28.1847	30.6468	0	30.6468	0	4.03009	43.7638	11.6259
N - nitramine	12	9.27298	29.4384	0	29.4384	83.2122	0	83.2122	0	7.18715	56.5901	14.4151
H	13	5.50911	47.3514	0	47.3514	76.3148	0	76.3148	0	7.39386	59.7201	25.2886
N - nitro	14	3.24707	19.1013	-8.53075	17.6815	48.8023	57.8669	106.669	0.248195	6.81213	32.9737	-28.6502
O - nitro	15	25.612	8.49073	-17.8133	-13.8501	35.51	55.2545	90.7646	0.23817	9.51779	23.0528	-29.6291
O - nitro	16	21.9773	8.82802	-15.0128	-10.3635	36.4086	60.8751	97.2837	0.234187	9.78957	27.606	-28.6596
NO ₂	6,7,8	50.7929	10.7788	-16.524	-10.6403	58.1738	59.5778	117.752	0.249964	11.071	32.5539	-29.6919
NO ₂	14,15,16	50.8364	11.221	-16.5242	-10.5827	59.2545	59.9495	119.204	0.249992	11.1777	32.9737	-29.6291

See figure A-4 for corresponding atom with atom number.

Table A-38. NQ atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
O - nitro	1	21.1844	4.43641	-23.8587	-22.0277	12.6489	136.701	149.35	0.07752	11.0749	14.1598	-45.4524
O - nitro	2	25.24	0	-36.485	-36.485	0	47.1409	47.1409	0	5.25152	-10.8942	-45.8804
N - amino	3	17.0768	24.2113	0	24.2113	139.451	0	139.451	0	9.93225	69.71	3.70105
N - amino	4	17.029	21.4318	-0.06087	21.4213	135.884	0	135.884	0	9.96212	67.2772	-0.06087
N - nitramine	5	16.058	3.96662	-18.4039	-14.5523	5.95098	125.95	131.901	0.043081	11.3625	9.42457	-41.0379
N - nitro	6	3.48516	2.36489	-8.91084	-6.46207	3.4866	53.4226	56.9092	0.057512	6.14071	7.71021	-45.4944
C	7	2.6842	13.4224	0	13.4224	27.5813	0	27.5813	0	4.02423	42.7842	2.50314
H - amino	8	5.74513	37.2311	0	37.2311	104.36	0	104.36	0	8.51112	50.5095	11.6867
H - amino	9	7.24657	56.3157	0	56.3157	73.4276	0	73.4276	0	7.2837	72.0889	37.3889
H - amino	10	6.89392	55.0549	0	55.0549	80.5895	0	80.5895	0	7.69509	72.0456	36.5612
H - amino	11	2.79033	23.5225	-0.5246	23.4536	75.8822	0	75.8822	0	7.45408	35.8942	-0.5246
NH ₂	3,8,9	30.0685	34.5727	0	34.5727	292.792	0	292.792	0	14.6476	72.0889	3.70105
NH ₂	4,10,11	26.7133	30.2125	-0.29273	30.1935	326.24	0.053761	326.293	0.000165	15.1644	72.0456	-0.5246
NO ₂	6,1,2	49.9096	3.71515	-29.7264	-28.3166	10.4327	147.049	157.482	0.061858	11.4307	14.1598	-45.8804

See figure A-5 for corresponding atom with atom number.

Table A-39. RDX atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	2.27461	29.6643	0	29.6643	14.4386	0	14.4386	0	2.57936	45.7197	18.5021
C	2	2.5669	30.4793	0	30.4793	6.6386	0	6.6386	0	1.62489	44.2859	19.7201
C	3	2.28378	31.1182	0	31.1182	15.3901	0	15.3901	0	2.47237	47.7095	24.075
H	4	9.40737	40.0886	0	40.0886	31.0491	0	31.0491	0	4.81701	50.3865	28.6289
H	5	4.99156	21.3257	-3.18812	21.0521	43.6713	5.24481	48.9162	0.095724	5.65346	29.828	-6.69741
H	6	5.70241	25.2781	-0.59049	25.2292	32.1796	0	32.1796	0	4.50543	30.7749	-0.59049
H	7	9.47639	40.4572	0	40.4572	25.8174	0	25.8174	0	4.41997	50.3865	31.0937
H	8	9.53207	39.8567	0	39.8567	25.9376	0	25.9376	0	4.37391	50.3514	30.3702
H	9	5.02409	22.5585	-4.35918	22.244	44.1943	3.23871	47.433	0.063618	5.66912	30.8396	-7.44666
N - nitramine	10	3.71152	24.8105	0	24.8105	126.648	0	126.648	0	10.37	46.6585	9.1334
N - nitramine	11	5.98331	20.4243	0	20.4243	31.7065	0	31.7065	0	4.51575	40.2133	12.7071
N - nitramine	12	6.0049	20.9172	0	20.9172	30.2794	0	30.2794	0	4.36589	40.2497	13.1626
N - nitro	13	3.28611	20.8077	-7.81245	19.6036	96.259	45.16	141.419	0.21736	9.23393	37.628	-22.9179
N - nitro	14	2.70134	21.5142	-5.32611	20.4575	53.6833	20.9645	74.6478	0.201971	6.1966	38.733	-15.0088
N - nitro	15	2.86736	21.8525	-9.81845	20.6436	58.5417	31.14	89.6818	0.226661	6.64908	39.1572	-19.5607
O - nitro	16	22.105	9.56327	-14.8029	-10.3985	58.6093	42.8357	101.445	0.243956	9.14383	32.2716	-25.2466
O - nitro	17	22.3086	8.99298	-15.2502	-11.3318	50.279	46.6069	96.8859	0.249641	8.9443	29.4415	-26.0479
O - nitro	18	19.6126	7.47784	-14.6543	-10.8393	24.9104	38.1799	63.0903	0.238941	8.41829	19.5852	-23.3132
O - nitro	19	21.4574	8.65201	-13.4523	-8.90666	33.1959	38.6727	71.8686	0.248548	8.85283	22.8068	-23.1275
O - nitro	20	19.606	9.01461	-14.3285	-10.0004	40.8649	35.7929	76.6577	0.248906	8.82615	29.4547	-22.6794
O - nitro	21	21.4547	8.00302	-12.9931	-8.6153	30.4863	35.0244	65.5107	0.2488	8.44563	21.3529	-22.3557
NO ₂	13,16,17	47.6996	12.7925	-15.0013	-8.66144	95.4092	45.0044	140.414	0.217784	11.005	37.628	-26.0479
NO ₂	14,18,19	43.7713	11.57	-13.9996	-7.88598	70.0472	38.987	109.034	0.229713	10.3965	38.733	-23.3132
NO ₂	16,20,21	63.1657	8.81785	-14.0484	-9.66535	43.2278	38.5954	81.8232	0.249199	8.83619	32.2716	-25.2466

See figure A-6 for corresponding atom with atom number.

Table A-40. CL20 atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
O - nitro	1	19.999	10.8034	-7.71971	-0.40947	65.3237	17.2765	82.6002	0.165411	8.85687	32.6876	-14.7898
O - nitro	2	19.4751	11.1592	-8.36455	-1.532	62.7466	14.1043	76.8509	0.149846	8.92828	30.7028	-14.8607
O - nitro	3	20.2949	10.4693	-6.91985	0.98793	63.0093	15.6026	78.6119	0.159084	8.65402	30.3106	-13.7061
O - nitro	4	17.7463	10.957	-7.33916	-0.61878	67.7498	14.1039	81.8537	0.142616	8.51104	33.9395	-13.792
O - nitro	5	20.6235	11.3607	-6.85003	1.04265	79.1132	13.9966	93.1098	0.127727	8.97913	37.591	-13.1884
O - nitro	6	19.8664	11.5989	-8.20254	-1.77961	93.7935	13.4852	107.279	0.109901	8.75115	39.8167	-14.3687
O - nitro	7	20.6256	13.2843	-7.95437	-0.82176	124.333	12.7074	137.04	0.084129	9.49218	49.0286	-14.0217
O - nitro	8	20.8848	9.1944	-7.20022	-1.62629	75.459	14.8182	90.2772	0.137199	7.43365	44.6711	-14.0732
O - nitro	9	22.1804	12.5499	-6.58331	2.42445	94.3494	14.5534	108.903	0.115778	9.69525	41.5643	-13.2279
O - nitro	10	20.5662	12.656	-7.6171	-0.22698	104.739	14.1792	118.918	0.105018	9.39368	45.7367	-14.0267
O - nitro	11	20.6133	8.63925	-6.91757	-2.64849	55.402	12.2805	67.6825	0.148521	6.4426	39.434	-13.5379
O - nitro	12	22.0776	12.6132	-5.74949	2.90644	113.875	11.1728	125.048	0.081365	9.41515	54.9428	-11.9264
N - nitramine	13	4.92298	30.0113	0	30.0113	22.2851	0	22.2851	0	3.77712	47.1642	23.3716
N - nitramine	14	5.20548	29.8286	0	29.8286	25.0235	0	25.0235	0	3.96885	45.234	22.7485
N - nitramine	15	3.19556	37.6424	0	37.6424	22.6049	0	22.6049	0	4.06214	49.033	31.3447
N - nitramine	16	0.952923	35.8378	0	35.8378	316.703	0	316.703	0	16.2304	65.1367	19.8983
N - nitramine	17	1.85761	38.7529	0	38.7529	34.5708	0	34.5708	0	4.68204	51.8348	24.4986
N - nitramine	18	1.45754	31.6286	0	31.6286	114.667	0	114.667	0	6.56103	64.9598	18.2279
N - nitro	19	1.90076	27.4847	-1.90637	27.2603	35.9051	0	35.9051	0	4.90863	33.7374	-1.90637
N - nitro	20	1.9565	28.0492	-9.7515	27.7562	40.8209	0	40.8209	0	5.08113	34.5777	-9.7515
N - nitro	21	1.83067	29.3506	-3.84695	28.7578	116.494	9.81469	126.309	0.071666	9.17214	41.8248	-6.97979
N - nitro	22	3.00171	33.2733	0	33.2733	198.03	0	198.03	0	12.2331	62.7993	4.35241
N - nitro	23	3.06198	30.3903	-6.76957	30.2199	92.0563	0	92.0563	0	7.91761	45.78	-6.76957
N - nitro	24	3.14219	33.0697	-1.4326	32.6685	200.016	0.137071	200.153	0.000684	11.8305	60.1568	-1.80283

See figure A-7 for corresponding atom with atom number.

Table A-40. CL20 atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	25	0.909746	51.6288	0	51.6288	21.7352	0	21.7352	0	3.4454	55.9594	35.1951
C	26	1.05784	50.2135	0	50.2135	28.6116	0	28.6116	0	4.42946	55.9833	35.421
C	27	0.463521	36.8251	0	36.8251	7.17714	0	7.17714	0	2.11423	42.665	29.9924
C	28	0.306849	33.9623	0	33.9623	49.694	0	49.694	0	6.04231	43.0792	19.8029
C	29	0.982357	51.5906	0	51.5906	62.4761	0	62.4761	0	5.70044	65.4009	32.1134
C	30	0.95363	54.3521	0	54.3521	24.3471	0	24.3471	0	4.24609	65.0445	46.3491
H	31	5.70752	43.4477	0	43.4477	71.4488	0	71.4488	0	6.75141	55.6137	14.4108
H	32	6.26724	44.5449	0	44.5449	50.4175	0	50.4175	0	5.66785	55.1468	21.7099
H	33	6.33996	37.0324	0	37.0324	15.3671	0	15.3671	0	3.13039	42.958	24.7992
H	34	3.58753	30.9149	0	30.9149	43.1	0	43.1	0	5.43777	42.4466	9.89143
H	35	3.83791	39.5928	0	39.5928	85.6273	0	85.6273	0	7.5185	54.5525	7.88152
H	36	4.41248	42.4784	0	42.4784	73.9179	0	73.9179	0	6.79824	57.584	13.295
NO ₂	19,1,2	41.3749	12.969	-8.04861	0.418356	89.7463	15.7573	105.504	0.127047	10.1178	33.7374	-14.8607
NO ₂	20,3,4	39.9977	12.6145	-7.13176	1.61716	92.3232	14.8901	107.213	0.119594	9.81383	34.5777	-13.792
NO ₂	21,5,6	42.3206	13.2374	-7.57393	0.835627	117.045	14.1874	131.233	0.096422	10.0415	41.8248	-14.3687
NO ₂	22,7,8	44.5122	15.1781	-7.57581	1.15204	192.463	13.9091	206.372	0.062856	10.7983	62.7993	-14.0732
NO ₂	23,9,10	45.8086	15.3985	-7.1261	3.27861	139.679	14.6143	154.293	0.085746	11.4386	45.78	-14.0267
NO ₂	24,11,12	45.8331	14.3637	-6.39629	2.19078	170.553	12.1433	182.696	0.062049	10.2002	60.1568	-13.5379

See figure A-7 for corresponding atom with atom number.

Table A-41. HNB atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	3.95538	40.9482	0	40.9482	17.3651	0	17.3651	0	3.26892	51.88	32.2829
C	2	3.9791	40.9292	0	40.9292	15.9188	0	15.9188	0	3.08168	51.8605	31.7664
C	3	3.92559	40.6699	0	40.6699	16.9582	0	16.9582	0	3.26192	51.4539	31.8643
N - nitro	4	0.752494	21.1978	0	21.1978	66.2866	0	66.2866	0	7.26831	37.606	7.76982
N - nitro	5	0.729956	21.7051	-0.9946	21.2847	75.8651	0	75.8651	0	7.36283	36.1885	-0.9946
N - nitro	6	0.634403	21.512	0	21.512	78.0047	0	78.0047	0	7.87978	35.0696	4.86132
O - nitro	7	20.9284	9.21254	-5.00868	0.679806	61.524	9.6373	71.1613	0.117088	6.8455	31.6491	-11.2556
O - nitro	8	19.922	9.5855	-3.11125	6.10955	63.3952	3.07764	66.4728	0.044156	6.93558	36.9245	-6.10002
O - nitro	9	20.7069	8.09384	-3.49873	4.10424	53.9595	5.08564	59.0451	0.078713	6.38189	33.6383	-7.63114
O - nitro	10	20.5049	8.80596	-3.46716	4.8693	58.7769	4.41799	63.1949	0.065023	6.72972	35.0113	-7.25777
O - nitro	11	20.3442	8.30958	-4.50405	2.94804	58.5313	8.02171	66.553	0.106003	6.78621	33.9407	-9.41578
O - nitro	12	21.0643	9.31397	-5.02327	0.753849	67.2383	9.79578	77.0341	0.110992	6.92867	31.8078	-11.3485
C	13	3.84076	40.9301	0	40.9301	15.2453	0	15.2453	0	3.04376	50.9519	31.4721
C	14	3.95961	40.5862	0	40.5862	16.428	0	16.428	0	3.16515	51.479	32.2383
C	15	4.02572	40.7637	0	40.7637	14.9851	0	14.9851	0	2.99898	51.4213	33.3151
N - nitro	16	0.752491	19.9162	0	19.9162	73.7647	0	73.7647	0	7.07593	37.0971	2.59914
N - nitro	17	0.784681	21.3902	-0.49009	21.0063	84.1842	0	84.1842	0	8.46563	35.1832	-0.49009
N - nitro	18	0.696901	21.2413	0	21.2413	65.9308	0	65.9308	0	6.7058	35.4555	0.062123
O - nitro	19	20.9073	9.2521	-4.99974	0.781668	61.5663	9.63928	71.2056	0.117047	6.8991	31.9942	-11.2581
O - nitro	20	20.0764	9.69872	-3.17393	6.23863	66.0746	2.95161	69.0262	0.040932	7.05807	37.0093	-6.11006
O - nitro	21	20.2634	7.99441	-4.49875	2.69187	55.3474	7.99681	63.3442	0.110306	6.5797	33.8799	-9.43963
O - nitro	22	21.0175	9.38901	-4.99519	0.77197	65.6644	9.85248	75.5169	0.113446	6.93952	32.6073	-11.3824
O - nitro	23	20.7228	7.96563	-3.5521	4.1212	52.4815	4.93649	57.418	0.078583	6.32961	33.8209	-7.63679
O - nitro	24	20.4997	8.84213	-3.53462	4.97649	59.5511	4.31401	63.8651	0.062986	6.78674	35.106	-7.25526
NO ₂	4,7,8	41.6029	9.8231	-4.43692	3.64149	67.1163	8.41859	75.5349	0.099031	7.5513	37.606	-11.2556
NO ₂	5,9,10	41.9417	8.80246	-3.48095	4.78806	61.5062	4.76469	66.2709	0.066728	6.80612	36.1885	-7.63114

See figure A-8 for corresponding atom with atom number.

Table A-41. HNB atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
NO ₂	6,11,12	42.043	9.12285	-4.81551	2.12307	67.7538	9.15063	76.9045	0.104829	7.21529	35.0696	-11.3485
NO ₂	16,19,20	41.7362	9.87236	-4.45098	3.74766	68.1599	8.33005	76.4899	0.097044	7.60917	37.0971	-11.2581
NO ₂	17,21,22	42.0656	9.073	-4.79287	2.07697	67.1152	9.17247	76.2877	0.105779	7.166	35.1832	-11.3824
NO ₂	18,23,24	41.9194	8.72303	-3.54366	4.82593	60.4111	4.63608	65.0472	0.066193	6.7883	35.4555	-7.63679

See figure A-8 for corresponding atom with atom number.

Table A-42. TATB atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	6.59266	21.3224	0	21.3224	3.90611	0	3.90611	0	1.53333	28.5548	18.2448
C	2	3.96684	21.6718	0	21.6718	1.40368	0	1.40368	0	0.87937	24.3831	16.9679
C	3	6.51089	19.9717	0	19.9717	2.05542	0	2.05542	0	1.10871	24.5212	17.6104
C	4	4.01896	20.9884	0	20.9884	0.76682	0	0.76682	0	0.662951	23.8498	18.9006
C	5	6.46614	21.0315	0	21.0315	1.50876	0	1.50876	0	1.03385	23.8278	18.8805
C	6	3.94678	22.0345	0	22.0345	2.75828	0	2.75828	0	1.29545	28.4908	17.9756
H - amino	7	2.1783	26.2256	0	26.2256	44.3777	0	44.3777	0	5.62024	35.8258	11.2305
H - amino	8	2.36096	27.2772	0	27.2772	43.2604	0	43.2604	0	5.54908	36.676	9.50049
H - amino	9	2.21339	26.1973	0	26.1973	57.2542	0	57.2542	0	6.34243	37.7045	7.59726
H - amino	10	3.3186	29.883	0	29.883	53.4748	0	53.4748	0	6.15534	39.8763	11.4069
H - amino	11	2.38884	26.6679	0	26.6679	46.4734	0	46.4734	0	5.78265	36.2236	10.1895
H - amino	12	2.95252	29.4378	0	29.4378	36.3629	0	36.3629	0	4.79905	37.2665	7.91227
N - nitro	13	3.8158	19.7625	-3.01727	19.5193	26.8797	1.60459	28.4843	0.053159	4.17612	27.6857	-4.59149
N - amino	14	15.198	19.4526	0	19.4526	59.339	0	59.339	0	6.12553	36.5769	4.19239
N - nitro	15	3.89951	17.6326	-6.61646	16.6901	23.5436	21.9977	45.5413	0.249712	4.81911	23.8134	-15.7423
N - amino	16	14.8215	18.5387	0	18.5387	54.1898	0	54.1898	0	5.80516	37.8533	9.15223
N - nitro	17	3.97942	19.0611	-10.0442	18.4589	22.5195	56.7443	79.2639	0.203391	4.35413	23.7701	-21.5669
N - amino	18	15.0078	19.1986	0	19.1986	70.3699	0	70.3699	0	6.94766	35.9149	3.52221
O - nitro	19	19.8384	9.12057	-12.9141	-6.63648	44.811	51.6453	96.4563	0.248745	10.071	27.7271	-25.9438
O - nitro	20	20.2107	8.49393	-13.355	-7.11247	31.8669	51.9787	83.8456	0.235616	10.0727	22.3983	-25.9889
O - nitro	21	20.1718	7.95741	-14.8111	-9.35114	30.5777	64.7605	95.3382	0.217862	10.2821	22.793	-28.6389
O - nitro	22	20.5098	7.15453	-15.0218	-9.87821	24.0615	61.8075	85.869	0.201693	10.0004	19.4829	-28.6182
O - nitro	23	19.5354	9.04567	-13.0999	-5.78398	37.337	50.4585	87.7955	0.244416	10.54	25.4719	-25.7856
O - nitro	24	20.315	7.97872	-13.6222	-7.582	28.3376	55.2505	83.5881	0.224084	10.034	21.2067	-26.0385
NH ₂	14,7,8	19.7373	21.1918	0	21.1918	65.3708	0	65.3708	0	6.74927	36.676	4.19239
NH ₂	16,9,10	20.3535	21.3444	0	21.3444	75.1474	0	75.1474	0	7.5221	39.8763	7.59726

See figure A-9 for corresponding atom with atom number.

Table A-42. TATB atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
NH ₂	18,11,12	20.3492	21.6831	0	21.6831	79.09	0	79.09	0	7.53796	37.2665	3.52221
NO ₂	13,19,20	43.8649	11.1684	-13.1252	-4.93619	56.2016	51.9242	108.126	0.249609	11.3888	27.7271	-25.9889
NO ₂	15,21,22	44.5811	10.0162	-14.8826	-7.68774	45.2439	63.4139	108.658	0.243009	11.4227	23.8134	-28.6389
NO ₂	17,23,24	43.8298	10.7467	-13.3737	-4.80048	49.4359	53.1486	102.584	0.249673	11.5201	25.4719	-26.0385

See figure A-9 for corresponding atom with atom number.

Table A-43. PNA atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	4.20051	37.9462	0	37.9462	6.7066	0	6.7066	0	1.78211	48.7581	31.944
C	2	5.12238	33.6636	0	33.6636	24.1563	0	24.1563	0	3.73823	49.1465	22.4046
C	3	3.50961	28.2426	0	28.2426	18.0826	0	18.0826	0	3.44544	38.583	20.539
C	4	4.45187	28.0972	0	28.0972	9.23431	0	9.23431	0	2.2338	37.7805	21.0347
N - amino	5	15.8907	36.8819	0	36.8819	53.0936	0	53.0936	0	5.99846	55.1261	26.7903
H - amino	6	2.8217	46.8596	0	46.8596	41.7604	0	41.7604	0	5.37696	55.5202	27.5765
N - nitro	7	2.72641	33.5515	0	33.5515	100.967	0	100.967	0	8.72626	49.6774	7.73782
N - nitro	8	0.267309	6.35636	-3.21614	3.96323	60.74	6.97422	67.7142	0.092387	5.90146	20.7624	-6.28639
N - nitro	9	1.95537	17.4626	-2.64725	17.019	39.1639	0.53618	39.7001	0.013323	5.40061	26.6553	-3.2756
O - nitro	10	21.013	13.7461	-5.17939	8.05044	104.305	8.03042	112.335	0.066376	10.1067	44.188	-9.63478
O - nitro	11	19.198	11.0233	-6.3938	-0.6053	76.2457	10.7984	87.0441	0.108667	7.74331	35.3633	-12.5383
O - nitro	12	21.0327	8.37964	-8.36865	-5.14608	39.7126	18.4507	58.1634	0.216592	6.07518	23.7563	-16.3642
O - nitro	13	20.2562	8.35473	-8.65314	-5.94871	42.0983	17.1099	59.2082	0.20547	5.63114	22.0582	-16.2914
O - nitro	14	19.5135	8.56702	-9.61258	-5.92609	37.9844	17.9843	55.9687	0.218076	6.69464	23.4023	-17.1806
C	15	5.13817	33.6032	0	33.6032	22.1449	0	22.1449	0	3.62062	48.8366	22.9468
C	16	3.53078	28.1585	0	28.1585	18.4809	0	18.4809	0	3.47784	38.6671	20.155
H - amino	17	2.7797	46.9062	0	46.9062	40.0597	0	40.0597	0	5.27426	55.5133	28.6377
N - nitro	18	2.70382	33.2165	-7.69138	33.0099	113.29	0	113.29	0	9.41708	49.8594	-7.69138
N - nitro	19	0.249717	3.86091	-5.25727	2.03727	23.8967	18.9632	42.8599	0.246688	3.84411	15.6112	-11.2575
O - nitro	20	20.9575	13.7619	-5.16445	8.0776	103.643	7.99943	111.643	0.066518	10.0997	44.4365	-9.63666
O - nitro	21	19.1636	11.1172	-6.45142	-0.66073	80.7076	10.5869	91.2945	0.102517	7.77571	34.7791	-12.5257
O - nitro	22	21.0454	8.31403	-8.35668	-5.16848	40.1068	18.4292	58.536	0.215714	6.04413	23.7694	-16.3749
O - nitro	23	20.1707	7.8718	-8.66226	-6.0622	38.8026	16.9764	55.7791	0.211722	5.49722	21.7187	-16.3234
O - nitro	24	19.4793	8.50261	-9.55632	-5.94186	37.8163	18.1729	55.9891	0.219227	6.63848	23.1049	-17.1825
NH ₂	5,6,17	22.2012	36.7238	0	36.7238	70.5315	0	70.5315	0	6.9853	55.5133	20.155
NO ₂	7,10,11	42.9374	15.3238	-5.99381	5.82341	141.606	10.2125	151.818	0.062743	11.4195	49.6774	-12.5383

See figure A-10 for corresponding atom with atom number.

Table A-43. PNA atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
NO ₂	8,12,13	41.5562	8.32228	-8.5019	-5.48663	41.3185	17.8299	59.1484	0.210575	5.90407	23.7563	-16.3642
NO ₂	9,14,24	40.9482	10.2787	-9.57496	-4.84094	50.6741	18.1212	68.7953	0.194024	7.71406	26.6553	-17.1825
NO ₂	18,20,21	42.8249	15.3559	-6.02782	5.8276	142.644	10.0936	152.737	0.061718	11.4649	49.8594	-12.5257
NO ₂	19,22,23	41.4659	8.02192	-8.50397	-5.56248	39.633	17.7477	57.3807	0.213632	5.81636	23.7694	-16.3749

See figure A-10 for corresponding atom with atom number.

Table A-44. TNT atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
O - nitro	1	20.6497	8.0021	-8.88637	-3.68866	40.3496	25.5363	65.8859	0.237363	7.62674	29.6567	-17.869
O - nitro	2	23.1105	9.61224	-9.55405	-3.70137	50.182	24.0969	74.2789	0.219169	8.4943	30.3388	-18.2135
O - nitro	3	23.2778	8.20121	-11.1171	-5.89096	37.9887	29.9922	67.9809	0.246541	8.39705	26.1954	-20.5434
O - nitro	4	23.3462	9.15815	-10.7389	-5.44695	49.5429	27.938	77.4809	0.230562	8.43501	31.4671	-19.9968
O - nitro	5	23.8611	9.69099	-9.03486	-3.29887	55.4851	18.1748	73.6599	0.185859	8.19677	33.723	-16.9967
O - nitro	6	21.9353	8.1356	-8.30397	-3.4458	40.7505	18.6202	59.3707	0.215265	7.20326	26.9886	-16.4018
N - nitro	7	3.2378	27.3409	-4.35856	26.403	48.7617	18.3914	67.1531	0.198867	6.29637	37.0231	-12.5289
N - nitro	8	3.64975	25.2995	-6.87813	24.7914	43.5491	24.9028	68.4519	0.231449	5.58822	35.1487	-13.243
N - nitro	9	1.81759	27.6956	-5.23719	27.3036	57.9341	0	57.9341	0	6.26827	39.7151	-5.23719
C	10	5.16076	23.144	0	23.144	15.5537	0	15.5537	0	2.95778	36.9057	12.5759
C	11	7.25404	21.3024	0	21.3024	19.8733	0	19.8733	0	3.29947	34.1579	10.2234
C	12	5.35326	22.6433	0	22.6433	14.6955	0	14.6955	0	2.84833	35.3256	11.0159
C	13	6.85507	21.2027	0	21.2027	47.4931	0	47.4931	0	6.0079	40.074	8.5699
C	14	4.55454	21.2052	0	21.2052	16.4924	0	16.4924	0	3.02673	36.4263	9.91653
C	15	4.61827	23.5788	0	23.5788	19.0533	0	19.0533	0	3.7045	35.0357	12.9938
C	16	4.00474	22.3744	0	22.3744	31.4834	0	31.4834	0	4.3218	32.6136	6.6334
H	17	6.98488	23.6282	0	23.6282	22.0802	0	22.0802	0	3.81574	32.3054	10.2799
H	18	7.68538	28.9577	0	28.9577	46.8943	0	46.8943	0	5.69416	39.7264	10.1023
H	19	8.23602	24.8738	0	24.8738	16.7975	0	16.7975	0	2.87454	35.3602	9.77911
H	20	9.40421	17.648	0	17.648	13.9463	0	13.9463	0	3.02786	22.5552	5.74171
H	21	7.84559	24.2055	0	24.2055	19.3832	0	19.3832	0	3.26027	32.3174	7.18498
NO ₂	7,1,2	46.9979	12.4864	-9.22398	-1.53545	100.696	24.9417	125.637	0.159111	9.99237	37.0231	-18.2135
NO ₂	8,3,4	50.2738	12.5399	-10.9213	-3.34592	93.1701	29.0257	122.196	0.181112	10.4615	35.1487	-20.5434
NO ₂	9,5,6	47.6141	10.9877	-8.67717	-2.2729	84.0405	18.5207	102.561	0.147972	8.76195	39.7151	-16.9967

See figure A-11 for corresponding atom with atom number.

Table A-45. TNA atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	4.25634	31.8498	0	31.8498	3.06115	0	3.06115	0	1.20822	39.7571	26.4602
C	2	5.5051	28.231	0	28.231	16.1091	0	16.1091	0	2.99152	41.5832	18.5015
C	3	3.46533	22.4699	0	22.4699	14.2613	0	14.2613	0	3.06326	32.3268	15.0169
C	4	5.66523	24.6647	0	24.6647	9.41119	0	9.41119	0	2.56167	32.0789	16.105
C	5	7.03358	25.2924	0	25.2924	6.68766	0	6.68766	0	1.98425	31.8016	13.4664
C	6	6.25382	30.3749	0	30.3749	7.42208	0	7.42208	0	2.20875	37.0544	24.2595
H - amino	7	3.53772	39.4908	0	39.4908	49.4433	0	49.4433	0	5.97793	49.1478	23.7067
H - amino	8	3.61676	40.9152	0	40.9152	49.0544	0	49.0544	0	5.79855	50.2008	20.4869
H	9	5.77677	21.5588	0	21.5588	10.714	0	10.714	0	2.64487	26.1383	11.2989
N - amino	10	15.6328	28.6184	0	28.6184	46.2483	0	46.2483	0	5.49666	45.6024	19.4716
N - nitro	11	3.23132	28.3169	-11.8555	28.1593	66.7087	0	66.7087	0	6.69284	41.9327	-11.8555
N - nitro	12	0.276007	14.7193	-5.3184	-2.31275	4.12598	7.57574	11.7017	0.228272	5.10961	16.4935	-11.6949
N - nitro	13	3.59825	22.3527	-9.42896	21.6929	41.3695	17.1309	58.5004	0.207082	5.672	31.6152	-12.4642
N - nitro	14	4.0714	29.918	-6.68078	29.4849	37.6532	19.6307	57.2839	0.225254	5.06893	36.9973	-13.1796
O - nitro	15	20.3143	12.7295	-7.00035	5.00238	81.673	15.4615	97.1346	0.133839	10.1876	37.9336	-13.3427
O - nitro	16	18.6114	10.0753	-9.36344	-4.70422	54.9941	15.5041	70.4982	0.171556	7.56908	28.6904	-16.026
O - nitro	17	20.9761	7.43278	-11.5048	-9.12984	26.9845	20.6188	47.6033	0.245529	5.72705	21.2023	-19.6793
O - nitro	18	20.4267	7.14688	-12.0074	-10.0662	21.1693	20.8798	42.0491	0.249988	5.36254	18.1865	-19.8883
O - nitro	19	18.9664	8.45929	-13.5639	-10.0072	35.6808	27.5847	63.2655	0.245906	7.56872	22.8319	-21.7037
O - nitro	20	22.5499	8.7276	-10.9232	-5.36968	37.8381	32.7922	70.6302	0.248724	8.69203	26.4953	-20.753
O - nitro	21	22.0783	10.2038	-8.08109	-0.77823	51.3156	19.8375	71.1531	0.201071	8.78601	27.5339	-15.699
O - nitro	22	20.2394	13.8191	-7.5814	5.63535	81.249	17.1567	98.4057	0.14395	10.9264	36.393	-14.1052
NH ₂	10,7,8	22.7873	32.1216	0	32.1216	75.6016	0	75.6016	0	7.57548	50.2008	19.4716
NO ₂	11,15,16	42.157	14.7418	-8.51592	2.57756	111.305	16.7713	128.076	0.113801	11.7585	41.9327	-16.026
NO ₂	12,17,18	41.6788	7.37101	-11.716	-9.5449	24.7341	20.9895	45.7237	0.248323	5.58571	21.2023	-19.8883
NO ₂	13,19,20	45.1146	12.5488	-12.219	-5.00446	76.6693	31.9485	108.618	0.20762	10.6827	31.6152	-21.7037
NO ₂	14,21,22	46.3891	15.3619	-7.89214	4.91969	110.24	18.9042	129.144	0.124954	12.063	36.9973	-15.699

See figure A-12 for corresponding atom with atom number.

Table A-46. NTO atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	4.17512	23.5675	0	23.5675	20.1067	0	20.1067	0	3.40664	29.7308	0.251004
N	2	11.3504	22.7532	0	22.7532	14.9191	0	14.9191	0	3.11803	33.4306	15.3257
C	3	2.97185	18.6332	0	18.6332	13.3293	0	13.3293	0	3.15353	26.5913	12.9963
N	4	11.555	22.0812	0	22.0812	29.2811	0	29.2811	0	4.59541	35.4066	13.0836
N	5	16.9578	10.0134	-10.5447	-0.85906	38.5938	37.9212	76.515	0.249981	10.2649	26.378	-21.8718
H	6	6.38553	43.3371	0	43.3371	60.872	0	60.872	0	6.67763	57.1548	24.3172
H	7	7.77444	45.8342	0	45.8342	56.789	0	56.789	0	6.45552	59.9353	29.7182
N - nitro	8	4.2177	21.4483	-4.48293	20.913	40.0873	12.7579	52.8452	0.183136	5.62114	29.7509	-12.4994
O - nitro	9	23.2592	10.2255	-11.3422	-4.54783	50.3132	37.8098	88.1229	0.244967	9.82102	28.9207	-21.6497
O - nitro	10	23.6247	6.60271	-15.2734	-12.9287	20.0293	28.8559	48.8852	0.24185	6.67779	16.5713	-22.5357
O	11	27.9777	7.83489	-16.7837	-11.6847	24.5147	57.1116	81.6263	0.210131	10.3836	22.1781	-26.826
NO ₂	8,9,210	51.1016	12.5627	-13.5557	-6.58316	72.7237	36.6392	109.363	0.222783	10.9955	29.7509	-22.5357

See figure A-13 for corresponding atom with atom number.

Table A-47. DATB atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	3.99486	22.4104	0	22.4104	0.468888	0	0.468888	0	0.482318	24.6059	20.4267
C	2	4.02696	22.4002	0	22.4002	0.452752	0	0.452752	0	0.47933	24.567	20.5315
C	3	6.46903	20.0441	0	20.0441	5.55271	0	5.55271	0	2.00026	24.9818	15.4468
C	4	6.80611	16.3151	0	16.3151	2.23948	0	2.23948	0	0.930457	22.965	11.7865
C	5	6.48521	20.0886	0	20.0886	5.43074	0	5.43074	0	1.97142	24.9561	16.3058
N - nitro	6	3.8601	22.5633	0	22.5633	21.5086	0	21.5086	0	3.43405	26.2945	5.71285
N - nitro	7	4.02531	19.1698	-7.68936	18.4024	25.2469	43.9435	69.1904	0.231745	4.73806	24.8011	-17.3682
N - nitro	8	4.01568	18.916	-6.70852	18.0786	27.9631	34.2154	62.1785	0.247472	5.00369	24.818	-18.4877
O - nitro	9	19.812	9.74851	-10.3839	-2.32646	41.5892	35.4144	77.0036	0.248392	9.81975	27.1605	-20.6626
O - nitro	10	19.8694	9.86868	-10.3788	-2.23935	42.8514	35.3081	78.1595	0.247671	9.87621	27.9279	-20.657
O - nitro	11	20.4461	9.3721	-12.3156	-4.82092	37.6806	47.9096	85.5902	0.246429	10.4027	25.999	-23.4563
O - nitro	12	22.1218	5.8721	-14.0674	-11.1025	18.1111	43.2487	61.3598	0.208042	7.73297	15.6645	-24.658
O - nitro	13	22.0672	6.11899	-14.0727	-11.0037	19.2997	42.8768	62.1765	0.214053	7.79964	16.3686	-24.6981
O - nitro	14	20.4359	9.42689	-12.3671	-4.65874	38.4748	47.8575	86.3323	0.247047	10.5132	25.8346	-23.4751
H	15	5.39709	11.1604	0	11.1604	7.05478	0	7.05478	0	2.18951	14.577	4.27397
C	16	6.71777	22.645	0	22.645	2.43763	0	2.43763	0	1.35043	25.6946	20.2911
N - amino	17	15.6837	19.9244	0	19.9244	41.7931	0	41.7931	0	5.2566	35.7486	11.7325
H - amino	18	3.35656	30.6761	0	30.6761	43.6064	0	43.6064	0	5.49427	39.9165	14.8444
H - amino	19	3.1119	29.146	0	29.146	43.548	0	43.548	0	5.5906	38.258	14.38
N - amino	20	15.6155	19.9581	0	19.9581	41.5939	0	41.5939	0	5.25637	36.2782	11.7225
H - amino	21	3.15971	29.123	0	29.123	44.1942	0	44.1942	0	5.65316	38.2517	14.3882
H - amino	22	3.41454	30.5476	0	30.5476	45.3111	0	45.3111	0	5.61434	40.0044	14.5538
NH ₂	17,18,19	22.1521	22.9372	0	22.9372	63.7257	0	63.7257	0	7.00736	39.9165	11.7325
NH ₂	20,21,22	22.1898	23.0034	0	23.0034	63.7479	0	63.7479	0	7.0024	40.0044	11.7225
NO ₂	6,9,10	43.5415	11.9592	-10.3814	-0.41387	61.536	35.3612	96.8972	0.231757	11.0452	27.9279	-20.6626
NO ₂	7,11,12	46.5932	10.9275	-13.3282	-6.11736	53.9789	46.0042	99.9831	0.24841	10.922	25.999	-24.658
NO ₂	8,13,14	46.5187	10.8326	-13.3443	-6.06605	53.0192	45.7545	98.7737	0.248648	10.9331	25.8346	-24.6981

See figure A-14 for corresponding atom with atom number.

Table A-48. Picric acid atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	4.32506	29.4672	0	29.4672	13.0391	0	13.0391	0	2.37775	38.0741	13.8661
C	2	6.243	30.9542	0	30.9542	10.9285	0	10.9285	0	2.73085	38.8861	25.7486
C	3	7.367	24.9854	0	24.9854	2.6782	0	2.6782	0	1.18018	29.5438	17.3318
C	4	6.10367	25.4193	0	25.4193	2.25143	0	2.25143	0	1.24261	29.2369	20.6225
C	5	7.21646	22.9659	0	22.9659	9.64652	0	9.64652	0	2.3193	30.0677	11.5951
C	6	5.81852	25.4694	0	25.4694	9.82245	0	9.82245	0	2.45423	31.826	15.2133
N - nitro	7	4.05575	32.2085	-0.62437	32.1019	37.9551	0	37.9551	0	4.66072	38.6621	-0.62437
N - nitro	8	4.1056	23.5608	-3.3486	23.0716	36.6088	1.90505	38.5139	0.047017	5.0812	30.1035	-5.50263
N - nitro	9	3.63347	23.4767	-4.21624	23.3138	41.1425	5.44326	46.5857	0.103192	5.28528	32.0369	-6.54932
O	10	17.4931	16.8346	-6.67547	10.6938	98.1008	18.0232	116.124	0.131118	11.6432	37.5175	-15.9099
O - nitro	11	20.3182	14.0729	-6.33954	6.24393	88.6551	11.4683	100.123	0.101422	10.7045	37.8991	-11.8028
O - nitro	12	22.1689	9.59893	-6.1598	1.03686	55.8606	13.5106	69.3712	0.156828	7.87247	29.6335	-12.9524
O - nitro	13	22.7596	8.32678	-11.2101	-6.27861	37.6989	30.7949	68.4938	0.24746	8.30623	27.3544	-20.9802
O - nitro	14	21.456	8.29377	-12.8392	-9.22266	32.9135	26.2385	59.1519	0.246816	7.54027	21.4615	-21.1421
H	15	1.63584	34.6707	0	34.6707	20.6705	0	20.6705	0	3.97519	41.8756	26.3516
H	16	6.3342	22.3601	0	22.3601	10.0934	0	10.0934	0	2.5449	27.3582	12.9487
H	17	6.47971	20.5846	0	20.5846	16.2133	0	16.2133	0	3.39071	26.9195	8.99221
O - nitro	18	22.487	8.36588	-10.867	-5.52764	35.6529	30.9608	66.6137	0.24876	8.45776	23.5787	-20.7266
O - nitro	19	22.6914	8.28865	-11.1888	-6.01326	35.2788	30.5602	65.839	0.248716	8.42044	23.4299	-20.79
NO ₂	7,11,12	46.5428	14.6128	-6.22612	5.55941	118.782	12.7404	131.523	0.087485	11.138	38.6621	-12.9524
NO ₂	8,18,19	49.284	11.699	-11.0155	-3.66976	75.711	30.8419	106.553	0.205669	10.2222	30.1035	-20.79
NO ₂	9,13,14	47.849	12.4773	-12.0317	-5.36714	83.097	29.1695	112.266	0.192316	10.2372	32.0369	-21.1421

See figure A-15 for corresponding atom with atom number.

A.8 Area Weighted B3LYP/6-31G* Training Set Data

Table A-49. FOX-7 area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.90143	21.312	0	21.312	25.8153	0	25.8153	0	3.46899
N - amino	2	16.112	30.2805	0	30.2805	166.359	0	166.359	0	10.9518
H - amino	3	5.8596	62.4536	0	62.4536	54.3925	0	54.3925	0	6.10558
H - amino	4	3.11972	37.1908	0	37.1908	86.3702	0	86.3702	0	7.8248
N - amino	5	16.2672	29.7572	0	29.7572	156.65	0	156.65	0	10.709
H - amino	6	2.73426	33.1977	0	33.1977	92.5031	0	92.5031	0	8.1795
H - amino	7	6.07142	62.785	0	62.785	59.5459	0	59.5459	0	6.49098
C	8	6.64294	9.20668	-2.20761	9.14871	23.208	2.28085	25.4889	0.081477	4.10524
N - nitro	9	3.34425	10.1168	-6.22948	5.11188	53.5607	23.6091	77.1697	0.21234	8.14115
O - nitro	10	20.344	3.07021	-28.6788	-28.2114	3.11019	89.1054	92.2156	0.03259	7.95015
O - nitro	11	19.7789	8.95943	-18.5301	-14.3468	43.9946	86.997	130.992	0.223057	10.8275
N - nitro	12	3.78496	6.14294	-6.1558	2.14465	12.6803	30.3652	43.0456	0.207802	5.59065
O - nitro	13	20.2858	0.317247	-31.0716	-31.0307	0.018153	87.3402	87.3584	0.000208	7.37347
O - nitro	14	19.8208	7.13932	-20.1864	-15.9118	21.489	111.187	132.676	0.135734	11.7356

See figure A-1 for corresponding atom with atom number.

Table A-50. HMX area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.22976	34.9489	0	34.9489	41.0339	0	41.0339	0	5.68514
C	2	1.61168	33.4374	0	33.4374	64.9277	0	64.9277	0	6.52796
H	3	7.26617	37.9487	0	37.9487	36.6084	0	36.6084	0	5.07436
H	4	6.21413	29.7713	0	29.7713	60.2249	0	60.2249	0	6.3736
H	5	7.20738	27.4672	0	27.4672	35.0349	0	35.0349	0	4.87408
H	6	7.44781	35.7715	0	35.7715	66.9832	0	66.9832	0	6.70424
N - nitro	7	2.40869	15.1633	-6.50343	12.7575	44.3778	53.8298	98.2075	0.247684	7.62607
N - nitramine	8	3.45288	15.1929	0	15.1929	31.5173	0	31.5173	0	4.49667
N - nitramine	9	2.54446	37.1331	0	37.1331	6.27251	0	6.27251	0	1.89077
N - nitro	10	2.59798	32.4771	0	32.4771	85.101	0	85.101	0	6.94545
O - nitro	11	19.9858	6.80851	-16.0945	-13.1829	20.883	46.1361	67.0191	0.214505	8.06462
O - nitro	12	20.7205	8.24238	-13.5408	-8.86489	36.6706	47.1211	83.7917	0.246111	9.11029
O - nitro	13	19.7343	10.9818	-8.90406	-2.03558	79.5859	22.477	102.063	0.171727	9.10202
O - nitro	14	18.1013	13.3594	-11.7564	-4.69586	97.1343	24.1276	121.262	0.159382	10.5649
N - nitramine	15	2.54018	37.2089	0	37.2089	6.37579	0	6.37579	0	1.91635
C	16	1.76288	33.0375	0	33.0375	74.0194	0	74.0194	0	6.94875
C	17	2.25333	34.6614	0	34.6614	41.6307	0	41.6307	0	5.66105
N - nitro	18	2.70531	31.3415	-4.56743	30.8181	93.7598	16.1672	109.927	0.125442	7.88096
H	19	7.24872	27.3779	0	27.3779	35.3555	0	35.3555	0	4.89725
H	20	7.31616	35.9514	0	35.9514	65.3839	0	65.3839	0	6.62393
N - nitramine	21	3.47811	15.6313	0	15.6313	38.0603	0	38.0603	0	4.75827
H	22	7.2104	37.9094	0	37.9094	36.2889	0	36.2889	0	5.05531
H	23	6.19097	29.657	0	29.657	62.8782	0	62.8782	0	6.45841
O - nitro	24	19.602	10.8859	-8.90497	-2.12303	77.8618	22.4652	100.327	0.17378	9.03444
O - nitro	25	18.0006	13.2796	-11.7938	-4.73561	95.0589	23.8244	118.883	0.160241	10.548
N - nitro	26	2.3948	15.197	-5.23725	12.8333	43.3747	33.3151	76.6898	0.245698	7.5393
O - nitro	27	20.045	6.77301	-16.1031	-13.2019	20.753	45.9887	66.7417	0.214258	8.05066
O - nitro	28	20.6815	8.38787	-13.5336	-8.8574	38.828	47.1321	85.9601	0.247667	9.12952

See figure A-2 for corresponding atom with atom number.

Table A-51. PETN area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.973351	29.3085	0	29.3085	47.9072	0	47.9072	0	5.95781
O - nitro	3	20.9062	10.1893	-6.33351	0.967361	64.3471	12.8219	77.1689	0.138546	8.18701
O - nitro	4	23.8737	8.0515	-9.3422	-5.63318	34.544	14.8863	49.4303	0.210461	6.62773
O - nitrate	5	9.24505	14.7222	-0.82941	14.2942	93.9473	0.344887	94.2922	0.003644	8.19903
N - nitro	6	3.64419	26.9532	-3.78911	26.7387	40.5587	2.55833	43.117	0.055814	5.23833
H	7	6.21711	28.6393	0	28.6393	28.1393	0	28.1393	0	4.15737
H	8	7.48494	28.6379	0	28.6379	22.1069	0	22.1069	0	3.70355
C	9	1.01708	28.0919	0	28.0919	55.568	0	55.568	0	6.41922
C	10	0.951943	28.0196	0	28.0196	58.8818	0	58.8818	0	6.7367
C	11	0.860056	27.6378	0	27.6378	49.2866	0	49.2866	0	6.13493
O - nitro	12	20.8826	10.2941	-6.33181	1.00227	66.2986	12.8585	79.1571	0.136055	8.23513
O - nitro	13	20.939	10.2545	-6.35538	1.00716	67.1841	12.6892	79.8732	0.133628	8.23828
O - nitro	14	20.8942	10.1889	-6.33207	0.953989	64.5417	12.8495	77.3912	0.138466	8.18021
O - nitro	15	23.833	8.19853	-9.31811	-5.63928	34.8044	15.0629	49.8672	0.210819	6.63006
O - nitro	16	23.8487	8.05355	-9.31243	-5.66748	33.8861	15.0653	48.9514	0.213044	6.58617
O - nitro	17	23.8017	8.06297	-9.33152	-5.68415	33.3431	14.9374	48.2805	0.213667	6.583
O - nitrate	18	9.2388	14.8248	-0.92581	14.4257	96.7215	0.252984	96.9745	0.002602	8.3193
O - nitrate	19	9.17597	14.6956	-0.9436	14.3177	93.4516	0.362647	93.8142	0.003851	8.16453
O - nitrate	20	9.28424	14.9465	-0.77326	14.5535	97.5389	0.261143	97.8001	0.002663	8.34639
N - nitro	21	3.62882	26.5716	-2.3065	26.0343	45.5521	4.62177	50.1739	0.08363	5.82383
N - nitro	22	3.61855	26.8706	-0.64006	26.805	43.501	0	43.501	0	5.27531
N - nitro	23	3.69384	26.7733	-2.03156	26.2908	43.7192	4.26388	47.9831	0.080966	5.61339
H	24	6.26075	28.6545	0	28.6545	28.3654	0	28.3654	0	4.18196
H	25	6.31999	28.7411	0	28.7411	28.6798	0	28.6798	0	4.20966
H	26	6.35663	28.7071	0	28.7071	28.7963	0	28.7963	0	4.20116
H	27	7.46085	28.6749	0	28.6749	21.4349	0	21.4349	0	3.66113
H	28	7.5804	28.7286	0	28.7286	22.0777	0	22.0777	0	3.722
H	29	7.57335	28.7079	0	28.7079	22.47	0	22.47	0	3.75069

See figure A-3 for corresponding atom with atom number.

Table A-52. EDNA area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.50214	31.6444	0	31.6444	54.7567	0	54.7567	0	5.5795
H	2	8.58945	32.2703	0	32.2703	36.5676	0	36.5676	0	4.50822
H	3	7.37389	26.9946	0	26.9946	34.3901	0	34.3901	0	4.29627
H	4	5.53685	48.8979	0	48.8979	63.4592	0	63.4592	0	6.6739
N - nitramine	5	9.31728	28.0182	0	28.0182	98.962	0	98.962	0	7.84693
N - nitro	6	3.4007	16.947	-7.24749	15.5377	45.9097	52.3841	98.2938	0.248915	6.61785
O - nitro	7	23.9956	8.86181	-19.2585	-15.2561	40.8297	64.0609	104.891	0.237737	10.0532
O - nitro	8	21.0157	8.11889	-16.4535	-11.8514	34.162	67.8207	101.983	0.222768	10.1429
C	9	2.57585	31.28	0	31.28	47.9063	0	47.9063	0	4.95194
H	10	8.44872	32.2975	0	32.2975	36.5716	0	36.5716	0	4.49642
H	11	7.26259	26.9714	0	26.9714	34.4937	0	34.4937	0	4.28622
N - nitramine	12	9.43822	28.119	0	28.119	101.242	0	101.242	0	7.93704
H	13	5.49556	48.8453	0	48.8453	65.3303	0	65.3303	0	6.73596
N - nitro	14	3.27238	17.1395	-7.24714	15.8344	44.8315	22.3543	67.1858	0.222019	6.44632
O - nitro	15	24.1201	8.71966	-19.2215	-15.2591	37.2473	65.0583	102.306	0.231525	10.0569
O - nitro	16	20.9365	8.00979	-16.4754	-11.8401	34.5716	67.2186	101.79	0.224283	10.1279

See figure A-4 for corresponding atom with atom number.

Table A-53. NQ area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.1288	3.92247	-26.0772	-24.5896	8.36055	153.678	162.038	0.048934	11.4632
O - nitro	2	23.6084	0	-39.4652	-39.4652	0	49.4486	49.4486	0	5.34807
N - amino	3	16.9156	23.964	0	23.964	176.727	0	176.727	0	11.3349
N - amino	4	16.8882	20.8122	-0.58547	20.773	153.512	0.364179	153.876	0.002361	10.6494
N - nitramine	5	15.6934	3.49573	-20.7349	-17.7053	5.23766	148.755	153.993	0.032856	11.9522
N - nitro	6	3.63554	2.18246	-9.85964	-8.47526	3.47106	45.6434	49.1144	0.065678	5.8172
C	7	2.6782	12.3081	0	12.3081	36.4075	0	36.4075	0	4.3335
H - amino	8	5.46852	38.0092	0	38.0092	97.2013	0	97.2013	0	8.25539
H - amino	9	6.93018	58.1828	0	58.1828	65.8805	0	65.8805	0	6.84654
H - amino	10	6.56807	56.6267	0	56.6267	79.8624	0	79.8624	0	7.59994
H - amino	11	2.74512	23.2173	0	23.2173	80.8219	0	80.8219	0	7.65433

See figure A-5 for corresponding atom with atom number.

Table A-54. RDX area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.53959	27.2625	0	27.2625	15.2111	0	15.2111	0	2.44265
C	2	2.45168	28.7216	0	28.7216	18.6935	0	18.6935	0	2.62779
C	3	2.70601	29.8417	0	29.8417	5.96379	0	5.96379	0	1.79714
H	4	2.34931	30.5354	0	30.5354	15.4785	0	15.4785	0	2.38489
H	5	9.28893	39.1606	0	39.1606	30.6349	0	30.6349	0	4.7298
H	6	4.87019	21.0151	-2.81812	20.4413	48.8909	3.26328	52.1542	0.058655	6.30341
H	7	5.58386	25.1823	-3.46009	25.1133	40.2191	0	40.2191	0	5.0656
H	8	9.29597	39.5667	0	39.5667	27.3212	0	27.3212	0	4.47745
H	9	9.52332	39.0455	0	39.0455	26.8494	0	26.8494	0	4.40882
N - nitramine	10	4.98455	22.6133	-3.3966	22.1231	49.7664	3.21399	52.9804	0.056984	6.21611
N - nitramine	11	4.06821	24.0908	0	24.0908	135.863	0	135.863	0	10.8355
N - nitramine	12	6.02802	18.6681	0	18.6681	38.8117	0	38.8117	0	4.92742
N - nitro	13	6.01144	19.0139	0	19.0139	34.1656	0	34.1656	0	4.62681
N - nitro	14	3.35512	19.7054	-5.41902	18.9086	97.2888	27.8246	125.113	0.172935	9.16027
N - nitro	15	2.83699	20.2421	-7.50879	19.5744	57.17	20.8648	78.0348	0.195887	6.05787
O - nitro	16	2.96216	21.0322	-11.6696	20.0913	55.6562	48.0529	103.709	0.248656	6.18218
O - nitro	17	21.2708	9.26563	-15.7414	-11.7185	55.2797	48.5797	103.859	0.24896	9.19507
O - nitro	18	21.3868	8.68188	-16.3424	-12.6491	52.5535	50.9063	103.46	0.249937	9.03959
O - nitro	19	19.0874	7.4634	-15.8186	-12.1167	23.9511	43.157	67.1081	0.229523	8.70805
O - nitro	20	20.6421	8.35915	-14.5455	-10.3631	34.0027	40.6566	74.6593	0.248014	8.81852
O - nitro	21	18.9582	9.09867	-15.566	-11.1286	39.4482	41.3198	80.7681	0.249866	9.3305

See figure A-6 for corresponding atom with atom number.

Table A-55. CL20 area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.6445	10.9192	-8.60016	-1.58181	62.9329	20.7523	83.6852	0.186486	9.05708
O - nitro	2	18.8643	10.9201	-9.62005	-3.18555	58.6673	17.6921	76.3595	0.178013	9.04907
O - nitro	3	19.8153	10.6209	-7.7471	-0.23707	59.6307	18.7706	78.4014	0.182096	8.88053
O - nitro	4	17.4912	10.8311	-8.58211	-2.09251	65.4229	16.3521	81.775	0.159979	8.73551
O - nitro	5	19.9424	11.6676	-7.70633	-0.20097	82.8137	16.2627	99.0764	0.1372	9.19647
O - nitro	6	19.5695	12.5928	-9.3335	-2.73589	102.129	17.3895	119.518	0.124328	9.42212
O - nitro	7	20.0701	13.6364	-9.03801	-1.43301	128.445	15.0326	143.478	0.093795	10.1468
O - nitro	8	20.562	9.9953	-7.95145	-2.31095	79.9292	16.0509	95.9801	0.139265	7.89854
O - nitro	9	21.4527	12.5637	-7.35872	1.54765	98.8411	15.6035	114.445	0.117752	9.92595
O - nitro	10	19.9414	12.6683	-8.7496	-1.50139	110.548	15.5034	126.052	0.107866	9.63811
O - nitro	11	20.4048	9.03301	-7.7112	-3.07676	59.8848	14.37	74.2548	0.156071	7.00401
O - nitro	12	21.3881	13.6153	-6.52886	2.79245	128.525	12.8825	141.407	0.082803	10.2272
N - nitramine	13	5.01433	27.277	0	27.277	29.0026	0	29.0026	0	4.36658
N - nitramine	14	5.37799	27.1865	0	27.1865	31.2993	0	31.2993	0	4.56718
N - nitramine	15	3.3236	36.955	0	36.955	27.615	0	27.615	0	4.47544
N - nitramine	16	1.14448	33.2309	0	33.2309	301.646	0	301.646	0	14.9657
N - nitramine	17	2.07566	37.7315	0	37.7315	48.6846	0	48.6846	0	5.62091
N - nitramine	18	1.57451	30.3035	0	30.3035	134.086	0	134.086	0	7.23746
N - nitro	19	2.00913	25.3082	-8.84461	24.4442	33.8046	14.4894	48.294	0.21001	5.46641
N - nitro	20	2.00609	26.6037	-7.33935	25.8811	28.4388	4.05975	32.4985	0.109316	5.01636
N - nitro	21	1.95402	29.0593	-3.63946	28.4318	106.636	0.477306	107.113	0.004436	8.78465
N - nitro	22	3.16299	32.9473	0	32.9473	221.037	0	221.037	0	13.1033
N - nitro	23	3.25057	29.6366	-9.76468	29.5499	92.2797	0	92.2797	0	8.0785
N - nitro	24	3.15186	33.2494	-5.48067	33.0547	198.177	-5.34E-15	198.177	-2.69E-17	12.1169
C	25	1.05559	51.3479	0	51.3479	33.7398	0	33.7398	0	4.46522
C	26	1.20759	50.2132	0	50.2132	30.6468	0	30.6468	0	4.6576
C	27	0.580999	36.6531	0	36.6531	11.591	0	11.591	0	2.53736
C	28	0.427561	35.288	0	35.288	32.7589	0	32.7589	0	4.97628

See figure A-7 for corresponding atom with atom number.

Table A-55. CL20 area weighted atom specific Politzer parameters using B3LYP/6-31G* (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	29	1.0423	52.7867	0	52.7867	67.8486	0	67.8486	0	5.88005
C	30	1.07034	55.2743	0	55.2743	29.4994	0	29.4994	0	4.07192
H	31	5.55513	43.3638	0	43.3638	83.9038	0	83.9038	0	7.35762
H	32	5.99654	43.786	0	43.786	59.2814	0	59.2814	0	6.22301
H	33	6.2256	36.7135	0	36.7135	13.4788	0	13.4788	0	2.86953
H	34	3.60268	30.9787	0	30.9787	50.3582	0	50.3582	0	5.86016
H	35	3.87401	40.265	0	40.265	108.876	0	108.876	0	8.6647
H	36	4.1894	43.8171	0	43.8171	81.8116	0	81.8116	0	7.18887

See figure A-7 for corresponding atom with atom number.

Table A-56. HNB area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.14893	44.1133	0	44.1133	18.0827	0	18.0827	0	3.25296
C	2	4.23515	44.3789	0	44.3789	18.1273	0	18.1273	0	3.28492
C	3	4.20832	43.9913	0	43.9913	17.4116	0	17.4116	0	3.21238
N - nitro	4	0.850367	21.1605	0	21.1605	89.9709	0	89.9709	0	7.93469
N - nitro	5	0.900335	22.8432	0	22.8432	82.2962	0	82.2962	0	7.83981
N - nitro	6	0.8501	22.751	-6.62211	22.4503	105.632	0	105.632	0	9.5829
O - nitro	7	20.2473	10.5845	-6.36598	-0.26008	77.4507	12.9394	90.3901	0.122658	7.8149
O - nitro	8	19.654	10.2824	-3.87174	5.33154	83.657	5.51153	89.1686	0.05799	7.83109
O - nitro	9	20.0921	9.65296	-4.20206	3.55784	73.4387	7.72747	81.1662	0.086141	7.45982
O - nitro	10	20.0179	9.75443	-4.14362	4.14499	79.6571	6.90175	86.5589	0.073377	7.62018
O - nitro	11	19.7715	9.60268	-5.33259	2.09665	76.3484	11.5665	87.9149	0.114256	7.68283
O - nitro	12	20.4264	10.6714	-6.36781	-0.23548	85.2006	13.2898	98.4904	0.116727	7.85279
C	13	4.16218	44.2564	0	44.2564	18.1709	0	18.1709	0	3.25469
C	14	4.17426	44.1161	0	44.1161	17.6014	0	17.6014	0	3.19819
C	15	4.3637	44.1723	0	44.1723	18.6996	0	18.6996	0	3.31349
N - nitro	16	0.860106	21.4597	0	21.4597	99.9378	0	99.9378	0	8.77003
N - nitro	17	0.868842	21.6416	0	21.6416	111.807	0	111.807	0	9.48613
N - nitro	18	0.852827	21.5985	-0.94185	20.9236	78.0447	0.000235	78.045	3.01E-06	7.43015
O - nitro	19	20.212	10.5096	-6.3497	-0.31952	76.5787	13.0407	89.6194	0.124338	7.75158
O - nitro	20	19.6484	10.2961	-3.87062	5.30506	84.4139	5.52129	89.9352	0.057623	7.8348
O - nitro	21	19.7582	9.74192	-5.30303	2.13493	79.016	11.6061	90.6222	0.111669	7.73144
O - nitro	22	20.4009	10.7685	-6.34321	-0.24957	84.3304	13.4068	97.7372	0.118356	7.85019
O - nitro	23	20.1989	9.57217	-4.23526	3.5767	72.6154	7.62029	80.2356	0.085954	7.4531
O - nitro	24	19.9547	9.75629	-4.12423	4.11516	77.2046	6.96715	84.1717	0.075922	7.59015

See figure A-8 for corresponding atom with atom number.

Table A-57. TATB area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.82838	19.9889	0	19.9889	6.16402	0	6.16402	0	1.95053
C	2	3.69986	20.9951	0	20.9951	2.68243	0	2.68243	0	1.22303
C	3	6.93822	18.5298	0	18.5298	4.33193	0	4.33193	0	1.62224
C	4	3.8635	20.3634	0	20.3634	1.81942	0	1.81942	0	0.981269
C	5	6.77723	19.6601	0	19.6601	3.25881	0	3.25881	0	1.45919
C	6	3.82579	21.4172	0	21.4172	4.6357	0	4.6357	0	1.80811
H - amino	7	2.25364	26.1974	0	26.1974	40.6549	0	40.6549	0	5.43836
H - amino	8	2.33373	27.4594	0	27.4594	40.6128	0	40.6128	0	5.33256
H - amino	9	2.27425	26.7818	0	26.7818	54.2819	0	54.2819	0	6.26214
H - amino	10	3.10124	31.8772	0	31.8772	48.7998	0	48.7998	0	5.85665
H - amino	11	2.28266	27.1538	0	27.1538	41.9118	0	41.9118	0	5.51911
H - amino	12	2.72465	30.2372	0	30.2372	34.5182	0	34.5182	0	4.59305
N - nitro	13	3.93538	18.0649	-3.14861	17.7767	26.4524	3.78043	30.2328	0.109408	4.21438
N - amino	14	15.0614	18.0958	0	18.0958	68.1314	0	68.1314	0	6.58678
N - nitro	15	3.99579	15.7609	-5.21373	15.0434	22.1684	21.4447	43.6132	0.249931	4.46962
N - amino	16	14.7312	17.7664	0	17.7664	65.5584	0	65.5584	0	6.42759
N - nitro	17	3.97011	17.7266	-4.61272	17.2562	21.1463	15.0995	36.2458	0.243042	4.11653
N - amino	18	15.1674	18.1365	0	18.1365	83.8827	0	83.8827	0	7.55865
O - nitro	19	19.0477	9.51324	-14.1308	-7.68718	48.6897	60.6612	109.351	0.247004	10.7305
O - nitro	20	19.2968	8.35221	-14.3915	-8.20208	29.8914	61.969	91.8603	0.219515	10.5298
O - nitro	21	19.2676	7.79797	-15.7472	-10.4198	30.467	71.1196	101.587	0.209965	10.5417
O - nitro	22	19.6186	7.08399	-15.5667	-10.6583	22.4088	70.0191	92.4279	0.183666	10.1736
O - nitro	23	18.77	9.15831	-13.8375	-6.11442	36.5139	60.2699	96.7838	0.234938	11.0822
O - nitro	24	19.4113	7.99799	-14.4748	-8.54021	27.604	62.5272	90.1312	0.212467	10.3818

See figure A-9 for corresponding atom with atom number.

Table A-58. PNA area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.07015	39.3958	0	39.3958	5.81739	0	5.81739	0	1.62956
C	2	5.47816	34.7826	0	34.7826	20.8928	0	20.8928	0	3.64442
C	3	3.64206	30.1943	0	30.1943	20.2102	0	20.2102	0	3.55362
C	4	4.93769	29.3424	0	29.3424	13.0534	0	13.0534	0	2.66041
N - amino	5	15.6271	37.3229	0	37.3229	62.3677	0	62.3677	0	6.60751
H - amino	6	2.83672	48.2796	0	48.2796	33.6787	0	33.6787	0	4.81547
N - nitro	7	3.00393	32.9069	0	32.9069	117.238	0	117.238	0	9.28587
N - nitro	8	0.32023	13.0051	-3.10204	6.15284	95.5063	10.0452	105.552	0.086112	10.1329
N - nitro	9	2.11705	17.9405	-1.77376	17.4367	46.3843	0.344315	46.7286	0.007314	6.11789
O - nitro	10	20.2586	13.9343	-5.24516	7.61842	111.022	8.95676	119.979	0.06908	10.3724
O - nitro	11	18.5129	11.7108	-7.42265	-1.35978	82.499	11.6629	94.1619	0.108519	8.32578
O - nitro	12	20.469	8.91856	-10.2376	-6.99643	42.0428	23.2963	65.3391	0.229421	6.65829
O - nitro	13	19.598	9.16564	-10.6779	-7.83288	44.7265	21.5344	66.2609	0.219373	6.28536
O - nitro	14	18.9174	8.81879	-11.3384	-7.5689	43.1868	21.7488	64.9356	0.222751	7.21787
C	15	5.37822	34.8775	0	34.8775	20.4295	0	20.4295	0	3.57913
C	16	3.70034	30.0039	0	30.0039	20.512	0	20.512	0	3.57062
H - amino	17	2.81291	48.2374	0	48.2374	36.8168	0	36.8168	0	4.93748
N - nitro	18	3.02278	32.8836	0	32.8836	113.74	0	113.74	0	9.08998
N - nitro	19	0.27137	9.43735	-3.86295	4.76383	90.0574	9.81825	99.8756	0.088641	8.64462
O - nitro	20	20.1433	13.8178	-5.24805	7.52878	108.442	8.99018	117.433	0.070695	10.279
O - nitro	21	18.5998	11.9219	-7.39046	-1.27988	83.0902	11.8228	94.9131	0.109048	8.39572
O - nitro	22	20.4489	8.92326	-10.2251	-6.99912	43.4385	23.3602	66.7987	0.227413	6.64852
O - nitro	23	19.5954	8.8387	-10.6685	-7.93808	42.6015	21.5711	64.1726	0.22315	6.17279
O - nitro	24	18.8637	8.89417	-11.3666	-7.54299	44.2427	21.599	65.8417	0.220431	7.26511

See figure A-9 for corresponding atom with atom number.

Table A-59. TNT area weighted atom specific Politzer parameters using B3LYP/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.8719	8.16217	-9.93947	-5.02413	37.5895	27.0437	64.6332	0.243344	7.86235
O - nitro	2	22.2275	9.417	-10.5156	-4.87119	47.5634	26.1013	73.6647	0.228779	8.6329
O - nitro	3	22.3041	8.86637	-11.8002	-6.91024	37.0798	33.3321	70.4119	0.249292	8.59544
O - nitro	4	22.3082	9.08938	-11.7521	-6.60931	48.5775	30.1155	78.693	0.23624	8.66867
O - nitro	5	22.8681	10.3147	-10.4476	-4.65592	57.058	23.4975	80.5555	0.206608	8.84472
O - nitro	6	20.9736	8.27681	-9.85383	-5.3792	41.1544	23.2841	64.4385	0.230773	7.51896
N - nitro	7	3.26306	27.2429	-4.4754	26.9494	38.2095	2.67E-15	38.2095	6.98E-17	5.24125
N - nitro	8	3.80442	24.761	-7.06738	24.0279	42.4684	29.6117	72.08	0.242046	5.89691
N - nitro	9	2.04249	27.1686	-5.0356	26.4573	52.4292	5.23275	57.662	0.082513	6.45417
C	10	5.34349	23.6023	0	23.6023	14.1649	0	14.1649	0	2.92836
C	11	7.29688	21.8896	0	21.8896	18.9004	0	18.9004	0	3.27974
C	12	5.49058	23.2235	0	23.2235	14.4746	0	14.4746	0	2.88332
C	13	7.0206	21.6703	0	21.6703	49.7006	0	49.7006	0	6.26467
C	14	4.83901	21.8832	0	21.8832	18.5198	0	18.5198	0	3.29026
C	15	4.69267	24.0714	0	24.0714	21.3019	0	21.3019	0	4.01314
C	16	4.15352	20.7645	0	20.7645	44.4535	0	44.4535	0	5.28607
H	17	6.8761	24.1425	0	24.1425	18.523	0	18.523	0	3.40029
H	18	7.45844	28.9134	0	28.9134	45.8163	0	45.8163	0	5.74136
H	19	8.02274	23.5903	0	23.5903	19.8208	0	19.8208	0	3.27629
H	20	9.32859	16.5281	0	16.5281	12.3517	0	12.3517	0	2.81261
H	21	7.75196	22.6292	0	22.6292	25.7902	0	25.7902	0	3.93343

See figure A-10 for corresponding atom with atom number.

A.9 Area Weighted B3LYP/6-31G** Training Set Data

Table A-60. FOX-7 area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number ^a	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.82177	24.7182	0	24.7182	18.3196	0	18.3196	0	3.36958
N - amino	2	16.3528	31.4935	0	31.4935	137.893	0	137.893	0	9.88909
H - amino	3	6.07973	61.5806	0	61.5806	58.69	0	58.69	0	6.37935
H - amino	4	3.24397	36.8508	0	36.8508	87.0431	0	87.0431	0	7.85911
N - amino	5	16.4664	31.0772	0	31.0772	133.638	0	133.638	0	9.817
H - amino	6	2.75515	33.7334	0	33.7334	84.9562	0	84.9562	0	7.83256
H - amino	7	6.27586	61.9533	0	61.9533	63.4038	0	63.4038	0	6.72596
C	8	6.34747	13.0499	0	13.0499	22.515	0	22.515	0	3.94283
N - nitro	9	3.0078	12.3935	-6.0527	8.68392	59.4323	32.9987	92.431	0.229554	8.28666
O - nitro	10	21.3815	4.01153	-27.3708	-26.3931	7.68078	80.8024	88.4832	0.07927	8.17699
O - nitro	11	20.8174	8.60995	-17.7442	-12.9603	44.2571	84.0298	128.287	0.225971	10.9861
N - nitro	12	3.64822	8.76679	-6.85481	5.53222	18.2958	57.4645	75.7603	0.183176	6.09124
O - nitro	13	21.3339	2.06834	-29.655	-29.2722	1.30809	82.5781	83.8862	0.015351	7.59528
O - nitro	14	20.9107	7.58483	-19.5926	-14.5139	26.5779	106.675	133.253	0.159672	12.0147

See figure A-1 for corresponding atom with atom number.

Table A-61. HMX area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.10725	37.404	0	37.404	43.6811	0	43.6811	0	5.88703
C	2	1.47325	36.3185	0	36.3185	76.2376	0	76.2376	0	7.33959
H	3	7.24045	40.548	0	40.548	35.2337	0	35.2337	0	5.00952
H	4	6.34817	31.2923	0	31.2923	61.8702	0	61.8702	0	6.34429
H	5	7.4262	29.4687	0	29.4687	36.7391	0	36.7391	0	4.93552
H	6	7.3348	38.3192	0	38.3192	66.5527	0	66.5527	0	6.68083
N - nitro	7	2.1551	16.6534	-7.49019	14.8862	63.5551	25.5895	89.1445	0.204655	8.28248
N - nitramine	8	3.1955	18.4054	0	18.4054	24.6326	0	24.6326	0	4.00977
N - nitramine	9	2.4579	40.9422	0	40.9422	6.41812	0	6.41812	0	1.90575
N - nitro	10	2.49593	34.9271	-7.54141	34.6048	104.693	0	104.693	0	8.10066
O - nitro	11	20.9793	7.77634	-15.642	-12.2779	27.6491	46.9567	74.6059	0.233256	8.47265
O - nitro	12	21.625	8.87996	-13.322	-7.96831	42.2382	48.6146	90.8528	0.248769	9.59262
O - nitro	13	20.4397	11.5651	-8.50686	-0.75874	87.7926	23.0675	110.86	0.164781	9.53838
O - nitro	14	18.5905	13.7625	-11.2424	-3.71199	112.181	21.9197	134.1	0.136739	10.7753
N - nitramine	15	2.43918	40.989	0	40.989	5.89059	0	5.89059	0	1.88115
C	16	1.53712	35.9339	0	35.9339	76.512	0	76.512	0	7.31698
C	17	2.06174	36.9668	0	36.9668	42.9581	0	42.9581	0	5.74918
N - nitro	18	2.37892	35.3965	-3.19821	34.8712	92.1571	4.68411	96.8412	0.046029	7.75716
H	19	7.27704	29.4715	0	29.4715	34.0385	0	34.0385	0	4.78322
H	20	7.42523	38.5247	0	38.5247	65.2604	0	65.2604	0	6.62999
N - nitramine	21	3.3125	18.8538	0	18.8538	28.8087	0	28.8087	0	4.32029
H	22	7.28765	40.517	0	40.517	35.848	0	35.848	0	5.04137
H	23	6.35851	31.3661	0	31.3661	58.9663	0	58.9663	0	6.27765
O - nitro	24	20.4874	11.4285	-8.63415	-0.71097	87.3474	22.4312	109.779	0.16258	9.60151
O - nitro	25	18.5858	13.3241	-11.2978	-3.73746	106.587	21.2933	127.88	0.138784	10.6973
N - nitro	26	2.03983	17.3373	-7.38704	15.3451	56.3245	44.9119	101.236	0.246823	8.11189
O - nitro	27	21.016	7.28762	-15.6733	-12.2765	25.2622	46.5594	71.8216	0.228017	8.45217
O - nitro	28	21.6727	8.60797	-13.3993	-8.00098	39.8875	47.7794	87.6669	0.247974	9.56067

See figure A-2 for corresponding atom with atom number.

Table A-62. PETN area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.871068	30.5786	0	30.5786	48.99	0	48.99	0	6.04693
O - nitro	3	21.6633	10.7768	-6.01873	2.161	72.5196	12.6718	85.1914	0.12662	8.55161
O - nitro	4	25.0257	8.39289	-8.77647	-4.95161	39.4219	13.8761	53.298	0.192568	6.61114
O - nitrate	5	9.21635	16.5892	-0.64326	16.4346	103.85	0.201855	104.051	0.001936	8.50235
N - nitro	6	3.3669	28.8986	-5.77725	28.5201	53.2841	1.5157	54.7998	0.026894	6.16438
H	7	6.3271	30.7825	0	30.7825	28.8885	0	28.8885	0	4.2555
H	8	7.51784	30.9538	0	30.9538	22.4531	0	22.4531	0	3.72854
C	9	0.880605	30.383	0	30.383	50.1432	0	50.1432	0	6.08399
C	10	0.790156	29.5611	0	29.5611	47.3134	0	47.3134	0	5.94825
C	11	0.732989	30.1887	0	30.1887	40.7078	0	40.7078	0	5.41357
O - nitro	12	21.7003	10.8104	-6.01592	2.17113	73.1822	12.6644	85.8466	0.12576	8.56378
O - nitro	13	21.6676	10.6377	-6.08078	2.13201	72.4092	12.4225	84.8317	0.124993	8.52914
O - nitro	14	21.8031	10.8309	-6.04388	2.24357	73.5443	12.5422	86.0865	0.124467	8.61382
O - nitro	15	24.9352	8.40658	-8.79347	-4.9727	40.3271	13.7948	54.1219	0.189918	6.60483
O - nitro	16	25.122	8.40778	-8.79895	-4.88326	40.4411	13.7124	54.1536	0.189097	6.67001
O - nitro	17	25.079	8.35863	-8.79261	-4.91256	39.9228	13.7802	53.703	0.190757	6.64269
O - nitrate	18	9.26795	16.7164	-0.78979	16.5183	105.736	0.113341	105.85	0.00107	8.60211
O - nitrate	19	9.14731	16.7153	-0.48756	16.4443	103.702	0.230492	103.933	0.002213	8.5324
O - nitrate	20	9.22434	16.8663	-0.55996	16.6479	106.11	0.14522	106.255	0.001365	8.62007
N - nitro	21	3.38766	28.5986	-3.74407	28.1848	56.8327	10.0674	66.9002	0.127839	6.3687
N - nitro	22	3.30186	29.1729	0	29.1729	49.9265	0	49.9265	0	5.64212
N - nitro	23	3.27678	28.9899	-8.41992	28.8389	51.9842	0	51.9842	0	5.89706
H	24	6.29203	30.8049	0	30.8049	28.4954	0	28.4954	0	4.23728
H	25	6.35544	30.9492	0	30.9492	29.6989	0	29.6989	0	4.32213
H	26	6.3177	30.9578	0	30.9578	28.812	0	28.812	0	4.26793
H	27	7.51295	30.8728	0	30.8728	22.6351	0	22.6351	0	3.72998
H	28	7.58533	30.991	0	30.991	22.596	0	22.596	0	3.74157
H	29	7.63361	30.9081	0	30.9081	23.397	0	23.397	0	3.80537

See figure A-3 for corresponding atom with atom number.

Table A-63. EDNA area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.39525	34.0174	0	34.0174	50.5098	0	50.5098	0	5.27356
H	2	8.69212	34.3994	0	34.3994	32.9263	0	32.9263	0	4.22234
H	3	7.4341	29.1751	0	29.1751	31.1069	0	31.1069	0	4.03129
H	4	5.42174	49.0639	0	49.0639	81.4046	0	81.4046	0	7.5858
N - nitramine	5	9.39721	30.4327	0	30.4327	92.4956	0	92.4956	0	7.51081
N - nitro	6	3.16012	20.0606	-5.81675	19.0041	58.7639	32.1922	90.956	0.228664	6.99449
O - nitro	7	25.5552	8.77416	-18.5005	-14.3789	35.0993	61.4522	96.5515	0.231376	9.98661
O - nitro	8	22.0772	9.09448	-15.7333	-10.0688	44.7102	64.9415	109.652	0.241489	10.6696
C	9	2.25025	34.0474	0	34.0474	45.3169	0	45.3169	0	4.97181
H	10	8.68947	34.4792	0	34.4792	34.5543	0	34.5543	0	4.31956
H	11	7.52846	29.1603	0	29.1603	31.667	0	31.667	0	4.05995
N - nitramine	12	9.49295	30.3831	0	30.3831	91.9403	0	91.9403	0	7.49848
H	13	5.43751	49.0471	0	49.0471	81.5923	0	81.5923	0	7.62854
N - nitro	14	3.11287	20.4981	-7.97461	19.1466	53.5277	43.6085	97.1362	0.247393	7.00557
O - nitro	15	25.6157	8.58808	-18.5273	-14.3313	35.6287	61.0377	96.6664	0.232727	10.0226
O - nitro	16	21.9795	9.13324	-15.5839	-10.1968	39.8153	66.7636	106.579	0.234017	10.5685

See figure A-4 for corresponding atom with atom number.

Table A-64. NQ area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	21.2304	4.52542	-24.8942	-22.9007	13.154	149.606	162.76	0.074287	11.6854
O - nitro	2	25.187	0	-37.7951	-37.7951	0	51.7182	51.7182	0	5.46047
N - amino	3	17.2283	25.0786	0	25.0786	145.928	0	145.928	0	10.2015
N - amino	4	17.1685	22.125	0	22.125	131.387	0	131.387	0	9.76041
N - nitramine	5	16.2652	4.67584	-19.1472	-14.7133	8.58317	129.573	138.156	0.058267	11.8806
N - nitro	6	3.37466	2.93216	-8.95517	-5.78523	4.77276	58.4004	63.1732	0.069843	6.43564
C	7	2.47261	15.5639	0	15.5639	34.2265	0	34.2265	0	4.28091
H - amino	8	5.70453	37.7557	0	37.7557	102.888	0	102.888	0	8.51672
H - amino	9	7.20981	57.2057	0	57.2057	73.635	0	73.635	0	7.26781
H - amino	10	6.87621	55.7502	0	55.7502	85.1915	0	85.1915	0	7.88403
H - amino	11	2.6931	23.908	-0.10228	23.7659	76.8996	0	76.8996	0	7.52342

See figure A-5 for corresponding atom with atom number.

Table A-65. RDX area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.20372	31.1509	0	31.1509	20.3854	0	20.3854	0	3.01414
C	2	2.46173	32.0166	0	32.0166	7.79754	0	7.79754	0	1.56783
C	3	2.13272	32.509	0	32.509	15.3865	0	15.3865	0	2.47187
H	4	9.47319	41.5017	0	41.5017	33.9464	0	33.9464	0	4.99834
H	5	5.00754	22.1125	-2.96533	21.6999	44.0281	3.91103	47.9391	0.074927	5.78372
H	6	5.7238	26.1574	0	26.1574	35.3883	0	35.3883	0	4.67616
H	7	9.50805	41.8144	0	41.8144	28.6385	0	28.6385	0	4.64093
H	8	9.59823	41.4455	0	41.4455	29.1534	0	29.1534	0	4.61555
H	9	5.06259	23.5858	-3.14509	23.3584	45.7793	1.40394	47.1832	0.02887	5.65785
N - nitramine	10	3.75951	27.2249	0	27.2249	142.474	0	142.474	0	11.1482
N - nitramine	11	6.09917	21.4454	0	21.4454	38.0308	0	38.0308	0	4.89163
N - nitramine	12	6.06321	21.7647	0	21.7647	33.4635	0	33.4635	0	4.60493
N - nitro	13	3.20025	22.4098	-8.37787	21.2757	108.533	64.3984	172.931	0.233717	9.76928
N - nitro	14	2.59596	22.9282	-6.23944	22.0801	68.3471	49.726	118.073	0.243782	6.71065
N - nitro	15	2.80996	23.5207	-8.63993	22.1946	69.514	27.4217	96.9357	0.202861	7.19004
O - nitro	16	22.2	9.80228	-15.4161	-10.8664	64.4557	47.5946	112.05	0.244339	9.51379
O - nitro	17	22.3775	9.4583	-15.9769	-11.9276	58.6563	51.4146	110.071	0.248918	9.32631
O - nitro	18	19.7166	8.01294	-15.364	-11.2943	29.4773	42.6163	72.0937	0.241696	8.9462
O - nitro	19	21.4191	8.91527	-14.2858	-9.76551	37.4676	41.0297	78.4972	0.249485	9.06413
O - nitro	20	19.6053	9.46886	-15.2204	-10.3677	47.1515	39.5218	86.6733	0.248063	9.53756
O - nitro	21	21.4749	8.55796	-13.7792	-9.18836	35.5327	38.1036	73.6363	0.249695	8.88271

See figure A-6 for corresponding atom with atom number.

Table A-66. CL20 area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.0251	11.3437	-8.0292	-0.3413	72.1979	18.6241	90.822	0.163011	9.27681
O - nitro	2	19.5267	11.8418	-8.72148	-1.4962	69.6932	15.5244	85.2176	0.148986	9.41554
O - nitro	3	20.3858	11.1376	-7.23615	1.06336	70.9452	16.7357	87.6809	0.154439	9.14165
O - nitro	4	17.8329	11.5275	-7.64297	-0.67877	76.1694	15.0567	91.2261	0.137807	8.87789
O - nitro	5	20.6222	12.06	-7.3532	0.796355	89.8527	15.8087	105.661	0.127231	9.47528
O - nitro	6	19.8996	12.2242	-8.91245	-2.09578	102.336	15.4874	117.823	0.114168	9.33274
O - nitro	7	20.7272	14.116	-8.59917	-0.60382	135.536	14.4068	149.943	0.08685	10.3687
O - nitro	8	20.9355	9.92873	-7.69062	-1.9219	83.241	16.3905	99.6314	0.137447	7.87456
O - nitro	9	22.2638	13.2396	-7.13888	2.31912	108.274	16.2229	124.497	0.113328	10.2754
O - nitro	10	20.5972	13.2388	-8.24206	-0.64316	115.219	15.6981	130.917	0.105531	9.82867
O - nitro	11	20.6855	9.41677	-7.36739	-2.61917	63.7034	14.6484	78.3519	0.152004	7.05516
O - nitro	12	22.1707	13.9809	-6.38551	3.53526	141.027	13.101	154.128	0.077776	10.5334
N - nitramine	13	4.93297	31.605	0	31.605	27.2286	0	27.2286	0	4.13774
N - nitramine	14	5.24399	31.376	0	31.376	28.3013	0	28.3013	0	4.23214
N - nitramine	15	3.2793	39.6297	0	39.6297	27.2848	0	27.2848	0	4.39749
N - nitramine	16	0.952927	37.5118	0	37.5118	350.464	0	350.464	0	16.7037
N - nitramine	17	1.92621	41.1612	0	41.1612	41.6451	0	41.6451	0	5.17534
N - nitramine	18	1.5474	34.0864	0	34.0864	139.821	0	139.821	0	7.33193
N - nitro	19	1.86702	28.8139	0	28.8139	41.3514	0	41.3514	0	4.81998
N - nitro	20	1.84453	29.1469	0	29.1469	53.4805	0	53.4805	0	5.39484
N - nitro	21	1.84477	31.0454	-6.43455	29.8009	121.47	16.1072	137.577	0.103371	9.99031
N - nitro	22	2.89805	37.0138	0	37.0138	237.911	0	237.911	0	13.6295
N - nitro	23	2.93851	31.8383	-8.02178	31.6012	110.826	1.69321	112.52	0.014822	8.70316
N - nitro	24	3.0126	35.2028	-5.5522	35.084	228.009	0	228.009	0	12.474
C	25	0.813401	55.1663	0	55.1663	24.4582	0	24.4582	0	3.51318
C	26	1.05366	53.198	0	53.198	32.2498	0	32.2498	0	4.62914
C	27	0.457938	39.2046	0	39.2046	9.67338	0	9.67338	0	2.46332
C	28	0.285441	37.7685	0	37.7685	32.1276	0	32.1276	0	4.7282

See figure A-7 for corresponding atom with atom number.

Table A-66. CL20 area weighted atom specific Politzer parameters using B3LYP/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	29	0.912986	55.5813	0	55.5813	73.7706	0	73.7706	0	6.28352
C	30	0.924783	57.9215	0	57.9215	30.3445	0	30.3445	0	4.75624
H	31	5.77699	45.5753	0	45.5753	79.8452	0	79.8452	0	7.19099
H	32	6.25425	46.0708	0	46.0708	57.5121	0	57.5121	0	6.11509
H	33	6.34408	38.7604	0	38.7604	15.4946	0	15.4946	0	3.1136
H	34	3.63514	32.934	0	32.934	48.1442	0	48.1442	0	5.7385
H	35	3.83136	42.1067	0	42.1067	87.7425	0	87.7425	0	7.68838
H	36	4.43815	45.0639	0	45.0639	78.8675	0	78.8675	0	6.97588

See figure A-7 for corresponding atom with atom number.

Table A-67. HNB area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.91595	46.1518	0	46.1518	20.5746	0	20.5746	0	3.52825
C	2	4.01251	46.2413	0	46.2413	20.0027	0	20.0027	0	3.4637
C	3	3.89221	45.8897	0	45.8897	19.746	0	19.746	0	3.46814
N - nitro	4	0.706133	21.2584	-1.10755	20.9414	97.9474	-1.67E-16	97.9474	-1.70E-18	8.33473
N - nitro	5	0.702257	24.3442	-2.31237	23.7423	100.359	0	100.359	0	8.97847
N - nitro	6	0.609493	23.541	0	23.541	117.89	0	117.89	0	9.8459
O - nitro	7	20.9679	10.2399	-5.84776	0.477902	78.4185	11.773	90.1914	0.113494	7.68687
O - nitro	8	19.9471	10.3162	-3.50572	6.25497	79.8286	4.11465	83.9432	0.046614	7.59942
O - nitro	9	20.7956	9.22047	-4.02124	4.262	70.9022	6.31084	77.2131	0.075053	7.28067
O - nitro	10	20.4976	9.64241	-3.84714	4.95699	75.0091	5.60938	80.6185	0.064738	7.44907
O - nitro	11	20.3858	9.36979	-4.86942	3.24788	77.9696	9.58017	87.5497	0.097452	7.56536
O - nitro	12	21.0974	10.2853	-5.58592	0.652987	80.8432	11.9354	92.7786	0.112094	7.58956
C	13	3.87758	45.9786	0	45.9786	18.628	0	18.628	0	3.34468
C	14	3.95631	45.7785	0	45.7785	18.9041	0	18.9041	0	3.38093
C	15	4.02845	46.0444	0	46.0444	17.7163	0	17.7163	0	3.27645
N - nitro	16	0.648215	20.9553	0	20.9553	96.5807	0	96.5807	0	7.94742
N - nitro	17	0.742839	23.9561	0	23.9561	104.951	0	104.951	0	9.55757
N - nitro	18	0.662175	21.7346	-0.29381	21.2015	72.1314	0.00517	72.1366	7.17E-05	6.66941
O - nitro	19	20.9267	10.1326	-5.83661	0.424675	77.8913	11.8577	89.749	0.114665	7.62232
O - nitro	20	20.1506	10.4433	-3.51448	6.34127	82.1356	4.05493	86.1905	0.044833	7.69665
O - nitro	21	20.298	9.18459	-4.86164	3.06582	74.2862	9.54549	83.8317	0.1009	7.43173
O - nitro	22	21.0401	10.3152	-5.59397	0.688542	81.5795	11.9524	93.5319	0.111459	7.61917
O - nitro	23	20.7968	9.25452	-3.97247	4.24328	71.3385	6.42757	77.7661	0.075821	7.26628
O - nitro	24	20.516	9.61148	-3.90445	4.9934	76.057	5.48824	81.5453	0.062773	7.47064

See figure A-8 for corresponding atom with atom number.

Table A-68. TATB area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.80055	23.4759	0	23.4759	4.01155	0	4.01155	0	1.57357
C	2	3.63684	24.3414	0	24.3414	1.74815	0	1.74815	0	0.942492
C	3	6.77441	22.0866	0	22.0866	2.63978	0	2.63978	0	1.26957
C	4	3.7772	23.7527	0	23.7527	1.2958	0	1.2958	0	0.858321
C	5	6.58696	23.1833	0	23.1833	1.86924	0	1.86924	0	1.11685
C	6	3.78539	24.7314	0	24.7314	2.78743	0	2.78743	0	1.32709
H - amino	7	2.16188	26.7657	0	26.7657	45.4076	0	45.4076	0	5.72102
H - amino	8	2.31467	27.8526	0	27.8526	41.558	0	41.558	0	5.42106
H - amino	9	2.19187	26.9873	0	26.9873	59.9305	0	59.9305	0	6.49727
H - amino	10	3.21232	31.2778	0	31.2778	53.8319	0	53.8319	0	6.10862
H - amino	11	2.30374	27.2135	0	27.2135	46.135	0	46.135	0	5.78016
H - amino	12	2.89449	30.1636	0	30.1636	35.2493	0	35.2493	0	4.67998
N - nitro	13	3.69768	21.2646	-3.25308	21.0253	27.7479	1.99724	29.7451	0.062637	4.22503
N - amino	14	15.4112	19.6545	0	19.6545	58.0655	0	58.0655	0	6.04186
N - nitro	15	3.79005	19.0781	-7.68347	18.1746	25.2186	38.4024	63.621	0.239265	4.85341
N - amino	16	15.0994	19.1437	0	19.1437	54.8564	0	54.8564	0	5.85709
N - nitro	17	3.90802	20.6822	-6.05703	20.2195	25.774	16.9421	42.7161	0.239313	4.42767
N - amino	18	15.2355	19.5564	0	19.5564	68.9707	0	68.9707	0	6.82848
O - nitro	19	19.8826	9.81208	-13.755	-6.68715	51.1753	58.7408	109.916	0.248816	10.9284
O - nitro	20	20.2212	8.81087	-14.0896	-7.30742	34.8298	59.8403	94.6701	0.232551	10.7431
O - nitro	21	20.2422	8.44783	-15.3536	-9.43477	34.1547	70.5549	104.71	0.219788	10.8469
O - nitro	22	20.5441	7.8201	-15.2436	-9.67611	27.2747	69.1201	96.3948	0.202888	10.5178
O - nitro	23	19.5878	9.77358	-13.357	-5.26649	40.7356	58.6279	99.3635	0.241894	11.1902
O - nitro	24	20.3258	8.40735	-14.1482	-7.745	31.2238	60.4458	91.6696	0.224596	10.5346

See figure A-9 for corresponding atom with atom number.

Table A-69. PNA area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.08328	42.1196	0	42.1196	6.21553	0	6.21553	0	1.72991
C	2	5.18688	37.424	0	37.424	24.6001	0	24.6001	0	3.87638
C	3	3.45234	32.1776	0	32.1776	21.3873	0	21.3873	0	3.71446
C	4	4.57443	31.7335	0	31.7335	12.0124	0	12.0124	0	2.58008
N - amino	5	16.0517	38.8245	0	38.8245	56.2108	0	56.2108	0	6.19328
H - amino	6	2.753	48.208	0	48.208	38.6953	0	38.6953	0	5.17022
N - nitro	7	2.73145	35.432	-2.92608	35.3177	126.273	0	126.273	0	9.70194
N - nitro	8	0.234	8.10103	-3.42832	4.31104	94.0642	23.7389	117.803	0.160906	7.36265
N - nitro	9	1.90051	19.1727	-1.69675	18.345	48.3284	1.94991	50.2784	0.037278	6.39691
O - nitro	10	21.0089	14.2741	-5.24044	8.25977	112.945	8.30508	121.25	0.063804	10.5131
O - nitro	11	19.1991	12.2862	-6.80292	-0.4368	92.5108	11.5809	104.092	0.098878	8.49225
O - nitro	12	21.0819	9.45634	-9.36284	-5.65251	50.8575	21.4576	72.3151	0.208679	6.84396
O - nitro	13	20.2918	9.27571	-9.65215	-6.51605	49.9425	20.0158	69.9583	0.204251	6.33783
O - nitro	14	19.4993	9.44709	-10.5798	-6.5206	47.7612	21.0693	68.8305	0.212404	7.35124
C	15	5.18721	37.4816	0	37.4816	24.0649	0	24.0649	0	3.82106
C	16	3.47138	32.1536	0	32.1536	21.5883	0	21.5883	0	3.73521
H - amino	17	2.77321	48.224	0	48.224	38.0606	0	38.0606	0	5.14406
N - nitro	18	2.60869	35.3514	0	35.3514	131.504	0	131.504	0	9.93288
N - nitro	19	0.229684	6.20342	-3.57397	2.07422	45.944	18.108	64.052	0.202784	5.20812
O - nitro	20	20.9846	14.3301	-5.15774	8.22339	111.664	8.56411	120.228	0.066158	10.4874
O - nitro	21	19.2165	12.4683	-6.82406	-0.34543	96.4066	11.488	107.895	0.095137	8.60957
O - nitro	22	21.0814	9.36187	-9.35475	-5.68059	50.1666	21.5772	71.7438	0.210301	6.81571
O - nitro	23	20.184	9.1144	-9.66702	-6.56677	50.6398	19.9674	70.6071	0.202822	6.29899
O - nitro	24	19.5302	9.48983	-10.5518	-6.52828	47.6009	21.1432	68.7441	0.212968	7.32319

See figure A-10 for corresponding atom with atom number.

Table A-70. TNT area weighted atom specific Politzer parameters using B3LYP/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.7121	8.79184	-9.65033	-4.0085	45.5341	27.8706	73.4047	0.235524	8.29228
O - nitro	2	23.1033	9.91827	-10.162	-4.09442	53.2846	26.741	80.0256	0.222496	8.87766
O - nitro	3	23.4109	9.35401	-11.5316	-6.15172	42.556	33.6562	76.2122	0.246591	8.90335
O - nitro	4	23.3247	9.73049	-11.3257	-5.69002	53.9738	30.6992	84.6729	0.231111	8.97566
O - nitro	5	23.8747	10.5692	-9.84293	-3.6668	64.142	22.2221	86.3641	0.1911	8.92282
O - nitro	6	21.9501	8.66684	-9.24997	-4.10368	45.6989	22.6011	68.3	0.221408	7.79985
N - nitro	7	3.24867	29.3332	-8.9511	28.1144	49.5838	30.4293	80.0131	0.235673	6.73721
N - nitro	8	3.54912	27.3044	-3.35846	26.6698	47.3152	8.63354	55.9487	0.1305	6.0389
N - nitro	9	1.79253	29.3179	-6.21987	28.9393	59.1154	0	59.1154	0	6.37129
C	10	5.21715	25.3466	0	25.3466	15.7863	0	15.7863	0	2.97845
C	11	7.17809	23.619	0	23.619	20.2327	0	20.2327	0	3.3153
C	12	5.41616	25.018	0	25.018	17.0031	0	17.0031	0	3.05262
C	13	6.81314	23.2897	0	23.2897	48.1154	0	48.1154	0	6.0609
C	14	4.56648	23.3422	0	23.3422	18.2747	0	18.2747	0	3.21397
C	15	4.6406	26.1557	0	26.1557	21.2121	0	21.2121	0	3.9177
C	16	3.70782	23.0914	0	23.0914	41.8257	0	41.8257	0	4.99271
H	17	6.99601	25.7338	0	25.7338	20.91	0	20.91	0	3.65754
H	18	7.77584	30.3248	0	30.3248	52.7478	0	52.7478	0	6.10292
H	19	8.26568	25.5476	0	25.5476	20.1926	0	20.1926	0	3.10195
H	20	9.50324	18.0045	0	18.0045	13.4191	0	13.4191	0	2.95419
H	21	7.90003	24.5841	0	24.5841	22.4232	0	22.4232	0	3.54904

See figure A-11 for corresponding atom with atom number.

A.10 Area Weighted PBE/6-31G* Training Set Data

Table A-71. FOX-7 area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.10049	18.1291	0	18.1291	18.9372	0	18.9372	0	3.35866
N - amino	2	16.0264	29.1004	0	29.1004	173.917	0	173.917	0	11.2369
H - amino	3	5.87179	61.352	0	61.352	51.2619	0	51.2619	0	5.93002
H - amino	4	3.13297	36.2675	0	36.2675	85.2234	0	85.2234	0	7.76156
N - amino	5	16.1221	28.529	0	28.529	161.846	0	161.846	0	10.9371
H - amino	6	2.75022	32.2431	0	32.2431	90.4588	0	90.4588	0	8.08028
H - amino	7	6.09525	61.5706	0	61.5706	56.1614	0	56.1614	0	6.30534
C	8	6.51004	7.04111	-1.82428	6.89046	18.897	1.02022	19.9173	0.048599	3.7338
N - nitro	9	3.47109	8.88887	-6.3363	3.38952	45.2453	26.7405	71.9858	0.23348	7.77585
O - nitro	10	20.284	2.30893	-27.7596	-27.3812	2.03211	80.096	82.1281	0.024131	7.45906
O - nitro	11	19.6603	8.92988	-17.7308	-13.9267	40.379	79.9296	120.309	0.222982	10.2403
N - nitro	12	3.85552	4.88232	-5.998	0.627362	9.41597	28.1091	37.5251	0.187961	5.2068
O - nitro	13	20.2358	0	-30.0975	-30.0975	0	77.2219	77.2219	0	6.88389
O - nitro	14	19.7749	6.66658	-19.3127	-15.373	19.9212	102.536	122.458	0.136214	11.138

See figure A-1 for corresponding atom with atom number.

Table A-72. HMX area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.32378	32.6215	0	32.6215	39.4214	0	39.4214	0	5.52721
C	2	1.68924	31.3375	0	31.3375	56.7995	0	56.7995	0	6.04683
H	3	7.23016	36.203	0	36.203	32.6775	0	32.6775	0	4.79136
H	4	6.20035	28.371	0	28.371	56.9217	0	56.9217	0	6.21025
H	5	7.17732	26.3787	0	26.3787	32.0336	0	32.0336	0	4.68905
H	6	7.43274	34.0665	0	34.0665	61.0102	0	61.0102	0	6.38797
N - nitro	7	2.47588	13.7888	-6.43927	11.5569	38.5499	46.6725	85.2224	0.247729	7.10129
N - nitramine	8	3.42078	13.8806	0	13.8806	28.401	0	28.401	0	4.2636
N - nitramine	9	2.4773	34.6403	0	34.6403	5.17872	0	5.17872	0	1.7468
N - nitro	10	2.67259	30.156	0	30.156	76.2528	0	76.2528	0	6.5772
O - nitro	11	19.8968	6.20334	-15.2923	-12.6215	17.4819	41.3634	58.8453	0.208825	7.54983
O - nitro	12	20.6396	7.72252	-12.8347	-8.50639	32.1435	42.6971	74.8406	0.245029	8.56663
O - nitro	13	19.6786	10.4138	-8.43446	-1.9764	71.5165	20.1894	91.706	0.171686	8.59795
O - nitro	14	18.0417	12.5834	-11.1834	-4.55936	85.4306	21.6985	107.129	0.161521	9.96439
N - nitramine	15	2.50557	34.7113	0	34.7113	5.58316	0	5.58316	0	1.78645
C	16	1.80091	30.5312	0	30.5312	67.0952	0	67.0952	0	6.68194
C	17	2.2641	32.4513	0	32.4513	38.7563	0	38.7563	0	5.48649
N - nitro	18	2.72376	29.3376	-4.53248	28.8484	79.627	14.974	94.601	0.133231	7.23857
H	19	7.21179	26.3188	0	26.3188	32.1387	0	32.1387	0	4.70853
H	20	7.3143	34.3462	0	34.3462	57.9788	0	57.9788	0	6.23919
N - nitramine	21	3.3951	14.1376	0	14.1376	32.6673	0	32.6673	0	4.40346
H	22	7.20933	36.1358	0	36.1358	33.2465	0	33.2465	0	4.82405
H	23	6.23671	28.3153	0	28.3153	59.0854	0	59.0854	0	6.28468
O - nitro	24	19.5455	10.3608	-8.40735	-2.07073	68.8449	20.3362	89.1811	0.176034	8.52116
O - nitro	25	17.9535	12.4433	-11.2299	-4.59124	83.6741	21.3424	105.016	0.161927	9.94846
N - nitro	26	2.45382	13.9885	-4.14372	11.9716	37.7902	13.8905	51.6807	0.196536	6.809
O - nitro	27	19.9742	6.2087	-15.3039	-12.6381	17.8967	41.2669	59.1635	0.210992	7.54603
O - nitro	28	20.6361	7.80031	-12.8426	-8.47859	33.1868	42.5689	75.7557	0.246165	8.5933

See figure A-2 for corresponding atom with atom number.

Table A-73. PETN area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.98498	26.8202	0	26.8202	39.1459	0	39.1459	0	5.34612
O - nitro	3	20.7969	9.48206	-5.88639	0.871252	56.0149	11.1609	67.1758	0.13854	7.60547
O - nitro	4	23.7897	7.53728	-8.77686	-5.31911	29.6794	13.0885	42.7679	0.212378	6.20598
O - nitrate	5	9.12924	13.4695	-0.78192	13.0742	78.9314	0.310736	79.2422	0.003906	7.52389
N - nitro	6	3.81821	24.9137	-3.59913	24.7266	35.439	2.32015	37.7592	0.05767	4.89066
H	7	6.22246	26.9178	0	26.9178	24.8203	0	24.8203	0	3.90587
H	8	7.46007	27.0715	0	27.0715	19.6981	0	19.6981	0	3.50178
C	9	1.00424	25.8528	0	25.8528	47.4848	0	47.4848	0	5.91487
C	10	0.97041	26.023	0	26.023	47.6453	0	47.6453	0	6.06036
C	11	0.995112	25.799	0	25.799	42.8261	0	42.8261	0	5.70136
O - nitro	12	20.7713	9.51868	-5.88807	0.8918	56.117	11.1927	67.3096	0.138635	7.62528
O - nitro	13	20.8477	9.59724	-5.87322	0.909162	57.3155	11.1826	68.498	0.136602	7.64944
O - nitro	14	20.7995	9.49949	-5.8728	0.860947	55.4759	11.2295	66.7054	0.140005	7.59677
O - nitro	15	23.7489	7.62151	-8.77217	-5.32425	30.2012	13.1185	43.3197	0.211124	6.20863
O - nitro	16	23.7985	7.5758	-8.75816	-5.31895	29.838	13.1853	43.0233	0.212545	6.1988
O - nitro	17	23.7923	7.50734	-8.75778	-5.34647	28.9959	13.1833	42.1792	0.214864	6.17018
O - nitrate	18	9.20857	13.6789	-0.8754	13.3111	82.7197	0.23391	82.9536	0.002812	7.69829
O - nitrate	19	9.09263	13.4806	-0.89145	13.1301	78.3239	0.327001	78.6509	0.00414	7.4903
O - nitrate	20	9.15262	13.6334	-0.72679	13.27	80.3203	0.216028	80.5364	0.002675	7.58619
N - nitro	21	3.77447	24.5693	-2.92412	23.9563	37.9172	5.37521	43.2924	0.108745	5.41393
N - nitro	22	3.69611	24.8962	-0.59049	24.8376	38.0189	0	38.0189	0	4.8638
N - nitro	23	3.74262	24.9419	-1.86619	24.7405	34.4249	0.870758	35.2957	0.024062	4.82026
H	24	6.26835	26.9906	0	26.9906	24.3603	0	24.3603	0	3.89405
H	25	6.32996	27.0283	0	27.0283	25.1904	0	25.1904	0	3.95523
H	26	6.33318	27.0178	0	27.0178	25.2731	0	25.2731	0	3.9418
H	27	7.44717	27.0842	0	27.0842	19.1458	0	19.1458	0	3.46415
H	28	7.58651	27.1317	0	27.1317	19.9461	0	19.9461	0	3.53528
H	29	7.5277	27.119	0	27.119	19.9791	0	19.9791	0	3.53961

See figure A-3 for corresponding atom with atom number.

Table A-74. EDNA area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.66498	29.5555	0	29.5555	49.1847	0	49.1847	0	5.19827
H	2	8.55133	30.9265	0	30.9265	34.9545	0	34.9545	0	4.4861
H	3	7.29847	25.6709	0	25.6709	30.9704	0	30.9704	0	4.09313
H	4	5.51812	47.6664	0	47.6664	57.8399	0	57.8399	0	6.36744
N - nitramine	5	9.26989	26.8024	0	26.8024	96.5529	0	96.5529	0	7.76083
N - nitro	6	3.4129	15.6172	-5.64244	14.2742	38.7755	25.3969	64.1724	0.239134	6.09965
O - nitro	7	23.9818	8.50255	-18.4735	-14.5793	39.923	58.4574	98.3804	0.241127	9.65203
O - nitro	8	20.967	7.54745	-15.793	-11.5331	29.3423	62.8453	92.1876	0.216981	9.61359
C	9	2.65933	29.5954	0	29.5954	47.7334	0	47.7334	0	5.02139
H	10	8.42198	30.9847	0	30.9847	35.5147	0	35.5147	0	4.50864
H	11	7.2376	25.6649	0	25.6649	31.2183	0	31.2183	0	4.09674
N - nitramine	12	9.31576	26.7113	0	26.7113	94.5579	0	94.5579	0	7.67866
H	13	5.51735	47.6597	0	47.6597	58.7923	0	58.7923	0	6.39723
N - nitro	14	3.3894	15.7014	-6.40064	14.3736	38.4424	22.7751	61.2176	0.233625	6.06268
O - nitro	15	24.005	8.19033	-18.4465	-14.6865	34.9949	59.1829	94.1778	0.233509	9.55833
O - nitro	16	20.8882	7.36652	-15.8318	-11.5277	29.3449	62.0276	91.3724	0.218015	9.59011

See figure A-4 for corresponding atom with atom number.

Table A-75. NQ area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.0701	3.77819	-25.052	-23.8517	8.23307	142.202	150.435	0.051733	10.8539
O - nitro	2	23.5677	0	-38.2007	-38.2007	0	44.4029	44.4029	0	5.06934
N - amino	3	16.7578	23.0787	0	23.0787	180.086	0	180.086	0	11.4687
N - amino	4	16.7284	19.843	-0.78052	19.7276	154.857	0.490977	155.348	0.003151	10.7863
N - nitramine	5	15.5379	2.77402	-20.1428	-18.0621	3.98784	142.632	146.62	0.026459	11.2581
N - nitro	6	3.68565	1.82087	-9.82431	-9.12319	1.98275	39.434	41.4167	0.045581	5.24246
C	7	2.92972	9.7829	-0.21854	9.68804	34.8021	0.018512	34.8206	0.000531	4.24464
H - amino	8	5.52053	37.3533	0	37.3533	97.6965	0	97.6965	0	8.26839
H - amino	9	6.93801	57.1844	0	57.1844	62.029	0	62.029	0	6.64535
H - amino	10	6.61878	55.4213	0	55.4213	76.1088	0	76.1088	0	7.41952
H - amino	11	2.8048	22.0701	-0.25477	21.9879	79.002	0	79.002	0	7.63782

See figure A-5 for corresponding atom with atom number.

Table A-76. RDX area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.53959	27.1141	0	27.1141	16.1971	0	16.1971	0	2.54639
C	2	2.83725	28.0983	0	28.0983	9.87442	0	9.87442	0	2.05058
C	3	2.42195	28.5589	0	28.5589	13.2785	0	13.2785	0	2.24208
H	4	9.25737	37.3599	0	37.3599	28.1337	0	28.1337	0	4.54704
H	5	4.88613	20.0231	-3.16336	19.4085	45.1395	3.72385	48.8634	0.070402	6.11929
H	6	5.57739	23.9685	-3.75627	23.9093	37.1742	2.67E-15	37.1742	7.18E-17	4.86641
H	7	9.23668	37.7901	0	37.7901	25.4603	0	25.4603	0	4.3428
H	8	9.47473	37.2611	0	37.2611	24.1802	0	24.1802	0	4.19733
H	9	4.9411	21.5191	-3.99162	21.1118	46.5452	3.53113	50.0763	0.065543	5.94117
N - nitramine	10	4.0675	21.9697	0	21.9697	127.694	0	127.694	0	10.4569
N - nitramine	11	5.95797	17.2426	0	17.2426	33.7822	0	33.7822	0	4.60251
N - nitramine	12	5.96246	17.6587	0	17.6587	30.9353	0	30.9353	0	4.38098
N - nitro	13	3.44368	17.7756	-4.507	16.9691	84.3487	22.7561	107.105	0.167324	8.51625
N - nitro	14	2.93678	18.428	-6.38165	17.7624	44.5415	20.4837	65.0252	0.215779	5.43313
N - nitro	15	3.06776	19.2212	-9.79375	18.5123	43.1038	37.058	80.1618	0.248578	5.3524
O - nitro	16	21.184	8.61573	-15.0109	-11.3215	46.709	43.8433	90.5523	0.24975	8.61925
O - nitro	17	21.2511	8.04138	-15.4857	-12.2258	43.5755	46.3501	89.9256	0.249762	8.39299
O - nitro	18	19.0274	6.84253	-14.972	-11.5348	20.5025	38.2719	58.7744	0.227149	8.15445
O - nitro	19	20.5345	7.70851	-13.7632	-9.91001	28.3027	36.1328	64.4355	0.246308	8.23726
O - nitro	20	18.8193	8.25363	-14.6859	-10.6788	30.3638	37.1907	67.5545	0.247447	8.65982
O - nitro	21	20.7314	7.47434	-13.2581	-9.23569	27.1475	33.332	60.4795	0.247386	8.13962

See figure A-6 for corresponding atom with atom number.

Table A-77. CL20 area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.5319	10.1444	-8.17742	-1.74312	54.4357	18.7482	73.1839	0.190552	8.43542
O - nitro	2	18.7943	10.2378	-9.18212	-3.27281	50.2054	16.3807	66.5861	0.185488	8.47396
O - nitro	3	19.7271	9.75696	-7.351	-0.43166	50.7504	16.8671	67.6176	0.187224	8.24758
O - nitro	4	17.4561	10.0717	-8.16323	-2.11492	56.8274	14.8025	71.6299	0.163947	8.18657
O - nitro	5	19.8358	10.8498	-7.09238	-0.08646	72.0638	14.0109	86.0747	0.13628	8.54081
O - nitro	6	19.4284	11.4932	-8.71698	-2.53352	89.528	14.556	104.084	0.120291	8.74264
O - nitro	7	20.0506	12.7274	-8.45685	-1.32406	110.968	13.1173	124.085	0.094537	9.49543
O - nitro	8	20.5185	9.3029	-7.39236	-2.16959	68.3437	13.9188	82.2624	0.140571	7.33315
O - nitro	9	21.3778	11.7372	-6.78532	1.48503	84.9306	13.638	98.5686	0.119217	9.22567
O - nitro	10	19.8787	11.869	-8.14185	-1.3774	95.6349	13.5074	109.142	0.108443	8.99987
O - nitro	11	20.3231	8.27034	-7.16835	-2.90661	49.103	12.174	61.277	0.159201	6.44616
O - nitro	12	21.3206	12.5269	-6.03599	2.61678	106.693	11.0119	117.705	0.084803	9.44843
N - nitramine	13	4.99373	25.1943	0	25.1943	25.9561	0	25.9561	0	4.14726
N - nitramine	14	5.33875	25.1105	0	25.1105	27.2542	0	27.2542	0	4.29468
N - nitramine	15	3.27032	33.8542	0	33.8542	22.3684	0	22.3684	0	4.01925
N - nitramine	16	1.06839	28.7971	0	28.7971	225.659	0	225.659	0	12.17
N - nitramine	17	2.02035	34.4358	0	34.4358	42.2507	0	42.2507	0	5.28691
N - nitramine	18	1.57985	28.0415	0	28.0415	130.808	0	130.808	0	7.43777
N - nitro	19	2.1177	23.0272	-8.7586	22.265	34.2044	13.4628	47.6672	0.202665	5.35979
N - nitro	20	2.03608	24.7226	-7.34011	24.0603	24.7826	3.62371	28.4063	0.111294	4.67388
N - nitro	21	2.03014	26.8514	-3.28743	26.2983	94.912	0.424305	95.3363	0.004431	8.35423
N - nitro	22	3.15932	30.3903	0	30.3903	183.056	0	183.056	0	11.9536
N - nitro	23	3.27506	27.4271	0	27.4271	80.1638	0	80.1638	0	7.45789
N - nitro	24	3.24451	30.7975	-5.14181	30.6292	163.283	0.00E+00	163.283	0.00E+00	11.0362
C	25	1.06216	47.4169	0	47.4169	28.3728	0	28.3728	0	4.09726
C	26	1.27737	46.2996	0	46.2996	27.4448	0	27.4448	0	4.41478
C	27	0.614418	33.9836	0	33.9836	10.7895	0	10.7895	0	2.49702
C	28	0.412063	32.2136	0	32.2136	32.9426	0	32.9426	0	4.93469

See figure A-7 for corresponding atom with atom number.

Table A-77. CL20 area weighted atom specific Politzer parameters using PBE/6-31G* (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	29	1.08571	48.1818	0	48.1818	63.4043	0	63.4043	0	5.76948
C	30	1.13166	50.7066	0	50.7066	23.1425	0	23.1425	0	3.43511
H	31	5.55672	40.8518	0	40.8518	75.1543	0	75.1543	0	6.96656
H	32	6.00719	41.3203	0	41.3203	53.4962	0	53.4962	0	5.90557
H	33	6.19856	34.6369	0	34.6369	12.657	0	12.657	0	2.79439
H	34	3.58745	28.7062	0	28.7062	46.1887	0	46.1887	0	5.56498
H	35	3.83755	37.6579	0	37.6579	98.2857	0	98.2857	0	8.14963
H	36	4.18348	40.9721	0	40.9721	74.7388	0	74.7388	0	6.80782

See figure A-7 for corresponding atom with atom number.

Table A-78. HNB area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.20308	37.9683	0	37.9683	13.8076	0	13.8076	0	2.81867
C	2	4.2641	38.0592	0	38.0592	13.2406	0	13.2406	0	2.78584
C	3	4.21499	37.7922	0	37.7922	12.7558	0	12.7558	0	2.73848
N - nitro	4	0.852592	19.2711	0	19.2711	58.7686	0	58.7686	0	6.26349
N - nitro	5	0.953352	20.7343	0	20.7343	49.4306	0	49.4306	0	5.9154
N - nitro	6	0.855616	20.4963	-1.53363	20.3135	72.297	0	72.297	0	7.85885
O - nitro	7	20.2032	9.29971	-5.52408	-0.04868	57.1409	10.5232	67.6641	0.131334	6.906
O - nitro	8	19.6342	9.13949	-3.43044	5.08525	63.6491	4.14091	67.79	0.057353	6.97157
O - nitro	9	19.9569	8.3657	-3.69045	3.37322	54.0292	6.07915	60.1084	0.090908	6.55202
O - nitro	10	19.9684	8.64132	-3.64478	3.91071	60.1662	5.58515	65.7513	0.077728	6.76186
O - nitro	11	19.7275	8.48403	-4.77176	1.84301	55.8917	9.75047	65.6422	0.126476	6.80974
O - nitro	12	20.3607	9.47112	-5.69132	-0.33088	61.8321	11.2476	73.0797	0.130221	6.93526
C	13	4.09897	37.9728	0	37.9728	12.8276	0	12.8276	0	2.72362
C	14	4.16621	37.8448	0	37.8448	13.1191	0	13.1191	0	2.74849
C	15	4.37588	37.9086	0	37.9086	13.6174	0	13.6174	0	2.80945
N - nitro	16	0.890557	19.1404	0	19.1404	66.2959	0	66.2959	0	6.82213
N - nitro	17	0.931045	19.4389	0	19.4389	75.018	0	75.018	0	7.71762
N - nitro	18	0.9124	19.739	-0.47879	19.4706	52.4905	0	52.4905	0	5.97651
O - nitro	19	20.166	9.19364	-5.51918	-0.10158	57.0192	10.5829	67.6021	0.13204	6.8458
O - nitro	20	19.57	9.11667	-3.44356	5.03437	64.0824	4.08855	68.171	0.056378	6.9628
O - nitro	21	19.6888	8.5191	-4.77846	1.86603	58.1913	9.70631	67.8976	0.122519	6.84146
O - nitro	22	20.3099	9.25992	-5.74357	-0.38129	61.4751	11.0675	72.5426	0.129289	6.89635
O - nitro	23	20.122	8.45949	-3.66504	3.44508	53.9771	6.106	60.0831	0.091298	6.59
O - nitro	24	19.888	8.57637	-3.63398	3.85017	57.6241	5.64201	63.2661	0.081226	6.70521

See figure A-8 for corresponding atom with atom number.

Table A-79. TATB area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.70507	17.0627	0	17.0627	5.70929	0	5.70929	0	1.84713
C	2	3.98949	17.6149	0	17.6149	2.22256	0	2.22256	0	1.13888
C	3	6.62977	15.6351	0	15.6351	3.44385	0	3.44385	0	1.43215
C	4	3.9925	16.9771	0	16.9771	1.1484	0	1.1484	0	0.768103
C	5	6.67657	16.7267	0	16.7267	2.73648	0	2.73648	0	1.37191
C	6	3.93386	17.9716	0	17.9716	4.30881	0	4.30881	0	1.73381
H - amino	7	2.27351	25.7264	0	25.7264	39.8595	0	39.8595	0	5.38016
H - amino	8	2.42832	26.7279	0	26.7279	43.8232	0	43.8232	0	5.51196
H - amino	9	2.29888	26.4456	0	26.4456	52.7767	0	52.7767	0	6.1815
H - amino	10	3.22938	30.8	0	30.8	47.5834	0	47.5834	0	5.76358
H - amino	11	2.35678	26.5469	0	26.5469	41.5213	0	41.5213	0	5.49153
H - amino	12	2.80143	29.3287	0	29.3287	34.1047	0	34.1047	0	4.67162
N - nitro	13	4.04981	16.1746	-2.98941	15.9223	21.1985	3.35638	24.5549	0.118005	3.76245
N - amino	14	14.8736	17.3522	0	17.3522	70.5158	0	70.5158	0	6.69798
N - nitro	15	4.12682	14.0405	-4.53816	13.3594	17.275	19.2056	36.4805	0.2493	3.98957
N - amino	16	14.5447	16.8927	0	16.8927	68.7786	0	68.7786	0	6.63948
N - nitro	17	4.13404	15.7892	-4.32744	15.3508	16.871	12.2653	29.1363	0.243753	3.70194
N - amino	18	15.0187	17.2945	0	17.2945	84.0273	0	84.0273	0	7.5515
O - nitro	19	18.8993	8.76571	-13.3053	-7.30838	42.5036	54.4796	96.9832	0.246188	10.0437
O - nitro	20	19.2253	7.76671	-13.5385	-7.67782	25.4071	55.9138	81.3209	0.214817	9.92615
O - nitro	21	19.2019	7.27475	-14.8201	-9.81597	26.1687	64.6997	90.8685	0.20505	9.95266
O - nitro	22	19.5109	6.53956	-14.6884	-10.0984	18.8436	63.3777	82.2213	0.176657	9.58346
O - nitro	23	18.6855	8.52406	-13.0182	-5.73689	32.0599	54.1963	86.2562	0.233535	10.4166
O - nitro	24	19.2737	7.37121	-13.625	-8.0376	23.8053	56.0659	79.8712	0.209215	9.75113

See figure A-9 for corresponding atom with atom number.

Table A-80. PNA area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.16643	34.1	0	34.1	5.59947	0	5.59947	0	1.55029
C	2	5.40905	29.8026	0	29.8026	17.5449	0	17.5449	0	3.25966
C	3	3.66538	25.2249	0	25.2249	15.7271	0	15.7271	0	3.13786
C	4	4.88956	24.8692	0	24.8692	8.96412	0	8.96412	0	2.15245
N - amino	5	15.5799	35.4401	0	35.4401	67.93	0	67.93	0	6.938
H - amino	6	2.82395	46.9292	0	46.9292	33.8837	0	33.8837	0	4.83985
N - nitro	7	3.10462	29.9043	-4.36998	29.8537	95.8397	0	95.8397	0	8.50483
N - nitro	8	0.312076	10.6747	-2.07209	5.70393	64.2286	7.13635	71.365	0.089998	8.22576
N - nitro	9	2.21634	16.2406	-1.30261	15.8269	31.3114	0.335071	31.6465	0.010476	4.97434
O - nitro	10	20.1917	13.046	-4.97769	7.07419	98.0129	8.43125	106.444	0.072934	9.71158
O - nitro	11	18.4363	10.6393	-6.93577	-1.56662	64.9831	10.7515	75.7346	0.121809	7.53761
O - nitro	12	20.4184	7.56185	-9.13522	-6.43964	29.3478	19.0547	48.4025	0.238694	5.78076
O - nitro	13	19.5594	7.59944	-9.55356	-7.19856	31.2573	17.3638	48.6211	0.229587	5.41524
O - nitro	14	18.8281	7.852	-10.342	-6.99583	32.3301	18.7926	51.1227	0.23247	6.5262
C	15	5.35479	29.9383	0	29.9383	16.809	0	16.809	0	3.19298
C	16	3.75574	25.1084	0	25.1084	15.8089	0	15.8089	0	3.14265
H - amino	17	2.83612	46.6681	0	46.6681	38.0332	0	38.0332	0	5.03761
N - nitro	18	3.03785	29.936	-0.02134	29.8561	93.0628	0	93.0628	0	8.43444
N - nitro	19	0.256429	6.47576	-2.53056	2.55755	44.8133	6.34322	51.1565	0.108621	5.13585
O - nitro	20	20.0688	12.8584	-5.03882	6.99186	95.9491	8.26856	104.218	0.073045	9.62463
O - nitro	21	18.5559	10.6614	-6.96793	-1.47055	66.5992	10.527	77.1261	0.117861	7.62175
O - nitro	22	20.3875	7.62029	-9.12166	-6.43371	30.577	19.1679	49.7449	0.236849	5.78586
O - nitro	23	19.541	7.28548	-9.5463	-7.28252	29.2836	17.4467	46.7303	0.233959	5.32954
O - nitro	24	18.775	7.823	-10.3513	-7.023	31.5571	18.7416	50.2987	0.233771	6.50574

See figure A-10 for corresponding atom with atom number.

Table A-81. TNT area weighted atom specific Politzer parameters using PBE/6-31G*.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.7548	7.40502	-9.15566	-4.53394	32.124	23.1004	55.2244	0.243325	7.25577
O - nitro	2	22.167	8.76555	-9.74085	-4.54852	41.2644	22.4602	63.7246	0.228231	7.98563
O - nitro	3	22.2154	8.13127	-11.0622	-6.65726	30.9036	29.5172	60.4208	0.249868	7.92417
O - nitro	4	22.2134	8.38328	-11.0063	-6.34906	40.4518	26.5828	67.0346	0.239299	8.00645
O - nitro	5	22.6341	9.22455	-9.58092	-4.27966	47.7925	18.9443	66.7368	0.203286	8.03343
O - nitro	6	20.8542	7.45287	-8.94004	-4.70864	35.5011	18.4304	53.9315	0.224953	6.86769
N - nitro	7	3.33468	24.9622	-6.46745	24.592	31.5714	21.8153	53.3867	0.241651	4.86673
N - nitro	8	3.87041	22.6583	-8.26045	21.8145	32.919	34.8393	67.7583	0.249799	5.39648
N - nitro	9	2.19509	25.7966	-4.07531	25.1859	38.4502	4.7395	43.1897	0.097695	5.39901
C	10	5.32651	20.5449	0	20.5449	13.3777	0	13.3777	0	2.81427
C	11	7.31312	18.8029	0	18.8029	17.3669	0	17.3669	0	3.16413
C	12	5.38221	20.1478	0	20.1478	13.5121	0	13.5121	0	2.77272
C	13	7.15169	18.6874	0	18.6874	46.5387	0	46.5387	0	6.02887
C	14	4.71821	18.9835	0	18.9835	16.9339	0	16.9339	0	3.07873
C	15	4.78661	20.8144	0	20.8144	18.8837	0	18.8837	0	3.73753
C	16	4.29799	19.3326	0	19.3326	33.4195	0	33.4195	0	4.5849
H	17	6.90587	22.1517	0	22.1517	17.5815	0	17.5815	0	3.32747
H	18	7.46801	26.9017	0	26.9017	42.6326	0	42.6326	0	5.49107
H	19	8.00253	22.686	0	22.686	15.3763	0	15.3763	0	2.88907
H	20	9.27976	16.185	0	16.185	12.4721	0	12.4721	0	2.82022
H	21	7.72638	21.845	0	21.845	22.4143	0	22.4143	0	3.67179

See figure A-11 for corresponding atom with atom number.

A.11 Area Weighted PBE/6-31G** Training Set Data

Table A-82. FOX-7 area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.08797	22.1906	0	22.1906	20.7249	0	20.7249	0	3.49848
N - amino	2	16.2059	30.5325	0	30.5325	140.476	0	140.476	0	10.04
H - amino	3	6.1334	60.6343	0	60.6343	57.0757	0	57.0757	0	6.29814
H - amino	4	3.277	36.028	0	36.028	89.6958	0	89.6958	0	7.94578
N - amino	5	16.283	30.1706	0	30.1706	136.789	0	136.789	0	9.98664
H - amino	6	2.80176	33.1047	0	33.1047	84.4902	0	84.4902	0	7.79661
H - amino	7	6.30246	60.9898	0	60.9898	60.4205	0	60.4205	0	6.56411
C	8	6.12987	11.4358	-0.82263	11.4077	18.924	0.001743	18.9257	9.21E-05	3.63816
N - nitro	9	3.07369	11.0106	-5.57967	7.5366	52.7508	19.1603	71.9111	0.195452	7.76046
O - nitro	10	21.4247	3.68077	-26.4645	-25.6238	6.01637	74.782	80.7984	0.068917	7.75421
O - nitro	11	20.7531	8.38773	-17.0023	-12.531	43.5242	77.8801	121.404	0.229979	10.4729
N - nitro	12	3.75617	7.84584	-5.72138	4.51547	14.0892	40.1516	54.2408	0.192281	5.61113
O - nitro	13	21.3102	1.32757	-28.6866	-28.375	0.848014	75.13	75.978	0.011037	7.18595
O - nitro	14	20.8875	7.19175	-18.8094	-13.9955	25.4383	99.6053	125.044	0.162049	11.5177
NH ₂	2,3,4	25.6163	38.4429	0	38.4429	272.255	0	272.255	0	14.159
NH ₂	5,6,7	25.3872	38.1454	0	38.1454	285.208	0	285.208	0	14.4405
NO ₂	9,10,11	45.2515	8.92064	-21.9212	-17.3668	47.7244	101.557	149.281	0.21749	12.0966
NO ₂	12,13,14	45.9538	7.27213	-23.8369	-19.1507	21.2737	116.459	137.732	0.1306	12.839

See figure A-1 for corresponding atom with atom number.

Table A-83. HMX area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.14135	35.579	0	35.579	42.1829	0	42.1829	0	5.7546
C	2	1.54093	34.7421	0	34.7421	67.785	0	67.785	0	6.92685
H	3	7.22805	39.0394	0	39.0394	31.139	0	31.139	0	4.71479
H	4	6.33796	30.3396	0	30.3396	58.2684	0	58.2684	0	6.21923
H	5	7.38939	28.5303	0	28.5303	34.5706	0	34.5706	0	4.82045
H	6	7.33524	36.8753	0	36.8753	60.0964	0	60.0964	0	6.35441
N - nitro	7	2.21659	15.9417	-6.92427	14.0272	55.0328	38.3102	93.3431	0.241976	7.9218
N - nitramine	8	3.14997	17.5255	0	17.5255	22.1054	0	22.1054	0	3.78476
N - nitramine	9	2.42791	39.0884	0	39.0884	4.9798	0	4.9798	0	1.72067
N - nitro	10	2.57662	33.0795	-7.28288	32.8189	92.2523	0	92.2523	0	7.55468
O - nitro	11	20.9855	7.26204	-14.8885	-11.6738	24.3209	42.5988	66.9197	0.23135	8.05613
O - nitro	12	21.5677	8.35483	-12.6782	-7.61215	37.4759	44.5368	82.0127	0.248147	9.1055
O - nitro	13	20.3989	10.9262	-8.06033	-0.66414	77.8478	20.9341	98.7819	0.167011	9.04982
O - nitro	14	18.4988	12.8194	-10.7465	-3.57766	100.303	19.2031	119.506	0.134867	10.1901
N - nitramine	15	2.42139	39.1524	0	39.1524	5.32418	0	5.32418	0	1.75626
C	16	1.65585	34.5811	0	34.5811	69.1522	0	69.1522	0	6.79111
C	17	2.1612	35.2887	0	35.2887	40.304	0	40.304	0	5.55774
N - nitro	18	2.47365	33.3413	-4.20628	32.7505	81.2584	9.17721	90.4356	0.09118	7.48559
H	19	7.28544	28.5942	0	28.5942	32.3393	0	32.3393	0	4.69809
H	20	7.32657	36.9282	0	36.9282	61.2436	0	61.2436	0	6.41944
N - nitramine	21	3.21693	17.8772	0	17.8772	24.285	0	24.285	0	3.97009
H	22	7.23336	39.0335	0	39.0335	32.0311	0	32.0311	0	4.7527
H	23	6.3629	30.3102	0	30.3102	57.7052	0	57.7052	0	6.25017
O - nitro	24	20.4432	10.7961	-8.18284	-0.62971	77.9776	20.3754	98.3531	0.164248	9.10322
O - nitro	25	18.5249	12.6437	-10.7166	-3.60156	95.1293	19.3482	114.478	0.140448	10.1139
N - nitro	26	2.11482	16.5015	-8.68033	14.0271	51.1084	52.5915	103.7	0.249949	8.3056
O - nitro	27	20.9494	6.93025	-14.8951	-11.6971	22.5209	42.5591	65.08	0.226299	8.02336
O - nitro	28	21.6134	8.12424	-12.7776	-7.59653	36.278	43.6249	79.9029	0.247886	9.11231

See figure A-2 for corresponding atom with atom number.

Table A-83. HMX area weighted atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
NO ₂	7,11,12	44.7698	9.53096	-13.7967	-8.44464	47.3991	44.9632	92.3623	0.249826	9.69695
NO ₂	10,13,14	41.4743	15.1017	-9.42424	0.116504	149.653	21.8464	171.499	0.111158	11.659
NO ₂	26,27,28	44.6776	9.31548	-13.8552	-8.49574	46.8832	44.399	91.2822	0.249815	9.65635
NO ₂	18,24,25	41.4417	14.8248	-9.47052	0.034302	145.728	21.4781	167.206	0.111953	11.5727

See figure A-2 for corresponding atom with atom number.

Table A-84. PETN area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	Zero surface area for atom								
C	2	0.935798	28.4376	0	28.4376	45.7016	0	45.7016	0	5.86054
O - nitro	3	21.5986	10.1233	-5.59377	2.16452	64.6051	11.1042	75.7093	0.125157	8.03734
O - nitro	4	24.9727	7.97294	-8.21671	-4.57436	35.1929	12.11	47.3029	0.190469	6.24997
O - nitrate	5	9.1362	15.5598	-0.72828	15.431	91.177	0.180035	91.357	0.001967	7.95445
N - nitro	6	3.50738	27.2895	-6.30744	26.6482	45.673	1.5508	47.2238	0.031761	5.94436
H	7	6.30875	29.1864	0	29.1864	25.962	0	25.962	0	4.03634
H	8	7.50773	29.5026	0	29.5026	19.8616	0	19.8616	0	3.51312
C	9	0.926774	28.4681	0	28.4681	46.2	0	46.2	0	5.80834
C	10	0.807007	27.7501	0	27.7501	44.8084	0	44.8084	0	5.78676
C	11	0.871611	27.3787	0	27.3787	45.4903	0	45.4903	0	5.78573
O - nitro	12	21.6509	10.2017	-5.59195	2.17282	65.8492	11.0911	76.9403	0.123372	8.07023
O - nitro	13	21.6677	10.1259	-5.60554	2.17508	64.5855	11.0611	75.6467	0.124841	8.04505
O - nitro	14	21.7146	10.2389	-5.5685	2.20526	64.936	11.1697	76.1057	0.125225	8.07585
O - nitro	15	24.9337	7.9687	-8.24212	-4.57468	36.6205	11.9479	48.5684	0.185485	6.25864
O - nitro	16	25.083	8.10679	-8.20876	-4.51115	36.311	12.1306	48.4415	0.187708	6.30424
O - nitro	17	25.086	7.98848	-8.23376	-4.51287	36.3068	11.9788	48.2857	0.186538	6.30201
O - nitrate	18	9.18371	15.6983	-0.67481	15.4959	92.0972	0.180613	92.2778	0.001953	8.03974
O - nitrate	19	9.1435	15.7241	-0.50983	15.4827	90.8321	0.234959	91.067	0.002573	7.98962
O - nitrate	20	9.11263	15.7349	-0.50489	15.5341	91.2578	0.160078	91.4178	0.001748	7.98882
N - nitro	21	3.45719	26.9326	-0.67646	26.7492	50.1355	0	50.1355	0	5.76724
N - nitro	22	3.36019	27.5204	0	27.5204	42.5731	0	42.5731	0	5.19345
N - nitro	23	3.34325	27.4384	0	27.4384	44.3989	0	44.3989	0	5.28301
H	24	6.31214	29.2475	0	29.2475	25.9812	0	25.9812	0	4.05226
H	25	6.30955	29.4052	0	29.4052	25.7452	0	25.7452	0	4.05675
H	26	6.28832	29.4077	0	29.4077	25.3319	0	25.3319	0	4.01947
H	27	7.45754	29.4411	0	29.4411	19.8917	0	19.8917	0	3.51169
H	28	7.6064	29.5466	0	29.5466	20.4826	0	20.4826	0	3.57039

See figure A-3 for corresponding atom with atom number.

Table A-84. PETN area weighted atom specific Politzer parameters using PBE/6-31G** (continued).

H	29	7.55368	29.5073	0	29.5073	20.5723	0	20.5723	0	3.57642
NO ₂	6,3,4	50.0787	12.5055	-7.26755	0.518815	99.975	13.3101	113.285	0.103688	9.44796
NO ₂	21,12,15	50.0418	12.4767	-7.27442	0.508714	99.752	13.2841	113.036	0.10371	9.43945
NO ₂	22,13,16	50.1109	12.5028	-7.26943	0.52782	99.6804	13.3076	112.988	0.103907	9.4514
NO ₂	23,14,17	50.1438	12.4918	-7.2652	0.52668	99.5427	13.3281	112.871	0.10414	9.44514

See figure A-3 for corresponding atom with atom number.

Table A-85. EDNA area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.48194	32.4915	0	32.4915	44.1941	0	44.1941	0	4.81919
H	2	8.64888	33.299	0	33.299	31.8424	0	31.8424	0	4.18601
H	3	7.4396	28.0883	0	28.0883	29.8413	0	29.8413	0	3.92977
H	4	5.47327	47.9639	0	47.9639	78.6663	0	78.6663	0	7.45386
N - nitramine	5	9.26452	29.4374	0	29.4374	86.8084	0	86.8084	0	7.28444
N - nitro	6	3.24695	18.9448	-6.05514	17.7334	51.5743	23.1326	74.7069	0.213765	6.75854
O - nitro	7	25.5741	8.4974	-17.7075	-13.706	33.534	56.7335	90.2675	0.233487	9.61218
O - nitro	8	21.9718	8.55968	-15.0886	-9.79896	39.4754	60.7877	100.263	0.238704	10.1532
C	9	2.58009	32.6353	0	32.6353	43.7892	0	43.7892	0	4.86584
H	10	8.58313	33.3269	0	33.3269	33.1502	0	33.1502	0	4.25715
H	11	7.376	28.1053	0	28.1053	30.0551	0	30.0551	0	3.96703
N - nitramine	12	9.27298	29.3178	0	29.3178	84.7299	0	84.7299	0	7.19355
H	13	5.50911	48.0008	0	48.0008	76.7346	0	76.7346	0	7.42353
N - nitro	14	3.24707	19.4449	-8.82556	18.0659	46.6896	63.8045	110.494	0.244002	6.66496
O - nitro	15	25.612	8.26004	-17.7341	-13.6609	33.7356	56.1098	89.8454	0.234496	9.63122
O - nitro	16	21.9773	8.69174	-14.9541	-9.84173	35.4712	62.3662	97.8374	0.231108	10.1151
NO ₂	6,7,8	50.7929	11.2334	-16.5115	-10.0062	61.4975	60.5036	122.001	0.249983	11.5764
NO ₂	14,15,16	50.8364	11.3475	-16.4695	-9.98333	60.9465	61.0438	121.99	0.25	11.5915

See figure A-4 for corresponding atom with atom number.

Table A-86. NQ area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	21.1844	4.31078	-23.9143	-22.1392	12.1204	140.055	152.175	0.073304	11.1885
O - nitro	2	25.24	0	-36.5716	-36.5716	0	47.8321	47.8321	0	5.25086
N - amino	3	17.0768	24.4398	0	24.4398	148.69	0	148.69	0	10.3043
N - amino	4	17.029	21.3189	-0.06087	21.3071	131.918	0	131.918	0	9.80642
N - nitramine	5	16.058	3.88538	-18.6246	-14.8555	5.8424	123.41	129.252	0.043158	11.2985
N - nitro	6	3.48516	2.36893	-8.69076	-6.21727	3.52673	52.4911	56.0178	0.058994	6.02578
C	7	2.6842	13.421	0	13.421	27.7659	0	27.7659	0	4.05027
H - amino	8	5.74513	37.2181	0	37.2181	103.915	0	103.915	0	8.55529
H - amino	9	7.24657	56.2386	0	56.2386	70.7335	0	70.7335	0	7.12552
H - amino	10	6.89392	54.6323	0	54.6323	80.8814	0	80.8814	0	7.68575
H - amino	11	2.79033	23.3547	-0.5246	23.2359	77.3976	0	77.3976	0	7.54517
NH ₂	3,8,9	30.0685	34.5449	0	34.5449	294.126	0	294.126	0	14.7301
NH ₂	4,10,11	26.7133	30.1354	-0.33783	30.1089	322.417	0.051727	322.468	0.00016	15.0951
NO ₂	6,1,2	49.9096	3.59404	-29.7363	-28.3261	9.82655	150.221	160.048	0.057628	11.573

See figure A-5 for corresponding atom with atom number.

Table A-87. RDX area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.27461	29.6476	0	29.6476	16.6459	0	16.6459	0	2.76187
C	2	2.5669	30.552	0	30.552	6.91583	0	6.91583	0	1.59066
C	3	2.28378	31.3951	0	31.3951	17.1733	0	17.1733	0	2.64936
H	4	9.40737	39.9778	0	39.9778	30.3001	0	30.3001	0	4.73368
H	5	4.99156	21.2685	-2.99696	20.9605	43.3512	4.37365	47.7249	0.083245	5.64601
H	6	5.70241	25.244	-0.59049	25.2002	33.8086	4.17E-17	33.8086	1.23E-18	4.61443
H	7	9.47639	40.3245	0	40.3245	26.0393	0	26.0393	0	4.44264
H	8	9.53207	39.9028	0	39.9028	25.8751	0	25.8751	0	4.36437
H	9	5.02409	22.7893	-4.16899	22.4759	43.0065	3.09663	46.1031	0.062656	5.58577
N - nitramine	10	3.71152	25.4481	0	25.4481	129.218	0	129.218	0	10.5912
N - nitramine	11	5.98331	20.4075	0	20.4075	31.8516	0	31.8516	0	4.52591
N - nitramine	12	6.0049	20.8	0	20.8	29.2352	0	29.2352	0	4.29467
N - nitro	13	3.28611	20.8738	-8.44874	19.7189	96.3722	58.8256	155.198	0.235368	9.23463
N - nitro	14	2.70134	21.547	-5.27545	20.6429	54.4499	23.5427	77.9926	0.21074	6.09701
N - nitro	15	2.86736	22.0951	-8.61087	20.7097	55.7228	27.8655	83.5883	0.222233	6.63632
O - nitro	16	22.105	9.28301	-14.7263	-10.4647	57.1697	43.4639	100.634	0.245363	9.0112
O - nitro	17	22.3086	8.87927	-15.2109	-11.4276	51.5681	46.7436	98.3117	0.249398	8.80726
O - nitro	18	19.6126	7.60233	-14.5551	-10.681	25.3342	38.5973	63.9315	0.23924	8.5025
O - nitro	19	21.4574	8.51245	-13.5254	-9.2251	32.8359	37.183	70.019	0.249036	8.61941
O - nitro	20	19.606	9.02656	-14.4014	-9.79334	40.226	35.9556	76.1816	0.249214	9.0694
O - nitro	21	21.4547	8.15285	-13.0455	-8.64868	31.8555	34.1494	66.0049	0.249698	8.44511
NO ₂	13,16,17	47.6996	12.6064	-14.9499	-8.83562	96.0866	45.3855	141.472	0.217891	10.7956
NO ₂	14,18,19	43.7713	11.5343	-13.9998	-8.03412	70.3496	38.2995	108.649	0.228246	10.2782
NO ₂	16,20,21	63.1657	8.79093	-14.0647	-9.63947	42.8595	38.5707	81.4302	0.249307	8.85727

See figure A-6 for corresponding atom with atom number.

Table A-88. CL20 area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	19.999	10.7561	-7.64499	-0.39036	65.0556	17.0929	82.1484	0.164778	8.79515
O - nitro	2	19.4751	11.165	-8.33757	-1.55076	62.6907	14.3016	76.9924	0.151249	8.89992
O - nitro	3	20.2949	10.5176	-6.84184	0.958366	63.1079	15.4144	78.5223	0.15777	8.62117
O - nitro	4	17.7463	10.8051	-7.25904	-0.73842	67.5137	13.8254	81.3391	0.141082	8.34572
O - nitro	5	20.6235	11.3011	-6.82151	0.972749	80.2143	13.639	93.8532	0.124204	8.91857
O - nitro	6	19.8664	11.6119	-8.26629	-1.74875	92.7922	1.35E+01	106.261	1.11E-01	8.83242
O - nitro	7	20.6256	13.2631	-8.02302	-0.52805	118.446	12.7626	131.208	0.087808	9.71923
O - nitro	8	20.8848	9.25412	-7.19199	-1.72362	74.4052	14.245	88.6502	0.134867	7.38687
O - nitro	9	22.1804	12.4231	-6.62334	2.29743	95.6301	14.2761	109.906	0.113021	9.63668
O - nitro	10	20.5662	12.5533	-7.6653	-0.42161	103.186	13.7996	116.985	0.104045	9.30179
O - nitro	11	20.6133	8.76189	-6.87134	-2.35577	56.4257	12.493	68.9187	0.148412	6.61314
O - nitro	12	22.0776	13.0181	-5.88777	3.40269	120.199	11.4814	131.68	0.07959	9.80664
N - nitramine	13	4.92298	30.0797	0	30.0797	23.4954	0	23.4954	0	3.85141
N - nitramine	14	5.20548	29.9112	0	29.9112	24.7326	0	24.7326	0	3.95582
N - nitramine	15	3.19556	37.1527	0	37.1527	22.1354	0	22.1354	0	3.98682
N - nitramine	16	0.952923	35.3117	0	35.3117	305.933	0	305.933	0	15.84
N - nitramine	17	1.85761	38.4356	0	38.4356	35.6892	0	35.6892	0	4.78172
N - nitramine	18	1.45754	31.7863	0	31.7863	119.77	0	119.77	0	6.77493
N - nitro	19	1.90076	27.4309	-1.90637	27.0551	32.6008	0	32.6008	0	4.93404
N - nitro	20	1.9565	27.6607	-9.7515	27.4216	46.8271	0	46.8271	0	5.39226
N - nitro	21	1.83067	29.7834	-3.65069	29.2869	105.514	9.77618	115.29	0.077606	8.53414
N - nitro	22	3.00171	33.9206	0	33.9206	204.799	0	204.799	0	12.5099
N - nitro	23	3.06198	30.0744	-6.76957	29.9288	94.8187	0	94.8187	0	8.00055
N - nitro	24	3.14219	32.9764	-1.45203	32.6322	190.984	0.136693	191.12	0.000715	11.453
C	25	0.909746	51.5868	0	51.5868	22.271	0	22.271	0	3.50277
C	26	1.05784	50.2318	0	50.2318	26.834	0	26.834	0	4.24476
C	27	0.463521	37.0296	0	37.0296	8.56111	0	8.56111	0	2.32152
C	28	0.306849	34.8217	0	34.8217	34.1272	0	34.1272	0	4.92032
C	29	0.982357	51.8018	0	51.8018	63.0588	0	63.0588	0	5.63885
C	30	0.95363	54.2221	0	54.2221	23.6112	0	23.6112	0	4.16044

See figure A-7 for corresponding atom with atom number.

Table A-88. CL20 area weighted atom specific Politzer parameters using PBE/6-31G** (continued).

H	31	5.70752	43.4528	0	43.4528	74.5348	0	74.5348	0	6.92115
H	32	6.26724	43.9778	0	43.9778	54.3818	0	54.3818	0	5.94376
H	33	6.33996	37.0098	0	37.0098	14.8951	0	14.8951	0	3.07291
H	34	3.58753	31.0556	0	31.0556	44.1964	0	44.1964	0	5.51786
H	35	3.83791	39.6633	0	39.6633	87.6337	0	87.6337	0	7.57775
H	36	4.41248	42.8898	0	42.8898	69.5979	0	69.5979	0	6.54513
NO ₂	19,1,2	41.3749	12.8156	-7.99345	0.324286	87.7783	15.8052	103.583	0.129302	9.989
NO ₂	20,3,4	39.9977	12.5307	-7.05346	1.49999	91.5934	14.6535	106.247	0.118898	9.69688
NO ₂	21,5,6	42.3206	13.3583	-7.58565	0.919991	119.285	14.0804	133.365	0.094431	10.1265
NO ₂	22,7,8	44.5122	15.2487	-7.59872	1.23407	192.716	13.692	206.408	0.061935	10.877
NO ₂	23,9,10	45.8086	15.0566	-7.17344	2.92365	136.928	14.2882	151.216	0.085561	11.2241
NO ₂	24,11,12	45.8331	14.8632	-6.43868	2.81673	176.424	12.3073	188.732	0.060958	10.6869

See figure A-7 for corresponding atom with atom number.

Table A-89. HNB area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.95538	40.8863	0	40.8863	16.6019	0	16.6019	0	3.1721
C	2	3.9791	41.0669	0	41.0669	16.0445	0	16.0445	0	3.10176
C	3	3.92559	40.5649	0	40.5649	16.1088	0	16.1088	0	3.15124
N - nitro	4	0.752494	20.9292	0	20.9292	64.8561	0	64.8561	0	7.01074
N - nitro	5	0.729956	21.3845	-0.9946	20.9571	69.0083	1.67E-16	69.0083	2.42E-18	6.88437
N - nitro	6	0.634403	21.6262	0	21.6262	76.0263	0	76.0263	0	7.73712
O - nitro	7	20.9284	9.04694	-5.03679	0.723924	59.0437	9.83838	68.882	0.122429	6.83217
O - nitro	8	19.922	9.40714	-3.10722	6.05452	62.0952	3.05089	65.1461	0.044638	6.83448
O - nitro	9	20.7069	8.36092	-3.51723	4.23268	55.0612	5.08972	60.151	0.077456	6.53952
O - nitro	10	20.5049	8.77557	-3.43743	4.83923	59.2816	4.46939	63.7509	0.065192	6.73051
O - nitro	11	20.3442	8.27881	-4.46594	2.9995	58.7888	8.11564	66.9044	0.106588	6.76704
O - nitro	12	21.0643	9.11559	-5.0404	0.641247	63.0032	10.1587	73.1619	0.119572	6.82308
C	13	3.84076	40.8539	0	40.8539	15.0251	0	15.0251	0	3.00964
C	14	3.95961	40.5672	0	40.5672	15.8381	0	15.8381	0	3.09194
C	15	4.02572	40.813	0	40.813	14.2566	0	14.2566	0	2.95124
N - nitro	16	0.752491	19.4955	0	19.4955	69.8897	0	69.8897	0	6.6355
N - nitro	17	0.784681	21.5275	-0.49009	21.3551	87.7726	-4.17E-17	87.7726	-4.75E-19	8.52535
N - nitro	18	0.696901	20.2108	0	20.2108	60.802	0	60.802	0	5.92246
O - nitro	19	20.9073	9.00745	-5.03375	0.718979	58.9788	9.89954	68.8783	0.123068	6.81613
O - nitro	20	20.0764	9.50045	-3.14049	6.12954	64.5222	2.94413	67.4663	0.041734	6.93348
O - nitro	21	20.2634	8.14842	-4.47814	2.86999	56.6114	8.03531	64.6467	0.108846	6.68375
O - nitro	22	21.0175	9.12062	-5.04503	0.670545	62.3941	10.188	72.582	0.120662	6.84275
O - nitro	23	20.7228	8.23961	-3.58259	4.20177	54.7824	4.91334	59.6957	0.075532	6.5115
O - nitro	24	20.4997	8.72545	-3.48803	4.84758	59.2895	4.36013	63.6497	0.06381	6.72613
NO ₂	4,7,8	41.6029	9.64092	-4.45513	3.642	65.2611	8.57635	73.8375	0.10266	7.46199
NO ₂	5,9,10	41.9417	8.8974	-3.47652	4.82029	61.6174	4.79574	66.4131	0.066996	6.86591
NO ₂	6,11,12	42.043	9.01871	-4.81027	2.09903	66.1204	9.41952	75.54	0.109147	7.15336
NO ₂	16,19,20	41.7362	9.63764	-4.46094	3.66016	65.9097	8.55154	74.4613	0.101656	7.47533
NO ₂	17,21,22	42.0656	9.03486	-4.81518	2.11589	66.3082	9.40002	75.7082	0.108745	7.1699
NO ₂	18,23,24	41.9194	8.77398	-3.53729	4.78373	60.5121	4.65055	65.1627	0.066275	6.82315

See figure A-8 for corresponding atom with atom number.

Table A-90. TATB area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.59266	21.1966	0	21.1966	3.68874	0	3.68874	0	1.48928
C	2	3.96684	21.6339	0	21.6339	1.33891	0	1.33891	0	0.849076
C	3	6.51089	19.8755	0	19.8755	2.04928	0	2.04928	0	1.11045
C	4	4.01896	21.0062	0	21.0062	0.766513	0	0.766513	0	0.662043
C	5	6.46614	20.9098	0	20.9098	1.536	0	1.536	0	1.04833
C	6	3.94678	22.0317	0	22.0317	2.66517	0	2.66517	0	1.29142
H - amino	7	2.1783	26.4616	0	26.4616	45.1882	0	45.1882	0	5.67584
H - amino	8	2.36096	27.6291	0	27.6291	41.001	0	41.001	0	5.41815
H - amino	9	2.21339	26.8201	0	26.8201	58.7543	0	58.7543	0	6.45185
H - amino	10	3.3186	30.2973	0	30.2973	53.4727	0	53.4727	0	6.12996
H - amino	11	2.38884	26.8074	0	26.8074	46.9303	0	46.9303	0	5.80102
H - amino	12	2.95252	29.4078	0	29.4078	35.7374	0	35.7374	0	4.77693
N - nitro	13	3.8158	19.6225	-2.98847	19.4092	25.4375	1.80147	27.239	0.061762	4.00806
N - amino	14	15.198	19.1527	0	19.1527	58.4935	0	58.4935	0	6.02257
N - nitro	15	3.89951	17.5246	-6.49934	16.7715	22.0853	21.1474	43.2327	0.249882	4.44973
N - amino	16	14.8215	18.5737	0	18.5737	56.6082	0	56.6082	0	5.94263
N - nitro	17	3.97942	19.2218	-9.23301	18.6071	21.2471	55.3909	76.638	0.200378	4.24619
N - amino	18	15.0078	18.9788	0	18.9788	67.858	0	67.858	0	6.73921
O - nitro	19	19.8384	9.31951	-13.0429	-6.25943	45.888	54.032	99.9199	0.248339	10.4201
O - nitro	20	20.2107	8.3826	-13.4223	-6.77311	31.4926	54.4871	85.9797	0.232119	10.2986
O - nitro	21	20.1718	7.94748	-14.6112	-8.92779	30.4694	64.9871	95.4565	0.21731	10.3527
O - nitro	22	20.5098	7.29099	-14.5936	-9.11509	24.9231	62.9409	87.864	0.203195	10.0772
O - nitro	23	19.5354	9.15202	-12.7432	-4.89511	36.9492	53.0912	90.0404	0.241965	10.6476
O - nitro	24	20.315	7.93442	-13.4801	-7.19152	28.4221	54.86	83.2821	0.224806	10.082
NH ₂	14,7,8	19.7373	20.9733	0	20.9733	66.1082	0	66.1082	0	6.7671
NH ₂	16,9,10	20.3535	21.382	0	21.382	78.2489	0	78.2489	0	7.71504
NH ₂	18,11,12	20.3492	21.411	0	21.411	77.8008	0	77.8008	0	7.43465
NO ₂	13,19,20	43.8649	11.3977	-13.2209	-4.2632	56.6451	54.3649	111.01	0.249895	11.7855
NO ₂	15,21,22	44.5811	10.2917	-14.57	-6.76604	45.5918	64.0448	109.637	0.242918	11.6459
NO ₂	17,23,24	43.8298	11.0464	-13.1241	-3.82566	50.6565	54.2228	104.879	0.249711	11.753

See figure A-9 for corresponding atom with atom number.

Table A-91. PNA area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.20051	37.9255	0	37.9255	6.69974	0	6.69974	0	1.77511
C	2	5.12238	33.474	0	33.474	22.6046	0	22.6046	0	3.63191
C	3	3.50961	28.2338	0	28.2338	17.9465	0	17.9465	0	3.41959
C	4	4.45187	28.0441	0	28.0441	9.0077	0	9.0077	0	2.1868
N - amino	5	15.8907	37.3528	0	37.3528	58.7865	0	58.7865	0	6.34856
H - amino	6	2.8217	47.1693	0	47.1693	39.9768	0	39.9768	0	5.24208
N - nitro	7	2.72641	32.8888	0	32.8888	103.139	0	103.139	0	8.81611
N - nitro	8	0.267309	5.98917	-2.86774	3.57047	58.9566	6.47868	65.4353	0.089206	5.4524
N - nitro	9	1.95537	17.4438	-2.66464	16.9914	40.8813	0.563982	41.4452	0.013423	5.50716
O - nitro	10	21.013	13.5901	-5.02699	7.88681	102.841	7.94442	110.785	0.066568	9.98831
O - nitro	11	19.198	11.2352	-6.41682	-0.56769	77.5896	10.6594	88.249	0.106198	7.83497
O - nitro	12	21.0327	8.37565	-8.34416	-5.12046	38.6028	18.1201	56.7229	0.217402	6.07512
O - nitro	13	20.2562	8.07571	-8.63973	-5.88665	38.8888	16.6798	55.5686	0.210066	5.6292
O - nitro	14	19.5135	8.59655	-9.67958	-5.92655	38.1856	18.3596	56.5452	0.219266	6.77005
C	15	5.13817	33.5135	0	33.5135	21.8935	0	21.8935	0	3.57809
C	16	3.53078	28.2154	0	28.2154	18.2532	0	18.2532	0	3.45033
H - amino	17	2.7797	47.2411	0	47.2411	38.5141	0	38.5141	0	5.17668
N - nitro	18	2.70382	32.7495	-7.69138	32.5294	110.5	0	110.5	0	9.347
N - nitro	19	0.249717	3.94027	-4.79017	1.81907	25.422	17.0422	42.4642	0.240264	4.04684
O - nitro	20	20.9575	13.515	-5.01595	7.82746	101.083	7.95703	109.04	0.067648	9.93303
O - nitro	21	19.1636	11.2628	-6.46372	-0.52158	81.1446	10.4497	91.5943	0.101071	7.90725
O - nitro	22	21.0454	8.12067	-8.37847	-5.14217	38.7082	17.9195	56.6277	0.216307	6.04944
O - nitro	23	20.1707	7.80968	-8.64907	-5.94834	37.899	16.6076	54.5066	0.211854	5.56349
O - nitro	24	19.4793	8.58725	-9.64049	-5.98541	37.0417	18.569	55.6108	0.222414	6.70007
NH ₂	5,6,17	22.2012	37.1377	0	37.1377	75.2764	0	75.2764	0	7.27494
NO ₂	7,10,11	42.9374	15.1806	-5.95263	5.69421	137.959	10.1823	148.141	0.06401	11.3102
NO ₂	8,12,13	41.5562	8.18261	-8.47961	-5.43803	39.3981	17.4673	56.8654	0.212816	5.90229
NO ₂	9,14,24	40.9482	10.3141	-9.65011	-4.86017	50.5336	18.5087	69.0423	0.196212	7.78112
NO ₂	18,20,21	42.8249	15.0911	-5.9793	5.65097	137.718	10.0752	147.793	0.063524	11.282
NO ₂	19,22,23	41.4659	7.88209	-8.50687	-5.4924	38.4459	17.3073	55.7532	0.214062	5.84751

See figure A-10 for corresponding atom with atom number.

Table A-92. TNT area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	1	20.6497	8.22307	-8.93408	-3.54921	40.1136	24.8411	64.9547	0.236179	7.7785
O - nitro	2	23.1105	9.38512	-9.48977	-3.75941	48.2742	23.5796	71.8539	0.220471	8.35071
O - nitro	3	23.2778	8.20993	-11.0527	-5.95999	37.9429	28.9962	66.9391	0.245534	8.27271
O - nitro	4	23.3462	9.03869	-10.7474	-5.38063	48.735	27.1263	75.8612	0.229716	8.46169
O - nitro	5	23.8611	9.99025	-9.01535	-3.13228	58.4521	18.7615	77.2137	0.183942	8.36325
O - nitro	6	21.9353	8.27234	-8.36535	-3.40528	42.0747	1.91E+01	61.1448	2.15E-01	7.30713
N - nitro	7	3.2378	27.7247	-4.91068	26.8217	41.475	21.2027	62.6778	0.223847	5.92084
N - nitro	8	3.64975	25.3077	-7.16542	24.7484	43.1705	19.7564	62.9269	0.215389	5.67335
N - nitro	9	1.81759	28.2478	-5.23719	27.9091	47.3522	0	47.3522	0	5.60131
C	10	5.16076	23.11	0	23.11	15.0617	0	15.0617	0	2.90554
C	11	7.25404	21.3236	0	21.3236	19.2143	0	19.2143	0	3.2405
C	12	5.35326	22.7146	0	22.7146	16.0221	0	16.0221	0	2.96172
C	13	6.85507	21.1547	0	21.1547	46.9073	0	46.9073	0	5.99927
C	14	4.55454	21.1893	0	21.1893	17.4527	0	17.4527	0	3.09635
C	15	4.61827	23.6336	0	23.6336	19.0141	0	19.0141	0	3.69831
C	16	4.00474	22.1067	0	22.1067	33.8575	0	33.8575	0	4.56584
H	17	6.98488	23.9225	0	23.9225	20.2619	0	20.2619	0	3.62782
H	18	7.68538	28.741	0	28.741	48.8664	0	48.8664	0	5.85277
H	19	8.23602	24.8467	0	24.8467	16.3413	0	16.3413	0	2.81464
H	20	9.40421	17.7303	0	17.7303	13.3952	0	13.3952	0	2.9483
H	21	7.84559	23.9632	0	23.9632	20.1438	0	20.1438	0	3.36404
NO ₂	7,1,2	46.9979	12.4013	-9.21686	-1.56024	98.8526	24.293	123.146	0.158355	9.95103
NO ₂	8,3,4	50.2738	12.3519	-10.8937	-3.4616	91.7115	28.0979	119.809	0.179521	10.3301
NO ₂	9,5,6	47.6141	11.3648	-8.69936	-2.0731	87.8491	19.012	106.861	0.14626	8.98472

See figure A-11 for corresponding atom with atom number.

Table A-93. TNA area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.25634	31.8605	0	31.8605	3.11851	0	3.11851	0	1.21737
C	2	5.5051	28.2248	0	28.2248	16.0977	0	16.0977	0	2.98721
C	3	3.46533	22.5714	0	22.5714	14.2865	0	14.2865	0	3.06882
C	4	5.66523	24.6455	0	24.6455	9.57129	0	9.57129	0	2.58299
C	5	7.03358	25.2425	0	25.2425	6.82471	0	6.82471	0	2.00902
C	6	6.25382	30.3988	0	30.3988	7.56171	0.00E+00	7.56171	0.00E+00	2.23896
H - amino	7	3.53772	39.5871	0	39.5871	47.8401	0	47.8401	0	5.86389
H - amino	8	3.61676	40.8748	0	40.8748	45.1805	0	45.1805	0	5.59494
H	9	5.77677	21.6292	0	21.6292	10.5509	0	10.5509	0	2.63152
N - amino	10	15.6328	28.7575	0	28.7575	46.2568	0	46.2568	0	5.51264
N - nitro	11	3.23132	28.0789	-11.8555	27.9634	69.9199	0	69.9199	0	6.81287
N - nitro	12	0.276007	14.3702	-5.57542	-2.25903	4.12067	7.73761	11.8583	0.226742	5.52993
N - nitro	13	3.59825	22.1618	-8.3788	21.7205	43.5447	22.724	66.2686	0.225322	5.61236
N - nitro	14	4.0714	29.7617	-6.69382	29.2266	39.972	16.964	56.936	0.209175	5.31729
O - nitro	15	20.3143	12.6268	-6.95903	4.80145	80.7648	15.508	96.2728	0.135136	10.1156
O - nitro	16	18.6114	10.0425	-9.45391	-4.80979	54.677	15.2257	69.9027	0.17037	7.55717
O - nitro	17	20.9761	7.40933	-11.4059	-8.88381	27.0074	21.5708	48.5782	0.246869	5.93949
O - nitro	18	20.4267	7.16152	-11.9598	-9.98802	22.4784	20.6523	43.1308	0.249552	5.3764
O - nitro	19	18.9664	8.45378	-13.5431	-10.0619	35.819	27.1299	62.949	0.245237	7.47619
O - nitro	20	22.5499	8.60427	-10.9521	-5.53951	37.7529	32.0371	69.79	0.248323	8.58076
O - nitro	21	22.0783	9.93761	-7.99524	-1.04919	50.3013	19.6461	69.9473	0.201982	8.54406
O - nitro	22	20.2394	13.6426	-7.51303	5.3233	81.4168	17.3671	98.7839	0.1449	10.8407
NH ₂	10,7,8	22.7873	32.362	0	32.362	74.8513	0	74.8513	0	7.55121
NO ₂	11,15,16	42.157	14.5575	-8.54703	2.33365	109.693	16.7671	126.46	0.115009	11.6389
NO ₂	12,17,18	41.6788	7.36853	-11.6457	-9.38111	25.3464	21.3344	46.6808	0.248153	5.71081
NO ₂	13,19,20	45.1146	12.3283	-12.2276	-5.26656	76.0099	31.2979	107.308	0.206596	10.4747
NO ₂	14,21,22	46.3891	14.9701	-7.81349	4.38829	108.932	18.8543	127.786	0.125776	11.7927

See figure A-12 for corresponding atom with atom number.

Table A-94. NTO area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	23.5542	23.5542	0	23.5542	20.1944	0	20.1944	0	3.38158
N	2	22.6552	22.6552	0	22.6552	14.6205	0	14.6205	0	3.08459
C	3	18.57	18.57	0	18.57	12.967	0	12.967	0	3.11702
N	4	21.7856	21.7856	0	21.7856	28.7757	0	28.7757	0	4.53794
N	5	10.0716	10.0716	-10.7193	-0.57912	38.9661	39.1207	78.0868	0.249999	10.3988
H	6	43.216	43.216	0	43.216	60.4438	0.00E+00	60.4438	0.00E+00	6.64476
H	7	46.321	46.321	0	46.321	59.234	0	59.234	0	6.62902
N - nitro	8	21.5217	21.5217	-4.60107	21.0159	38.0795	15.1885	53.268	0.203833	5.46747
O - nitro	9	10.1619	10.1619	-11.35	-4.35424	48.5773	37.8805	86.4578	0.246173	9.90636
O - nitro	10	6.51749	6.51749	-15.1596	-12.6858	19.575	29.7155	49.2905	0.239419	6.8671
O	11	7.79792	7.79792	-16.6788	-11.461	24.6063	58.4907	83.097	0.208431	10.4822
NO ₂	8,9,210	12.7431	12.7431	-13.5071	-6.11205	73.0298	36.8977	109.927	0.222991	11.283

See figure A-13 for corresponding atom with atom number.

Table A-95. DATB area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.99486	22.3714	0	22.3714	0.441027	0	0.441027	0	0.469282
C	2	4.02696	22.3726	0	22.3726	0.420632	0	0.420632	0	0.460164
C	3	6.46903	19.9751	0	19.9751	5.40951	0	5.40951	0	1.96176
C	4	6.80611	16.3662	0	16.3662	2.32296	0	2.32296	0	0.922131
C	5	6.48521	20.0166	0	20.0166	5.38049	0	5.38049	0	1.96029
N - nitro	6	3.8601	22.5057	0	22.5057	20.6723	0.00E+00	20.6723	0.00E+00	3.40987
N - nitro	7	4.02531	19.1447	-8.89325	18.5585	24.308	45.3315	69.6395	0.227215	4.47036
N - nitro	8	4.01568	19.0827	-6.57719	18.2956	25.459	31.0426	56.5016	0.247559	4.7422
O - nitro	9	19.812	9.80129	-10.6413	-2.07596	40.64	36.8636	77.5035	0.249406	10.0721
O - nitro	10	19.8694	9.83741	-10.6751	-2.02581	41.8857	36.695	78.5808	0.248909	10.1132
O - nitro	11	20.4461	9.47405	-12.1756	-4.29015	38.6178	47.486	86.1037	0.247348	10.4894
O - nitro	12	22.1218	6.15372	-13.9997	-10.6923	18.2977	43.6056	61.9034	0.208215	8.00844
O - nitro	13	22.0672	6.24603	-14.0203	-10.6613	19.7989	43.0985	62.8974	0.215694	8.02253
O - nitro	14	20.4359	9.51838	-12.224	-4.31357	38.7983	47.7533	86.5516	0.247324	10.534
H	15	5.39709	11.2294	0	11.2294	6.87526	0	6.87526	0	2.15353
C	16	6.71777	22.5267	0	22.5267	2.39644	0	2.39644	0	1.3291
N - amino	17	15.6837	19.6501	0	19.6501	41.2791	0	41.2791	0	5.15942
H - amino	18	3.35656	30.7253	0	30.7253	46.1134	0	46.1134	0	5.67092
H - amino	19	3.1119	29.433	0	29.433	43.5352	0	43.5352	0	5.56648
N - amino	20	15.6155	19.6386	0	19.6386	41.1927	0	41.1927	0	5.1568
H - amino	21	3.15971	29.3542	0	29.3542	44.649	0	44.649	0	5.66409
H - amino	22	3.41454	30.5378	0	30.5378	47.1666	0	47.1666	0	5.74535
NH ₂	17,18,19	22.1521	22.7025	0	22.7025	65.0415	0	65.0415	0	7.0715
NH ₂	20,21,22	22.1898	22.6992	0	22.6992	64.9574	0	64.9574	0	7.06332
NO ₂	6,9,10	43.5415	12.2036	-10.6582	0.126172	61.9579	36.7797	98.7375	0.233744	11.3946
NO ₂	7,11,12	46.5932	11.2092	-13.2351	-5.35584	54.1465	46.0626	100.209	0.248373	11.2724
NO ₂	8,13,14	46.5187	11.2041	-13.2506	-5.37305	54.2299	45.9248	100.155	0.248281	11.2703

See figure A-14 for corresponding atom with atom number.

Table A-96. Picric acid area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.32506	29.5121	0	29.5121	11.4647	0	11.4647	0	2.24226
C	2	6.243	30.8191	0	30.8191	10.7588	0	10.7588	0	2.71608
C	3	7.367	25.0298	0	25.0298	2.52865	0	2.52865	0	1.15016
C	4	6.10367	25.3957	0	25.3957	2.27097	0	2.27097	0	1.24635
C	5	7.21646	23.0023	0	23.0023	9.27978	0	9.27978	0	2.27673
C	6	5.81852	25.2184	0	25.2184	9.65676	0.00E+00	9.65676	0.00E+00	2.4147
N - nitro	7	4.05575	32.5222	-0.62437	32.453	31.9481	0	31.9481	0	4.236
N - nitro	8	4.1056	23.8732	-3.48394	23.4411	34.0305	1.97343	36.0039	0.051807	4.86324
N - nitro	9	3.63347	23.6541	-5.5339	23.5152	39.5639	3.70702	43.2709	0.078331	5.11697
O	10	17.4931	17.0825	-6.67025	11.4595	97.4221	18.4914	115.913	0.134078	11.4896
O - nitro	11	20.3182	14.3201	-6.38442	6.94774	91.2441	11.8008	103.045	0.101406	10.7942
O - nitro	12	22.1689	10.2384	-6.30921	1.5572	58.7769	13.6736	72.4505	0.153111	8.3517
O - nitro	13	22.7596	8.42802	-11.2419	-6.20863	37.5154	31.8817	69.3971	0.248352	8.41925
O - nitro	14	21.456	8.32058	-12.8415	-9.14047	33.1034	26.1985	59.3019	0.246611	7.61324
H	15	1.63584	34.9416	0	34.9416	20.7658	0	20.7658	0	3.97315
H	16	6.3342	22.4181	0	22.4181	9.98324	0	9.98324	0	2.51765
H	17	6.47971	20.644	0	20.644	16.3194	0	16.3194	0	3.416
O - nitro	18	22.487	8.55108	-10.874	-5.28154	35.549	32.8421	68.3912	0.249608	8.66818
O - nitro	19	22.6914	8.52701	-11.0901	-5.68785	36.2019	32.5266	68.7285	0.249285	8.61929
NO ₂	7,11,12	46.5428	15.4279	-6.3355	6.60269	123.786	12.9655	136.751	0.085822	11.6696
NO ₂	8,18,19	49.284	12.2354	-10.9685	-3.07587	78.4416	32.7446	111.186	0.207771	10.6202
NO ₂	9,13,14	47.849	12.5711	-12.0562	-5.26618	83.208	29.6248	112.833	0.19362	10.3486

See figure A-15 for corresponding atom with atom number.

A.12 Minimum, Maximum, Average PBE/6-31G** Training Set Data

Table A-97. FOX-7 minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	4.60892	16.8727	-0.41573	16.8515	19.90175	0.00091	19.90265	4.72E-05	3.56709	33.696	4.06187
C max	6.12987	22.008	0	22.008	20.5216	0.001821	20.5216	9.44E-05	3.67304	42.3738	8.99786
C min	3.08797	11.7374	-0.83145	11.695	19.2819	0	19.2837	0	3.46114	25.0182	-0.87412
N - amino avg	16.24445	30.4464	0	30.4464	137.152	0	137.152	0	9.9398	71.3864	9.40513
N - amino max	16.283	30.4986	0	30.4986	140.31	0	140.31	0	10.1316	74.235	11.1057
N - amino min	16.2059	30.3942	0	30.3942	133.994	0	133.994	0	9.748	68.5378	7.70456
H - amino avg	4.628655	47.5414	0	47.5414	74.15335	0	74.15335	0	7.225733	62.48458	26.39665
H - amino max	6.30246	61.1717	0	61.1717	91.608	0	91.608	0	8.03735	76.4325	44.2463
H - amino min	2.80176	33.0238	0	33.0238	57.561	0	57.561	0	6.32836	47.2182	7.24271
N - nitro avg	3.41493	9.43605	-5.63176	5.88279	35.35475	28.093	63.44775	0.195429	6.84815	20.453	-26.048
N - nitro max	3.75617	11.1252	-5.59186	7.45558	56.1164	37.2555	75.0469	0.202238	8.03335	25.1223	-21.2682
N - nitro min	3.07369	7.7469	-5.67165	4.31	14.5931	18.9305	51.8486	0.18862	5.66295	15.7837	-30.8277
O - nitro avg	21.09388	5.180423	-22.82	-20.2983	18.99498	79.8401	98.83515	0.120767	9.062485	15.21617	-37.7444
O - nitro max	21.4247	8.23248	-17.0716	-12.7531	42.3736	95.8663	122.342	0.22718	11.3606	26.0247	-33.1413
O - nitro min	20.7531	1.34802	-28.5457	-28.2734	0.87663	70.6508	74.6577	0.011604	7.07476	2.77924	-40.5804
NH ₂ avg	25.50175	38.3633	0	38.3633	278.269	0	278.269	0	14.269	76.3861	8.717055
NH ₂ max	25.6163	38.4242	0	38.4242	284.911	0	284.911	0	14.3992	76.4325	10.1914
NH ₂ min	25.3872	38.3024	0	38.3024	271.627	0	271.627	0	14.1388	76.3397	7.24271
NO ₂ avg	45.60265	8.10565	-22.959	-18.5528	35.2032	107.452	142.6545	0.177504	12.28315	24.68875	-40.5704
NO ₂ max	45.9538	8.86879	-22.1769	-17.8831	48.2928	113.434	149.762	0.218481	12.6047	26.0247	-40.5603
NO ₂ min	45.2515	7.34251	-23.741	-19.2224	22.1136	101.47	135.547	0.136527	11.9616	23.3528	-40.5804

Table A-98. HMX minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	1.874833	35.24205	0	35.24205	55.56745	0	55.56745	0	6.299438	46.5391	17.0416
C max	2.1612	36.0932	0	36.0932	70.2873	0	70.2873	0	7.09932	46.7331	21.7137
C min	1.54093	34.4694	0	34.4694	40.3688	0	40.3688	0	5.59508	46.3391	11.7564
H avg	7.062364	33.80558	0	33.80558	45.79946	0	45.79946	0	5.497255	45.46235	13.64724
H max	7.38939	39.135	0	39.135	60.7724	0	60.7724	0	6.37154	50.6676	23.1074
H min	6.33796	28.5004	0	28.5004	30.5413	0	30.5413	0	4.61492	39.0813	2.87023
N - nitramine avg	2.80405	28.50283	0	28.50283	14.85173	0	14.85173	0	2.866195	40.4408	20.41275
N - nitramine max	3.21693	39.2213	0	39.2213	26.4466	0	26.4466	0	4.09356	49.8726	34.0713
N - nitramine min	2.42139	17.5937	0	17.5937	5.06851	0	5.06851	0	1.74413	31.4677	7.36947
N - nitro avg	2.34542	24.83705	-6.61205	23.55093	66.25783	22.47325	88.7311	0.14608	7.6121	38.648	-15.481
N - nitro max	2.57662	33.5728	-5.18909	33.2514	82.947	48.5929	98.4694	0.249958	8.2461	50.7881	-7.28288
N - nitro min	2.11482	15.7379	-7.94754	13.5612	49.8765	0	82.947	0	7.08802	25.9582	-22.8715
O - nitro avg	20.37273	9.98993	-11.6406	-5.5953	59.72913	32.10026	91.82953	0.195097	9.35164	32.22958	-20.4612
O - nitro max	21.6134	13.304	-8.17127	-0.35531	100.284	44.1804	119.512	0.248743	10.742	43.9426	-15.93
O - nitro min	18.4988	7.03266	-14.8135	-11.4072	22.7396	19.2276	66.819	0.135001	8.25022	18.9972	-25.1236
NO ₂ avg	43.09085	12.47114	-11.6563	-3.83427	97.8596	33.66688	131.5266	0.181032	10.91997	38.77978	-21.0882
NO ₂ max	44.7698	15.6002	-9.57029	0.643338	150.193	45.4481	172.47	0.249943	12.1499	50.7881	-17.0607
NO ₂ min	41.4417	9.49347	-13.7327	-8.27105	46.67	21.6661	91.9467	0.111807	9.75039	26.4853	-25.1236

Table A-99. PETN minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	0.885298	27.70033	0	27.70033	46.5182	0	46.5182	0	5.9411	38.06205	15.2604
C max	0.935798	28.0531	0	28.0531	48.0705	0	48.0705	0	6.04918	38.2442	15.5296
C min	0.807007	27.1321	0	27.1321	44.0351	0	44.0351	0	5.75027	37.9549	14.9542
H avg	6.918014	29.37709	0	29.37709	22.67934	0	22.67934	0	3.776159	38.35755	15.83474
H max	7.6064	29.4622	0	29.4622	26.1707	0	26.1707	0	4.0688	38.4632	16.7758
H min	6.28832	29.2549	0	29.2549	19.0265	0	19.0265	0	3.46493	38.2222	14.7333
N - nitro avg	3.417003	27.57393	-1.74793	27.4177	42.47058	0.54303	43.01363	0.011453	5.338528	37.00738	-0.60633
N - nitro max	3.50738	27.7852	0	27.7852	46.4357	2.17212	46.4357	0.045812	5.69439	37.0802	4.24447
N - nitro min	3.34325	27.2313	-6.31526	27.0106	40.1681	0	40.1681	0	5.07452	36.8555	-8.02961
O - nitro avg	23.3384	9.356829	-6.93125	-0.91473	51.59799	11.7367	63.33466	0.155609	7.397081	29.19386	-12.8663
O - nitro max	25.086	10.6081	-5.5959	2.5175	67.5373	12.3961	78.7398	0.191185	8.3249	35.0232	-11.4753
O - nitro min	21.5986	8.0761	-8.25828	-4.37486	35.5286	11.0707	47.8488	0.122031	6.43789	22.6443	-14.2539
O - nitrate avg	9.14401	16.05165	-0.50853	15.82943	94.7827	0.165043	94.94773	0.001736	8.217975	37.21915	-1.24639
O - nitrate max	9.18371	16.1178	-0.40275	15.8751	95.3812	0.188618	95.5566	0.002008	8.27231	37.323	-1.09375
O - nitrate min	9.11263	15.894	-0.61609	15.7589	93.5684	0.125283	93.757	0.001315	8.18621	37.1661	-1.41252
NO ₂ avg	50.0938	12.9813	-7.28996	1.005616	102.402	13.4871	115.889	0.102836	9.828738	37.00738	-14.2465
NO ₂ max	50.1438	13.0004	-7.28549	1.02071	102.661	13.502	116.127	0.103234	9.83555	37.0802	-14.2388
NO ₂ min	50.0418	12.9621	-7.29544	0.997982	101.999	13.4662	115.501	0.102514	9.8226	36.8555	-14.2539

Table A-100. EDNA minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	2.48194	32.8933	0	32.8933	46.513	0	46.513	0	5.04565	52.8307	24.53
C max	2.48194	32.8933	0	32.8933	46.513	0	46.513	0	5.04565	52.8307	24.53
C min	2.48194	32.8933	0	32.8933	46.513	0	46.513	0	5.04565	52.8307	24.53
N - nitramine avg	9.26875	29.55625	0	29.55625	85.5077	0	85.5077	0	7.286435	56.66885	14.7411
N - nitramine max	9.27298	29.6741	0	29.6741	87.8032	0	87.8032	0	7.38572	56.7476	15.0671
N - nitramine min	9.26452	29.4384	0	29.4384	83.2122	0	83.2122	0	7.18715	56.5901	14.4151
H avg	7.171665	36.34708	0	36.34708	46.9755	0	46.9755	0	5.244502	51.83783	17.63688
H max	8.64888	47.3958	0	47.3958	78.7889	0	78.7889	0	7.45673	60.0326	25.2886
H min	5.47327	28.1847	0	28.1847	30.6468	0	30.6468	0	4.0259	43.7638	11.383
N - nitro avg	3.24701	18.84325	-7.43553	17.4212	51.61465	42.3686	93.98315	0.234736	6.9713	32.7638	-23.1887
N - nitro max	3.24707	19.1013	-6.34031	17.6815	54.427	57.8669	106.669	0.248195	7.13047	32.9737	-17.7271
N - nitro min	3.24695	18.5852	-8.53075	17.1609	48.8023	26.8703	81.2973	0.221276	6.81213	32.5539	-28.6502
O - nitro avg	23.7838	8.542325	-16.4179	-12.0931	35.46793	57.91818	93.38613	0.235542	9.642513	25.7994	-29.1841
O - nitro max	25.612	8.82802	-15.0128	-10.3477	36.4086	60.8751	97.2837	0.23817	9.78957	28.7964	-28.6596
O - nitro min	21.9718	8.16434	-17.8133	-13.8501	34.0628	55.2545	90.0855	0.234187	9.51779	23.0528	-29.6919
NO ₂ avg	50.81465	10.9999	-16.5241	-10.6115	58.71415	59.76365	118.478	0.249978	11.12435	32.7638	-29.6605
NO ₂ max	50.8364	11.221	-16.524	-10.5827	59.2545	59.9495	119.204	0.249992	11.1777	32.9737	-29.6291
NO ₂ min	50.7929	10.7788	-16.5242	-10.6403	58.1738	59.5778	117.752	0.249964	11.071	32.5539	-29.6919

Table A-101. NQ minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
N - amino avg	17.0529	22.82155	-0.03043	22.8163	137.6675	0	137.6675	0	9.947185	68.4936	1.820091
N - amino max	17.0768	24.2113	0	24.2113	139.451	0	139.451	0	9.96212	69.71	3.70105
N - amino min	17.029	21.4318	-0.06087	21.4213	135.884	0	135.884	0	9.93225	67.2772	-0.06087
H - amino avg	5.668988	43.03105	-0.13115	43.01383	83.56483	0	83.56483	0	7.735998	57.63455	21.27805
H - amino max	7.24657	56.3157	0	56.3157	104.36	0	104.36	0	8.51112	72.0889	37.3889
H - amino min	2.79033	23.5225	-0.5246	23.4536	73.4276	0	73.4276	0	7.2837	35.8942	-0.5246
N - nitro avg	3.48516	2.36489	-8.91084	-6.46207	3.4866	53.4226	56.9092	0.057512	6.14071	7.71021	-45.4944
N - nitro max	3.48516	2.36489	-8.91084	-6.46207	3.4866	53.4226	56.9092	0.057512	6.14071	7.71021	-45.4944
N - nitro min	3.48516	2.36489	-8.91084	-6.46207	3.4866	53.4226	56.9092	0.057512	6.14071	7.71021	-45.4944
O - nitro avg	23.2122	2.218205	-30.1719	-29.2564	6.32445	91.92095	98.24545	0.03876	8.16321	1.6328	-45.6664
O - nitro max	25.24	4.43641	-23.8587	-22.0277	12.6489	136.701	149.35	0.07752	11.0749	14.1598	-45.4524
O - nitro min	21.1844	0	-36.485	-36.485	0	47.1409	47.1409	0	5.25152	-10.8942	-45.8804
NH ₂ avg	28.3909	32.3926	-0.14637	32.3831	309.516	0.026881	309.5425	8.24E-05	14.906	72.06725	1.588226
NH ₂ max	30.0685	34.5727	0	34.5727	326.24	0.053761	326.293	0.000165	15.1644	72.0889	3.70105
NH ₂ min	26.7133	30.2125	-0.29273	30.1935	292.792	0	292.792	0	14.6476	72.0456	-0.5246
NO ₂ avg	49.9096	3.71515	-29.7264	-28.3166	10.4327	147.049	157.482	0.061858	11.4307	14.1598	-45.8804
NO ₂ max	49.9096	3.71515	-29.7264	-28.3166	10.4327	147.049	157.482	0.061858	11.4307	14.1598	-45.8804
NO ₂ min	49.9096	3.71515	-29.7264	-28.3166	10.4327	147.049	157.482	0.061858	11.4307	14.1598	-45.8804

Table A-102. RDX minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	2.375097	30.4206	0	30.4206	12.15577	0	12.15577	0	2.22554	45.90503	20.76573
C max	2.5669	31.1182	0	31.1182	15.3901	0	15.3901	0	2.57936	47.7095	24.075
C min	2.27461	29.6643	0	29.6643	6.6386	0	6.6386	0	1.62489	44.2859	18.5021
H avg	7.355648	31.59413	-1.3563	31.48797	33.80822	1.41392	35.22215	0.026557	4.906483	40.42782	12.55971
H max	9.53207	40.4572	0	40.4572	44.1943	5.24481	48.9162	0.095724	5.66912	50.3865	31.0937
H min	4.99156	21.3257	-4.35918	21.0521	25.8174	0	25.8174	0	4.37391	29.828	-7.44666
N - nitramine avg	5.233243	22.05067	0	22.05067	62.87797	0	62.87797	0	6.417213	42.37383	11.6677
N - nitramine max	6.0049	24.8105	0	24.8105	126.648	0	126.648	0	10.37	46.6585	13.1626
N - nitramine min	3.71152	20.4243	0	20.4243	30.2794	0	30.2794	0	4.36589	40.2133	9.1334
N - nitro avg	2.951603	21.39147	-7.65234	20.2349	69.49467	32.4215	101.9162	0.215331	7.35987	38.50607	-19.1625
N - nitro max	3.28611	21.8525	-5.32611	20.6436	96.259	45.16	141.419	0.226661	9.23393	39.1572	-15.0088
N - nitro min	2.70134	20.8077	-9.81845	19.6036	53.6833	20.9645	74.6478	0.201971	6.1966	37.628	-22.9179
O - nitro avg	21.09072	8.617288	-14.2469	-10.0153	39.7243	39.51875	79.24303	0.246465	8.771838	25.81878	-23.7951
O - nitro max	22.3086	9.56327	-12.9931	-8.6153	58.6093	46.6069	101.445	0.249641	9.14383	32.2716	-22.3557
O - nitro min	19.606	7.47784	-15.2502	-11.3318	24.9104	35.0244	63.0903	0.238941	8.41829	19.5852	-26.0479
NO ₂ avg	51.54553	11.06012	-14.3498	-8.73759	69.5614	40.86227	110.4237	0.232232	10.07923	36.21087	-24.8692
NO ₂ max	63.1657	12.7925	-13.9996	-7.88598	95.4092	45.0044	140.414	0.249199	11.005	38.733	-23.3132
NO ₂ min	43.7713	8.81785	-15.0013	-9.66535	43.2278	38.5954	81.8232	0.217784	8.83619	32.2716	-26.0479

Table A-103. CL20 minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	0.778991	46.42873	0	46.42873	32.34019	0	32.34019	0	4.329655	54.68872	33.14565
C max	1.05784	54.3521	0	54.3521	62.4761	0	62.4761	0	6.04231	65.4009	46.3491
C min	0.306849	33.9623	0	33.9623	7.17714	0	7.17714	0	2.11423	42.665	19.8029
H avg	5.02544	39.66852	0	39.66852	56.64643	0	56.64643	0	5.884027	51.3836	15.33131
H max	6.33996	44.5449	0	44.5449	85.6273	0	85.6273	0	7.5185	57.584	24.7992
H min	3.58753	30.9149	0	30.9149	15.3671	0	15.3671	0	3.13039	42.4466	7.88152
N - nitramine avg	2.932016	33.95027	0	33.95027	89.30905	0	89.30905	0	6.54693	53.89375	23.34827
N - nitramine max	5.20548	38.7529	0	38.7529	316.703	0	316.703	0	16.2304	65.1367	31.3447
N - nitramine min	0.952923	29.8286	0	29.8286	22.2851	0	22.2851	0	3.77712	45.234	18.2279
N - nitro avg	2.482302	30.26963	-3.95117	29.98933	113.8871	1.658627	115.5457	0.012058	8.523852	46.47933	-3.80961
N - nitro max	3.14219	33.2733	0	33.2733	200.016	9.81469	200.153	0.071666	12.2331	62.7993	4.35241
N - nitro min	1.83067	27.4847	-9.7515	27.2603	35.9051	0	35.9051	0	4.90863	33.7374	-9.7515
O - nitro avg	20.41276	11.2738	-7.28483	-0.19183	83.32446	14.02338	97.34785	0.127216	8.71275	40.03548	-13.7933
O - nitro max	22.1804	13.2843	-5.74949	2.90644	124.333	17.2765	137.04	0.165411	9.69525	54.9428	-11.9264
O - nitro min	17.7463	8.63925	-8.36455	-2.64849	55.402	11.1728	67.6825	0.081365	6.4426	30.3106	-14.8607
NO ₂ avg	43.30785	13.9602	-7.30875	1.582096	133.6349	14.25025	147.8852	0.092286	10.40171	46.47933	-14.1099
NO ₂ max	45.8331	15.3985	-6.39629	3.27861	192.463	15.7573	206.372	0.127047	11.4386	62.7993	-13.5379
NO ₂ min	39.9977	12.6145	-8.04861	0.418356	89.7463	12.1433	105.504	0.062049	9.81383	33.7374	-14.8607

Table A-104. HNB minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	3.947693	40.80455	0	40.80455	16.15008	0	16.15008	0	3.136735	51.50777	32.15652
C max	4.02572	40.9482	0	40.9482	17.3651	0	17.3651	0	3.26892	51.88	33.3151
C min	3.84076	40.5862	0	40.5862	14.9851	0	14.9851	0	2.99898	50.9519	31.4721
N - nitro avg	0.725154	21.16043	-0.24745	21.02638	74.00602	0	74.00602	0	7.459713	36.09998	2.301286
N - nitro max	0.784681	21.7051	0	21.512	84.1842	0	84.1842	0	8.46563	37.606	7.76982
N - nitro min	0.634403	19.9162	-0.9946	19.9162	65.9308	0	65.9308	0	6.7058	35.0696	-0.9946
O - nitro avg	20.57982	8.871949	-4.11396	3.253884	60.34254	6.643895	66.98643	0.087106	6.766693	33.94911	-8.84092
O - nitro max	21.0643	9.69872	-3.11125	6.23863	67.2383	9.85248	77.0341	0.117088	7.05807	37.0093	-6.10002
O - nitro min	19.922	7.96563	-5.02327	0.679806	52.4815	2.95161	57.418	0.040932	6.32961	31.6491	-11.3824
NO ₂ avg	41.8848	9.236133	-4.25348	3.533863	65.34375	7.412085	72.75585	0.089934	7.189363	36.09998	-10.0854
NO ₂ max	42.0656	9.87236	-3.48095	4.82593	68.1599	9.17247	76.9045	0.105779	7.60917	37.606	-7.63114
NO ₂ min	41.6029	8.72303	-4.81551	2.07697	60.4111	4.63608	65.0472	0.066193	6.7883	35.0696	-11.3824

Table A-105. TATB minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.250378	21.17005	0	21.17005	2.066512	0	2.066512	0	1.08561	25.60458	18.09663
C max	6.59266	22.0345	0	22.0345	3.90611	0	3.90611	0	1.53333	28.5548	18.9006
C min	3.94678	19.9717	0	19.9717	0.76682	0	0.76682	0	0.662951	23.8278	16.9679
N - amino avg	15.0091	19.0633	0	19.0633	61.29957	0	61.29957	0	6.292783	36.7817	5.622277
N - amino max	15.198	19.4526	0	19.4526	70.3699	0	70.3699	0	6.94766	37.8533	9.15223
N - amino min	14.8215	18.5387	0	18.5387	54.1898	0	54.1898	0	5.80516	35.9149	3.52221
H - amino avg	2.568768	27.6148	0	27.6148	46.86723	0	46.86723	0	5.708132	37.26212	9.639487
H - amino max	3.3186	29.883	0	29.883	57.2542	0	57.2542	0	6.34243	39.8763	11.4069
H - amino min	2.1783	26.1973	0	26.1973	36.3629	0	36.3629	0	4.79905	35.8258	7.59726
N - nitro avg	3.898243	18.81873	-6.55931	18.22277	24.31427	26.7822	51.0965	0.168754	4.449787	25.08973	-13.9669
N - nitro max	3.97942	19.7625	-3.01727	19.5193	26.8797	56.7443	79.2639	0.249712	4.81911	27.6857	-4.59149
N - nitro min	3.8158	17.6326	-10.0442	16.6901	22.5195	1.60459	28.4843	0.053159	4.17612	23.7701	-21.5669
O - nitro avg	20.09685	8.291805	-13.804	-7.72405	32.83195	55.9835	88.81545	0.228736	10.1667	23.17998	-26.8357
O - nitro max	20.5098	9.12057	-12.9141	-5.78398	44.811	64.7605	96.4563	0.248745	10.54	27.7271	-25.7856
O - nitro min	19.5354	7.15453	-15.0218	-9.87821	24.0615	50.4585	83.5881	0.201693	10.0004	19.4829	-28.6389
NH ₂ avg	20.14667	21.40643	0	21.40643	73.20273	0	73.20273	0	7.269777	37.9396	5.103953
NH ₂ max	20.3535	21.6831	0	21.6831	79.09	0	79.09	0	7.53796	39.8763	7.59726
NH ₂ min	19.7373	21.1918	0	21.1918	65.3708	0	65.3708	0	6.74927	36.676	3.52221
NO ₂ avg	44.09193	10.64377	-13.7938	-5.80814	50.2938	56.16223	106.456	0.24743	11.44387	25.6708	-26.8888
NO ₂ max	44.5811	11.1684	-13.1252	-4.80048	56.2016	63.4139	108.658	0.249673	11.5201	27.7271	-25.9889
NO ₂ min	43.8298	10.0162	-14.8826	-7.68774	45.2439	51.9242	102.584	0.243009	11.3888	23.8134	-28.6389

Table A-106. PNA minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	4.325553	31.61855	0	31.61855	16.4676	0	16.4676	0	3.049673	43.62863	23.17068
C max	5.13817	37.9462	0	37.9462	24.1563	0	24.1563	0	3.73823	49.1465	31.944
C min	3.50961	28.0972	0	28.0972	6.7066	0	6.7066	0	1.78211	37.7805	20.155
N - amino avg	15.8907	36.8819	0	36.8819	53.0936	0	53.0936	0	5.99846	55.1261	26.7903
N - amino max	15.8907	36.8819	0	36.8819	53.0936	0	53.0936	0	5.99846	55.1261	26.7903
N - amino min	15.8907	36.8819	0	36.8819	53.0936	0	53.0936	0	5.99846	55.1261	26.7903
H - amino avg	2.8007	46.8829	0	46.8829	40.91005	0	40.91005	0	5.32561	55.51675	28.1071
H - amino max	2.8217	46.9062	0	46.9062	41.7604	0	41.7604	0	5.37696	55.5202	28.6377
H - amino min	2.7797	46.8596	0	46.8596	40.0597	0	40.0597	0	5.27426	55.5133	27.5765
N - nitro avg	1.580525	18.88957	-3.76241	17.91618	67.61152	5.29472	72.90624	0.07048	6.657904	32.51314	-4.15461
N - nitro max	2.72641	33.5515	0	33.5515	113.29	18.9632	113.29	0.246688	9.41708	49.8594	7.73782
N - nitro min	0.249717	3.86091	-7.69138	2.03727	23.8967	0	39.7001	0	3.84411	15.6112	-11.2575
O - nitro avg	20.18299	9.963833	-7.63987	-1.93314	60.14223	14.45386	74.59611	0.163088	7.230621	29.65767	-14.4052
O - nitro max	21.0454	13.7619	-5.16445	8.0776	104.305	18.4507	112.335	0.219227	10.1067	44.4365	-9.63478
O - nitro min	19.1636	7.8718	-9.61258	-6.0622	37.8163	7.99943	55.7791	0.066376	5.49722	21.7187	-17.1825
NH ₂ avg	22.2012	36.7238	0	36.7238	70.5315	0	70.5315	0	6.9853	55.5133	20.155
NH ₂ max	22.2012	36.7238	0	36.7238	70.5315	0	70.5315	0	6.9853	55.5133	20.155
NH ₂ min	22.2012	36.7238	0	36.7238	70.5315	0	70.5315	0	6.9853	55.5133	20.155
NO ₂ avg	41.94652	11.46052	-7.72049	-0.84781	83.17512	14.80098	97.97588	0.148538	8.463778	34.74356	-14.9971
NO ₂ max	42.9374	15.3559	-5.99381	5.8276	142.644	18.1212	152.737	0.213632	11.4649	49.8594	-12.5257
NO ₂ min	40.9482	8.02192	-9.57496	-5.56248	39.633	10.0936	57.3807	0.061718	5.81636	23.7563	-17.1825

Table A-107. TNT minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.400097	22.20726	0	22.20726	23.52067	0	23.52067	0	3.738073	35.79126	10.27555
C max	7.25404	23.5788	0	23.5788	47.4931	0	47.4931	0	6.0079	40.074	12.9938
C min	4.00474	21.2027	0	21.2027	14.6955	0	14.6955	0	2.84833	32.6136	6.6334
H avg	8.031216	23.86264	0	23.86264	23.8203	0	23.8203	0	3.734514	32.45292	8.6176
H max	9.40421	28.9577	0	28.9577	46.8943	0	46.8943	0	5.69416	39.7264	10.2799
H min	6.98488	17.648	0	17.648	13.9463	0	13.9463	0	2.87454	22.5552	5.74171
N - nitro avg	2.901713	26.77867	-5.49129	26.166	50.08163	14.4314	64.51303	0.143439	6.050953	37.29563	-10.3364
N - nitro max	3.64975	27.6956	-4.35856	27.3036	57.9341	24.9028	68.4519	0.231449	6.29637	39.7151	-5.23719
N - nitro min	1.81759	25.2995	-6.87813	24.7914	43.5491	0	57.9341	0	5.58822	35.1487	-13.243
O - nitro avg	22.69677	8.800048	-9.60588	-4.24544	45.71647	24.05973	69.7762	0.22246	8.058855	29.72827	-18.3369
O - nitro max	23.8611	9.69099	-8.30397	-3.29887	55.4851	29.9922	77.4809	0.246541	8.4943	33.723	-16.4018
O - nitro min	20.6497	8.0021	-11.1171	-5.89096	37.9887	18.1748	59.3707	0.185859	7.20326	26.1954	-20.5434
NO ₂ avg	48.29527	12.00467	-9.60748	-2.38476	92.63553	24.1627	116.798	0.162732	9.738607	37.29563	-18.5845
NO ₂ max	50.2738	12.5399	-8.67717	-1.53545	100.696	29.0257	125.637	0.181112	10.4615	39.7151	-16.9967
NO ₂ min	46.9979	10.9877	-10.9213	-3.34592	84.0405	18.5207	102.561	0.147972	8.76195	35.1487	-20.5434

Table A-108. TNA minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.363233	27.14712	0	27.14712	9.49208	0	9.49208	0	2.336278	35.767	18.96825
C max	7.03358	31.8498	0	31.8498	16.1091	0	16.1091	0	3.06326	41.5832	26.4602
C min	3.46533	22.4699	0	22.4699	3.06115	0	3.06115	0	1.20822	31.8016	13.4664
H avg	5.77677	21.5588	0	21.5588	10.714	0	10.714	0	2.64487	26.1383	11.2989
H max	5.77677	21.5588	0	21.5588	10.714	0	10.714	0	2.64487	26.1383	11.2989
H min	5.77677	21.5588	0	21.5588	10.714	0	10.714	0	2.64487	26.1383	11.2989
N - amino avg	15.6328	28.6184	0	28.6184	46.2483	0	46.2483	0	5.49666	45.6024	19.4716
N - amino max	15.6328	28.6184	0	28.6184	46.2483	0	46.2483	0	5.49666	45.6024	19.4716
N - amino min	15.6328	28.6184	0	28.6184	46.2483	0	46.2483	0	5.49666	45.6024	19.4716
H - amino avg	3.57724	40.203	0	40.203	49.24885	0	49.24885	0	5.88824	49.6743	22.0968
H - amino max	3.61676	40.9152	0	40.9152	49.4433	0	49.4433	0	5.97793	50.2008	23.7067
H - amino min	3.53772	39.4908	0	39.4908	49.0544	0	49.0544	0	5.79855	49.1478	20.4869
N - nitro avg	2.794244	23.82673	-8.32091	19.25609	37.46435	11.08434	48.54868	0.165152	5.635845	31.75968	-12.2986
N - nitro max	4.0714	29.918	-5.3184	29.4849	66.7087	19.6307	66.7087	0.228272	6.69284	41.9327	-11.6949
N - nitro min	0.276007	14.7193	-11.8555	-2.31275	4.12598	0	11.7017	0	5.06893	16.4935	-13.1796
O - nitro avg	20.52031	9.824281	-10.0032	-3.6772	48.86305	21.22941	70.09246	0.20507	8.102429	27.40836	-17.6497
O - nitro max	22.5499	13.8191	-7.00035	5.63535	81.673	32.7922	98.4057	0.249988	10.9264	37.9336	-13.3427
O - nitro min	18.6114	7.14688	-13.5639	-10.0662	21.1693	15.4615	42.0491	0.133839	5.36254	18.1865	-21.7037
NH ₂ avg	22.7873	32.1216	0	32.1216	75.6016	0	75.6016	0	7.57548	50.2008	19.4716
NH ₂ max	22.7873	32.1216	0	32.1216	75.6016	0	75.6016	0	7.57548	50.2008	19.4716
NH ₂ min	22.7873	32.1216	0	32.1216	75.6016	0	75.6016	0	7.57548	50.2008	19.4716
NO ₂ avg	43.83488	12.50588	-10.0858	-1.76303	80.7371	22.15338	102.8904	0.173675	10.02248	32.93688	-18.3293
NO ₂ max	46.3891	15.3619	-7.89214	4.91969	111.305	31.9485	129.144	0.248323	12.063	41.9327	-15.699
NO ₂ min	41.6788	7.37101	-12.219	-9.5449	24.7341	16.7713	45.7237	0.113801	5.58571	21.2023	-21.7037

Table A-109. NTO minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	3.573485	21.10035	0	21.10035	16.718	0	16.718	0	3.280085	28.16105	6.623652
C max	4.17512	23.5675	0	23.5675	20.1067	0	20.1067	0	3.40664	29.7308	12.9963
C min	2.97185	18.6332	0	18.6332	13.3293	0	13.3293	0	3.15353	26.5913	0.251004
H avg	7.079985	44.58565	0	44.58565	58.8305	0	58.8305	0	6.566575	58.54505	27.0177
H max	7.77444	45.8342	0	45.8342	60.872	0	60.872	0	6.67763	59.9353	29.7182
H min	6.38553	43.3371	0	43.3371	56.789	0	56.789	0	6.45552	57.1548	24.3172
N avg	13.28773	18.2826	-3.5149	14.65845	27.598	12.6404	40.2384	0.083327	5.99278	31.7384	2.179167
N max	16.9578	22.7532	0	22.7532	38.5938	37.9212	76.515	0.249981	10.2649	35.4066	15.3257
N min	11.3504	10.0134	-10.5447	-0.85906	14.9191	0	14.9191	0	3.11803	26.378	-21.8718
O avg	27.9777	7.83489	-16.7837	-11.6847	24.5147	57.1116	81.6263	0.210131	10.3836	22.1781	-26.826
O max	27.9777	7.83489	-16.7837	-11.6847	24.5147	57.1116	81.6263	0.210131	10.3836	22.1781	-26.826
O min	27.9777	7.83489	-16.7837	-11.6847	24.5147	57.1116	81.6263	0.210131	10.3836	22.1781	-26.826
N - nitro avg	4.2177	21.4483	-4.48293	20.913	40.0873	12.7579	52.8452	0.183136	5.62114	29.7509	-12.4994
N - nitro max	4.2177	21.4483	-4.48293	20.913	40.0873	12.7579	52.8452	0.183136	5.62114	29.7509	-12.4994
N - nitro min	4.2177	21.4483	-4.48293	20.913	40.0873	12.7579	52.8452	0.183136	5.62114	29.7509	-12.4994
O - nitro avg	23.44195	8.414105	-13.3078	-8.73827	35.17125	33.33285	68.50405	0.243409	8.249405	22.746	-22.0927
O - nitro max	23.6247	10.2255	-11.3422	-4.54783	50.3132	37.8098	88.1229	0.244967	9.82102	28.9207	-21.6497
O - nitro min	23.2592	6.60271	-15.2734	-12.9287	20.0293	28.8559	48.8852	0.24185	6.67779	16.5713	-22.5357
NO ₂ avg	51.1016	12.5627	-13.5557	-6.58316	72.7237	36.6392	109.363	0.222783	10.9955	29.7509	-22.5357
NO ₂ max	51.1016	12.5627	-13.5557	-6.58316	72.7237	36.6392	109.363	0.222783	10.9955	29.7509	-22.5357
NO ₂ min	51.1016	12.5627	-13.5557	-6.58316	72.7237	36.6392	109.363	0.222783	10.9955	29.7509	-22.5357

Table A-110. DATB minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.74999	20.65057	0	20.65057	2.7637	0	2.7637	0	1.202369	24.6284	17.46473
C max	6.80611	22.645	0	22.645	5.55271	0	5.55271	0	2.00026	25.6946	20.5315
C min	3.99486	16.3151	0	16.3151	0.452752	0	0.452752	0	0.47933	22.965	11.7865
H avg	5.39709	11.1604	0	11.1604	7.05478	0	7.05478	0	2.18951	14.577	4.27397
H max	5.39709	11.1604	0	11.1604	7.05478	0	7.05478	0	2.18951	14.577	4.27397
H min	5.39709	11.1604	0	11.1604	7.05478	0	7.05478	0	2.18951	14.577	4.27397
N - amino avg	15.6496	19.94125	0	19.94125	41.6935	0	41.6935	0	5.256485	36.0134	11.7275
N - amino max	15.6837	19.9581	0	19.9581	41.7931	0	41.7931	0	5.2566	36.2782	11.7325
N - amino min	15.6155	19.9244	0	19.9244	41.5939	0	41.5939	0	5.25637	35.7486	11.7225
H - amino avg	3.260678	29.87318	0	29.87318	44.16493	0	44.16493	0	5.588093	39.10765	14.5416
H - amino max	3.41454	30.6761	0	30.6761	45.3111	0	45.3111	0	5.65316	40.0044	14.8444
H - amino min	3.1119	29.123	0	29.123	43.548	0	43.548	0	5.49427	38.2517	14.38
N - nitro avg	3.96703	20.21637	-4.79929	19.68143	24.9062	26.05297	50.95917	0.159739	4.391933	25.30453	-10.0477
N - nitro max	4.02531	22.5633	0	22.5633	27.9631	43.9435	69.1904	0.247472	5.00369	26.2945	5.71285
N - nitro min	3.8601	18.916	-7.68936	18.0786	21.5086	0	21.5086	0	3.43405	24.8011	-18.4877
O - nitro avg	20.79207	8.401212	-12.2643	-6.02528	33.00113	42.10252	75.10365	0.235272	9.357412	23.15918	-22.9345
O - nitro max	22.1218	9.86868	-10.3788	-2.23935	42.8514	47.9096	86.3323	0.248392	10.5132	27.9279	-20.657
O - nitro min	19.812	5.8721	-14.0727	-11.1025	18.1111	35.3081	61.3598	0.208042	7.73297	15.6645	-24.6981
NH ₂ avg	22.17095	22.9703	0	22.9703	63.7368	0	63.7368	0	7.00488	39.96045	11.7275
NH ₂ max	22.1898	23.0034	0	23.0034	63.7479	0	63.7479	0	7.00736	40.0044	11.7325
NH ₂ min	22.1521	22.9372	0	22.9372	63.7257	0	63.7257	0	7.0024	39.9165	11.7225
NO ₂ avg	45.55113	11.23977	-12.3513	-4.19909	56.17803	42.3733	98.55133	0.242938	10.96677	26.58717	-23.3396
NO ₂ max	46.5932	11.9592	-10.3814	-0.41387	61.536	46.0042	99.9831	0.248648	11.0452	27.9279	-20.6626
NO ₂ min	43.5415	10.8326	-13.3443	-6.11736	53.0192	35.3612	96.8972	0.231757	10.922	25.8346	-24.6981

Table A-111. Picric acid minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	6.178952	26.54357	0	26.54357	8.061033	0	8.061033	0	2.05082	32.9391	17.39623
C max	7.367	30.9542	0	30.9542	13.0391	0	13.0391	0	2.73085	38.8861	25.7486
C min	4.32506	22.9659	0	22.9659	2.25143	0	2.25143	0	1.18018	29.2369	11.5951
H avg	4.816583	25.8718	0	25.8718	15.65907	0	15.65907	0	3.3036	32.0511	16.0975
H max	6.47971	34.6707	0	34.6707	20.6705	0	20.6705	0	3.97519	41.8756	26.3516
H min	1.63584	20.5846	0	20.5846	10.0934	0	10.0934	0	2.5449	26.9195	8.99221
O avg	17.4931	16.8346	-6.67547	10.6938	98.1008	18.0232	116.124	0.131118	11.6432	37.5175	-15.9099
O max	17.4931	16.8346	-6.67547	10.6938	98.1008	18.0232	116.124	0.131118	11.6432	37.5175	-15.9099
O min	17.4931	16.8346	-6.67547	10.6938	98.1008	18.0232	116.124	0.131118	11.6432	37.5175	-15.9099
N - nitro avg	3.931607	26.41533	-2.72974	26.16243	38.5688	2.449437	41.01823	0.05007	5.009067	33.60083	-4.22544
N - nitro max	4.1056	32.2085	-0.62437	32.1019	41.1425	5.44326	46.5857	0.103192	5.28528	38.6621	-0.62437
N - nitro min	3.63347	23.4767	-4.21624	23.0716	36.6088	0	37.9551	0	4.66072	30.1035	-6.54932
O - nitro avg	21.98018	9.491152	-9.76741	-3.29356	47.67663	23.92222	71.59877	0.208334	8.550278	27.22618	-18.0657
O - nitro max	22.7596	14.0729	-6.1598	6.24393	88.6551	30.9608	100.123	0.24876	10.7045	37.8991	-11.8028
O - nitro min	20.3182	8.28865	-12.8392	-9.22266	32.9135	11.4683	59.1519	0.101422	7.54027	21.4615	-21.1421
NO ₂ avg	47.89193	12.9297	-9.75777	-1.15916	92.53	24.2506	116.7807	0.161823	10.53247	33.60083	-18.2948
NO ₂ max	49.284	14.6128	-6.22612	5.55941	118.782	30.8419	131.523	0.205669	11.138	38.6621	-12.9524
NO ₂ min	46.5428	11.699	-12.0317	-5.36714	75.711	12.7404	106.553	0.087485	10.2222	30.1035	-21.1421

A.13 Minimum, Maximum, Average Area Weighted PBE/6-31G** Training Set Data

Table A-112. FOX-7 minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	4.60892	16.8132	-0.41132	16.79915	19.82445	0.000872	19.8253	4.6E-05	3.56832
C max	6.12987	22.1906	0	22.1906	20.7249	0.001743	20.7249	9.21E-05	3.63816
C min	3.08797	11.4358	-0.82263	11.4077	18.924	0	18.9257	0	3.49848
N - amino avg	16.24445	30.35155	0	30.35155	138.6325	0	138.6325	0	10.01332
N - amino max	16.283	30.5325	0	30.5325	140.476	0	140.476	0	10.04
N - amino min	16.2059	30.1706	0	30.1706	136.789	0	136.789	0	9.98664
H - amino avg	4.628655	47.6892	0	47.6892	72.92055	0	72.92055	0	7.15116
H - amino max	6.30246	60.9898	0	60.9898	89.6958	0	89.6958	0	7.94578
H - amino min	2.80176	33.1047	0	33.1047	57.0757	0	57.0757	0	6.29814
N - nitro avg	3.41493	9.42822	-5.65053	6.026035	33.42	29.65595	63.07595	0.193867	6.685795
N - nitro max	3.75617	11.0106	-5.57967	7.5366	52.7508	40.1516	71.9111	0.195452	7.76046
N - nitro min	3.07369	7.84584	-5.72138	4.51547	14.0892	19.1603	54.2408	0.192281	5.61113
O - nitro avg	21.09388	5.146955	-22.7407	-20.1313	18.95672	81.84935	100.8061	0.117995	9.23269
O - nitro max	21.4247	8.38773	-17.0023	-12.531	43.5242	99.6053	125.044	0.229979	11.5177
O - nitro min	20.7531	1.32757	-28.6866	-28.375	0.848014	74.782	75.978	0.011037	7.18595
NH ₂ avg	25.50175	38.29415	0	38.29415	278.7315	0	278.7315	0	14.29975
NH ₂ max	25.6163	38.4429	0	38.4429	285.208	0	285.208	0	14.4405
NH ₂ min	25.3872	38.1454	0	38.1454	272.255	0	272.255	0	14.159
NO ₂ avg	45.60265	8.096385	-22.8791	-18.2588	34.49905	109.008	143.5065	0.174045	12.4678
NO ₂ max	45.9538	8.92064	-21.9212	-17.3668	47.7244	116.459	149.281	0.21749	12.839
NO ₂ min	45.2515	7.27213	-23.8369	-19.1507	21.2737	101.557	137.732	0.1306	12.0966

Table A-113. HMX minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	1.874833	35.04773	0	35.04773	54.85603	0	54.85603	0	6.257575
C max	2.1612	35.579	0	35.579	69.1522	0	69.1522	0	6.92685
C min	1.54093	34.5811	0	34.5811	40.304	0	40.304	0	5.55774
H avg	7.062364	33.70634	0	33.70634	45.9242	0	45.9242	0	5.52866
H max	7.38939	39.0394	0	39.0394	61.2436	0	61.2436	0	6.41944
H min	6.33796	28.5303	0	28.5303	31.139	0	31.139	0	4.69809
N - nitramine avg	2.80405	28.41088	0	28.41088	14.1736	0	14.1736	0	2.807945
N - nitramine max	3.21693	39.1524	0	39.1524	24.285	0	24.285	0	3.97009
N - nitramine min	2.42139	17.5255	0	17.5255	4.9798	0	4.9798	0	1.72067
N - nitro avg	2.34542	24.716	-6.77344	23.40593	69.91298	25.01973	94.93275	0.145776	7.816918
N - nitro max	2.57662	33.3413	-4.20628	32.8189	92.2523	52.5915	103.7	0.249949	8.3056
N - nitro min	2.11482	15.9417	-8.68033	14.0271	51.1084	0	90.4356	0	7.48559
O - nitro avg	20.37273	9.732095	-11.6182	-5.88158	58.98168	31.64755	90.62929	0.195032	9.094293
O - nitro max	21.6134	12.8194	-8.06033	-0.62971	100.303	44.5368	119.506	0.248147	10.1901
O - nitro min	18.4988	6.93025	-14.8951	-11.6971	22.5209	19.2031	65.08	0.134867	8.02336
NO ₂ avg	43.09085	12.19324	-11.6367	-4.19739	97.41583	33.17168	130.5874	0.180688	10.64625
NO ₂ max	44.7698	15.1017	-9.42424	0.116504	149.653	44.9632	171.499	0.249826	11.659
NO ₂ min	41.4417	9.31548	-13.8552	-8.49574	46.8832	21.4781	91.2822	0.111158	9.65635

Table A-114. PETN minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	0.885298	28.00863	0	28.00863	45.55008	0	45.55008	0	5.810343
C max	0.935798	28.4681	0	28.4681	46.2	0	46.2	0	5.86054
C min	0.807007	27.3787	0	27.3787	44.8084	0	44.8084	0	5.78573
H avg	6.918014	29.40555	0	29.40555	22.97856	0	22.97856	0	3.792055
H max	7.6064	29.5466	0	29.5466	25.9812	0	25.9812	0	4.05675
H min	6.28832	29.1864	0	29.1864	19.8616	0	19.8616	0	3.51169
N - nitro avg	3.417003	27.29523	-1.74597	27.08905	45.69513	0.3877	46.08283	0.00794	5.547015
N - nitro max	3.50738	27.5204	0	27.5204	50.1355	1.5508	50.1355	0.031761	5.94436
N - nitro min	3.34325	26.9326	-6.30744	26.6482	42.5731	0	42.5731	0	5.19345
O - nitro avg	23.3384	9.090839	-6.90764	-1.18192	50.55088	11.57418	62.12506	0.156099	7.167916
O - nitro max	25.086	10.2389	-5.5685	2.20526	65.8492	12.1306	76.9403	0.190469	8.07585
O - nitro min	21.5986	7.9687	-8.24212	-4.57468	35.1929	11.0611	47.3029	0.123372	6.24997
O - nitrate avg	9.14401	15.67928	-0.60445	15.48593	91.34103	0.188921	91.5299	0.00206	7.993158
O - nitrate max	9.18371	15.7349	-0.50489	15.5341	92.0972	0.234959	92.2778	0.002573	8.03974
O - nitrate min	9.11263	15.5598	-0.72828	15.431	90.8321	0.160078	91.067	0.001748	7.95445
NO ₂ avg	50.0938	12.4942	-7.26915	0.520507	99.73753	13.30748	113.045	0.103861	9.445988
NO ₂ max	50.1438	12.5055	-7.2652	0.52782	99.975	13.3281	113.285	0.10414	9.4514
NO ₂ min	50.0418	12.4767	-7.27442	0.508714	99.5427	13.2841	112.871	0.103688	9.43945

Table A-115. EDNA minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	2.48194	32.4915	0	32.4915	44.1941	0	44.1941	0	4.81919
C max	2.48194	32.4915	0	32.4915	44.1941	0	44.1941	0	4.81919
C min	2.48194	32.4915	0	32.4915	44.1941	0	44.1941	0	4.81919
N - nitramine avg	9.26875	29.3776	0	29.3776	85.76915	0	85.76915	0	7.238995
N - nitramine max	9.27298	29.4374	0	29.4374	86.8084	0	86.8084	0	7.28444
N - nitramine min	9.26452	29.3178	0	29.3178	84.7299	0	84.7299	0	7.19355
H avg	7.171665	36.46403	0	36.46403	46.71498	0	46.71498	0	5.202892
H max	8.64888	48.0008	0	48.0008	78.6663	0	78.6663	0	7.45386
H min	5.47327	28.0883	0	28.0883	29.8413	0	29.8413	0	3.92977
N - nitro avg	3.24701	19.19485	-7.44035	17.89965	49.13195	43.46855	92.60045	0.228884	6.71175
N - nitro max	3.24707	19.4449	-6.05514	18.0659	51.5743	63.8045	110.494	0.244002	6.75854
N - nitro min	3.24695	18.9448	-8.82556	17.7334	46.6896	23.1326	74.7069	0.213765	6.66496
O - nitro avg	23.7838	8.502215	-16.3711	-11.7519	35.55405	58.9993	94.55333	0.234449	9.877925
O - nitro max	25.612	8.69174	-14.9541	-9.79896	39.4754	62.3662	100.263	0.238704	10.1532
O - nitro min	21.9718	8.26004	-17.7341	-13.706	33.534	56.1098	89.8454	0.231108	9.61218
NO ₂ avg	50.81465	11.29045	-16.4905	-9.99477	61.222	60.7737	121.9955	0.249992	11.58395
NO ₂ max	50.8364	11.3475	-16.4695	-9.98333	61.4975	61.0438	122.001	0.25	11.5915
NO ₂ min	50.7929	11.2334	-16.5115	-10.0062	60.9465	60.5036	121.99	0.249983	11.5764

Table A-116. NQ minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
N - amino avg	17.0529	22.87935	-0.03043	22.87345	140.304	0	140.304	0	10.05536
N - amino max	17.0768	24.4398	0	24.4398	148.69	0	148.69	0	10.3043
N - amino min	17.029	21.3189	-0.06087	21.3071	131.918	0	131.918	0	9.80642
H - amino avg	5.668988	42.86093	-0.13115	42.83123	83.23188	0	83.23188	0	7.727933
H - amino max	7.24657	56.2386	0	56.2386	103.915	0	103.915	0	8.55529
H - amino min	2.79033	23.3547	-0.5246	23.2359	70.7335	0	70.7335	0	7.12552
N - nitro avg	3.48516	2.36893	-8.69076	-6.21727	3.52673	52.4911	56.0178	0.058994	6.02578
N - nitro max	3.48516	2.36893	-8.69076	-6.21727	3.52673	52.4911	56.0178	0.058994	6.02578
N - nitro min	3.48516	2.36893	-8.69076	-6.21727	3.52673	52.4911	56.0178	0.058994	6.02578
O - nitro avg	23.2122	2.15539	-30.243	-29.3554	6.0602	93.94355	100.0036	0.036652	8.21968
O - nitro max	25.24	4.31078	-23.9143	-22.1392	12.1204	140.055	152.175	0.073304	11.1885
O - nitro min	21.1844	0	-36.5716	-36.5716	0	47.8321	47.8321	0	5.25086
NH ₂ avg	28.3909	32.34015	-0.16892	32.3269	308.2715	0.025864	308.297	8.02E-05	14.9126
NH ₂ max	30.0685	34.5449	0	34.5449	322.417	0.051727	322.468	0.00016	15.0951
NH ₂ min	26.7133	30.1354	-0.33783	30.1089	294.126	0	294.126	0	14.7301
NO ₂ avg	49.9096	3.59404	-29.7363	-28.3261	9.82655	150.221	160.048	0.057628	11.573
NO ₂ max	49.9096	3.59404	-29.7363	-28.3261	9.82655	150.221	160.048	0.057628	11.573
NO ₂ min	49.9096	3.59404	-29.7363	-28.3261	9.82655	150.221	160.048	0.057628	11.573

Table A-117. RDX minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	2.375097	30.53157	0	30.53157	13.57834	0	13.57834	0	2.333963
C max	2.5669	31.3951	0	31.3951	17.1733	0	17.1733	0	2.76187
C min	2.27461	29.6476	0	29.6476	6.91583	0	6.91583	0	1.59066
H avg	7.355648	31.58448	-1.29274	31.47362	33.73013	1.245047	34.97518	0.024317	4.897817
H max	9.53207	40.3245	0	40.3245	43.3512	4.37365	47.7249	0.083245	5.64601
H min	4.99156	21.2685	-4.16899	20.9605	25.8751	0	25.8751	0	4.36437
N - nitramine avg	5.233243	22.21853	0	22.21853	63.43493	0	63.43493	0	6.470593
N - nitramine max	6.0049	25.4481	0	25.4481	129.218	0	129.218	0	10.5912
N - nitramine min	3.71152	20.4075	0	20.4075	29.2352	0	29.2352	0	4.29467
N - nitro avg	2.951603	21.5053	-7.44502	20.35717	68.8483	36.7446	105.593	0.22278	7.322653
N - nitro max	3.28611	22.0951	-5.27545	20.7097	96.3722	58.8256	155.198	0.235368	9.23463
N - nitro min	2.70134	20.8738	-8.61087	19.7189	54.4499	23.5427	77.9926	0.21074	6.09701
O - nitro avg	21.09072	8.576078	-14.2441	-10.0401	39.83157	39.3488	79.18045	0.246992	8.74248
O - nitro max	22.3086	9.28301	-13.0455	-8.64868	57.1697	46.7436	100.634	0.249698	9.0694
O - nitro min	19.606	7.60233	-15.2109	-11.4276	25.3342	34.1494	63.9315	0.23924	8.44511
NO ₂ avg	51.54553	10.97721	-14.3381	-8.8364	69.76523	40.7519	110.5171	0.231815	9.977023
NO ₂ max	63.1657	12.6064	-13.9998	-8.03412	96.0866	45.3855	141.472	0.249307	10.7956
NO ₂ min	43.7713	8.79093	-14.9499	-9.63947	42.8595	38.2995	81.4302	0.217891	8.85727

Table A-118. CL20 minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	0.778991	46.61563	0	46.61563	29.74389	0	29.74389	0	4.131443
C max	1.05784	54.2221	0	54.2221	63.0588	0	63.0588	0	5.63885
C min	0.306849	34.8217	0	34.8217	8.56111	0	8.56111	0	2.32152
H avg	5.02544	39.67485	0	39.67485	57.53995	0	57.53995	0	5.92976
H max	6.33996	43.9778	0	43.9778	87.6337	0	87.6337	0	7.57775
H min	3.58753	31.0556	0	31.0556	14.8951	0	14.8951	0	3.07291
N - nitramine avg	2.932016	33.77953	0	33.77953	88.62593	0	88.62593	0	6.531783
N - nitramine max	5.20548	38.4356	0	38.4356	305.933	0	305.933	0	15.84
N - nitramine min	0.952923	29.9112	0	29.9112	22.1354	0	22.1354	0	3.85141
N - nitro avg	2.482302	30.30773	-3.92169	30.04087	112.5906	1.652146	114.2426	0.013053	8.470648
N - nitro max	3.14219	33.9206	0	33.9206	204.799	9.77618	204.799	0.077606	12.5099
N - nitro min	1.83067	27.4309	-9.7515	27.0551	32.6008	0	32.6008	0	4.93404
O - nitro avg	20.41276	11.28587	-7.28617	-0.15217	83.30553	13.9	97.20536	0.126459	8.739775
O - nitro max	22.1804	13.2631	-5.88777	3.40269	120.199	17.0929	131.68	0.164778	9.80664
O - nitro min	17.7463	8.76189	-8.33757	-2.35577	56.4257	11.4814	68.9187	0.07959	6.61314
NO ₂ avg	43.30785	13.97885	-7.30723	1.619786	134.1208	14.13777	148.2585	0.091847	10.4334
NO ₂ max	45.8331	15.2487	-6.43868	2.92365	192.716	15.8052	206.408	0.129302	11.2241
NO ₂ min	39.9977	12.5307	-7.99345	0.324286	87.7783	12.3073	103.583	0.060958	9.69688

Table A-119. HNB minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	3.947693	40.79203	0	40.79203	15.64583	0	15.64583	0	3.079653
C max	4.02572	41.0669	0	41.0669	16.6019	0	16.6019	0	3.1721
C min	3.84076	40.5649	0	40.5649	14.2566	0	14.2566	0	2.95124
N - nitro avg	0.725154	20.86228	-0.24745	20.76232	71.3925	2.08E-17	71.3925	3.24E-19	7.119257
N - nitro max	0.784681	21.6262	0	21.6262	87.7726	1.67E-16	87.7726	2.42E-18	8.52535
N - nitro min	0.634403	19.4955	-0.9946	19.4955	60.802	-4.2E-17	60.802	-4.7E-19	5.92246
O - nitro avg	20.57982	8.810581	-4.11442	3.244125	59.48768	6.755264	66.24292	0.089127	6.753378
O - nitro max	21.0643	9.50045	-3.10722	6.12954	64.5222	10.188	73.1619	0.123068	6.93348
O - nitro min	19.922	8.14842	-5.04503	0.641247	54.7824	2.94413	59.6957	0.041734	6.5115
NO ₂ avg	41.8848	9.167252	-4.25922	3.520183	64.28815	7.56562	71.8538	0.09258	7.158273
NO ₂ max	42.0656	9.64092	-3.47652	4.82029	66.3082	9.41952	75.7082	0.109147	7.47533
NO ₂ min	41.6029	8.77398	-4.81518	2.09903	60.5121	4.65055	65.1627	0.066275	6.82315

Table A-120. TATB minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.250378	21.10895	0	21.10895	2.007436	0	2.007436	0	1.0751
C max	6.59266	22.0317	0	22.0317	3.68874	0	3.68874	0	1.48928
C min	3.94678	19.8755	0	19.8755	0.766513	0	0.766513	0	0.662043
N - amino avg	15.0091	18.90173	0	18.90173	60.98657	0	60.98657	0	6.234803
N - amino max	15.198	19.1527	0	19.1527	67.858	0	67.858	0	6.73921
N - amino min	14.8215	18.5737	0	18.5737	56.6082	0	56.6082	0	5.94263
H - amino avg	2.568768	27.90388	0	27.90388	46.84732	0	46.84732	0	5.708958
H - amino max	3.3186	30.2973	0	30.2973	58.7543	0	58.7543	0	6.45185
H - amino min	2.1783	26.4616	0	26.4616	35.7374	0	35.7374	0	4.77693
N - nitro avg	3.898243	18.78963	-6.24027	18.2626	22.9233	26.11326	49.03657	0.170674	4.23466
N - nitro max	3.97942	19.6225	-2.98847	19.4092	25.4375	55.3909	76.638	0.249882	4.44973
N - nitro min	3.8158	17.5246	-9.23301	16.7715	21.2471	1.80147	27.239	0.061762	4.00806
O - nitro avg	20.09685	8.337837	-13.6489	-7.19368	33.02407	57.39972	90.42377	0.227956	10.31303
O - nitro max	20.5098	9.31951	-12.7432	-4.89511	45.888	64.9871	99.9199	0.248339	10.6476
O - nitro min	19.5354	7.29099	-14.6112	-9.11509	24.9231	53.0912	83.2821	0.203195	10.0772
NH ₂ avg	20.14667	21.25543	0	21.25543	74.05263	0	74.05263	0	7.305597
NH ₂ max	20.3535	21.411	0	21.411	78.2489	0	78.2489	0	7.71504
NH ₂ min	19.7373	20.9733	0	20.9733	66.1082	0	66.1082	0	6.7671
NO ₂ avg	44.09193	10.91193	-13.6383	-4.95163	50.96447	57.54417	108.5087	0.247508	11.72813
NO ₂ max	44.5811	11.3977	-13.1241	-3.82566	56.6451	64.0448	111.01	0.249895	11.7855
NO ₂ min	43.8298	10.2917	-14.57	-6.76604	45.5918	54.2228	104.879	0.242918	11.6459

Table A-121. PNA minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	4.325553	31.56772	0	31.56772	16.06754	0	16.06754	0	3.006972
C max	5.13817	37.9255	0	37.9255	22.6046	0	22.6046	0	3.63191
C min	3.50961	28.0441	0	28.0441	6.69974	0	6.69974	0	1.77511
N - amino avg	15.8907	37.3528	0	37.3528	58.7865	0	58.7865	0	6.34856
N - amino max	15.8907	37.3528	0	37.3528	58.7865	0	58.7865	0	6.34856
N - amino min	15.8907	37.3528	0	37.3528	58.7865	0	58.7865	0	6.34856
H - amino avg	2.8007	47.2052	0	47.2052	39.24545	0	39.24545	0	5.20938
H - amino max	2.8217	47.2411	0	47.2411	39.9768	0	39.9768	0	5.24208
H - amino min	2.7797	47.1693	0	47.1693	38.5141	0	38.5141	0	5.17668
N - nitro avg	1.580525	18.60231	-3.60279	17.55983	67.77978	4.816972	72.59674	0.068579	6.633902
N - nitro max	2.72641	32.8888	0	32.8888	110.5	17.0422	110.5	0.240264	9.347
N - nitro min	0.249717	3.94027	-7.69138	1.81907	25.422	0	41.4452	0	4.04684
O - nitro avg	20.18299	9.916861	-7.6255	-1.93846	59.19843	14.32662	73.52501	0.163879	7.245093
O - nitro max	21.0454	13.5901	-5.01595	7.88681	102.841	18.569	110.785	0.222414	9.98831
O - nitro min	19.1636	7.80968	-9.67958	-5.98541	37.0417	7.94442	54.5066	0.066568	5.56349
NH ₂ avg	22.2012	37.1377	0	37.1377	75.2764	0	75.2764	0	7.27494
NH ₂ max	22.2012	37.1377	0	37.1377	75.2764	0	75.2764	0	7.27494
NH ₂ min	22.2012	37.1377	0	37.1377	75.2764	0	75.2764	0	7.27494
NO ₂ avg	41.94652	11.3301	-7.7137	-0.88908	80.81092	14.70816	95.51898	0.150125	8.424624
NO ₂ max	42.9374	15.1806	-5.95263	5.69421	137.959	18.5087	148.141	0.214062	11.3102
NO ₂ min	40.9482	7.88209	-9.65011	-5.4924	38.4459	10.0752	55.7532	0.063524	5.84751

Table A-122. TNT minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.400097	22.17607	0	22.17607	23.93281	0	23.93281	0	3.781076
C max	7.25404	23.6336	0	23.6336	46.9073	0	46.9073	0	5.99927
C min	4.00474	21.1547	0	21.1547	15.0617	0	15.0617	0	2.90554
H avg	8.031216	23.84074	0	23.84074	23.80172	0	23.80172	0	3.721514
H max	9.40421	28.741	0	28.741	48.8664	0	48.8664	0	5.85277
H min	6.98488	17.7303	0	17.7303	13.3952	0	13.3952	0	2.81464
N - nitro avg	2.901713	27.0934	-5.7711	26.49307	43.99923	13.65303	57.6523	0.146412	5.731833
N - nitro max	3.64975	28.2478	-4.91068	27.9091	47.3522	21.2027	62.9269	0.223847	5.92084
N - nitro min	1.81759	25.3077	-7.16542	24.7484	41.475	0	47.3522	0	5.60131
O - nitro avg	22.69677	8.853233	-9.60078	-4.1978	45.93208	23.72913	69.66123	0.221742	8.088998
O - nitro max	23.8611	9.99025	-8.36535	-3.13228	58.4521	28.9962	77.2137	0.245534	8.46169
O - nitro min	20.6497	8.20993	-11.0527	-5.95999	37.9429	18.7615	61.1448	0.183942	7.30713
NO ₂ avg	48.29527	12.03933	-9.60331	-2.36498	92.8044	23.80097	116.6053	0.161379	9.755283
NO ₂ max	50.2738	12.4013	-8.69936	-1.56024	98.8526	28.0979	123.146	0.179521	10.3301
NO ₂ min	46.9979	11.3648	-10.8937	-3.4616	87.8491	19.012	106.861	0.14626	8.98472

Table A-123. TNA minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.363233	27.15725	0	27.15725	9.576737	0	9.576737	0	2.350728
C max	7.03358	31.8605	0	31.8605	16.0977	0	16.0977	0	3.06882
C min	3.46533	22.5714	0	22.5714	3.11851	0	3.11851	0	1.21737
H avg	5.77677	21.6292	0	21.6292	10.5509	0	10.5509	0	2.63152
H max	5.77677	21.6292	0	21.6292	10.5509	0	10.5509	0	2.63152
H min	5.77677	21.6292	0	21.6292	10.5509	0	10.5509	0	2.63152
N - amino avg	15.6328	28.7575	0	28.7575	46.2568	0	46.2568	0	5.51264
N - amino max	15.6328	28.7575	0	28.7575	46.2568	0	46.2568	0	5.51264
N - amino min	15.6328	28.7575	0	28.7575	46.2568	0	46.2568	0	5.51264
H - amino avg	3.57724	40.23095	0	40.23095	46.5103	0	46.5103	0	5.729415
H - amino max	3.61676	40.8748	0	40.8748	47.8401	0	47.8401	0	5.86389
H - amino min	3.53772	39.5871	0	39.5871	45.1805	0	45.1805	0	5.59494
N - nitro avg	2.794244	23.59315	-8.12589	19.16287	39.38932	11.8564	51.2457	0.16531	5.818113
N - nitro max	4.0714	29.7617	-5.57542	29.2266	69.9199	22.724	69.9199	0.226742	6.81287
N - nitro min	0.276007	14.3702	-11.8555	-2.25903	4.12067	0	11.8583	0	5.31729
O - nitro avg	20.52031	9.734801	-9.97276	-3.77593	48.7772	21.14213	69.91934	0.205296	8.053796
O - nitro max	22.5499	13.6426	-6.95903	5.3233	81.4168	32.0371	98.7839	0.249552	10.8407
O - nitro min	18.6114	7.16152	-13.5431	-10.0619	22.4784	15.2257	43.1308	0.135136	5.3764
NH ₂ avg	22.7873	32.362	0	32.362	74.8513	0	74.8513	0	7.55121
NH ₂ max	22.7873	32.362	0	32.362	74.8513	0	74.8513	0	7.55121
NH ₂ min	22.7873	32.362	0	32.362	74.8513	0	74.8513	0	7.55121
NO ₂ avg	43.83488	12.30611	-10.0585	-1.98143	79.99533	22.06343	102.0587	0.173884	9.904278
NO ₂ max	46.3891	14.9701	-7.81349	4.38829	109.693	31.2979	127.786	0.248153	11.7927
NO ₂ min	41.6788	7.36853	-12.2276	-9.38111	25.3464	16.7671	46.6808	0.115009	5.71081

Table A-124. NTO minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	3.573485	21.0621	0	21.0621	16.5807	0	16.5807	0	3.2493
C max	4.17512	23.5542	0	23.5542	20.1944	0	20.1944	0	3.38158
C min	2.97185	18.57	0	18.57	12.967	0	12.967	0	3.11702
H avg	7.079985	44.7685	0	44.7685	59.8389	0	59.8389	0	6.63689
H max	7.77444	46.321	0	46.321	60.4438	0	60.4438	0	6.64476
H min	6.38553	43.216	0	43.216	59.234	0	59.234	0	6.62902
N avg	13.28773	18.1708	-3.5731	14.62056	27.4541	13.04023	40.49433	0.083333	6.00711
N max	16.9578	22.6552	0	22.6552	38.9661	39.1207	78.0868	0.249999	10.3988
N min	11.3504	10.0716	-10.7193	-0.57912	14.6205	0	14.6205	0	3.08459
O avg	27.9777	7.79792	-16.6788	-11.461	24.6063	58.4907	83.097	0.208431	10.4822
O max	27.9777	7.79792	-16.6788	-11.461	24.6063	58.4907	83.097	0.208431	10.4822
O min	27.9777	7.79792	-16.6788	-11.461	24.6063	58.4907	83.097	0.208431	10.4822
N - nitro avg	4.2177	21.5217	-4.60107	21.0159	38.0795	15.1885	53.268	0.203833	5.46747
N - nitro max	4.2177	21.5217	-4.60107	21.0159	38.0795	15.1885	53.268	0.203833	5.46747
N - nitro min	4.2177	21.5217	-4.60107	21.0159	38.0795	15.1885	53.268	0.203833	5.46747
O - nitro avg	23.44195	8.339695	-13.2548	-8.52002	34.07615	33.798	67.87415	0.242796	8.38673
O - nitro max	23.6247	10.1619	-11.35	-4.35424	48.5773	37.8805	86.4578	0.246173	9.90636
O - nitro min	23.2592	6.51749	-15.1596	-12.6858	19.575	29.7155	49.2905	0.239419	6.8671
NO ₂ avg	51.1016	12.7431	-13.5071	-6.11205	73.0298	36.8977	109.927	0.222991	11.283
NO ₂ max	51.1016	12.7431	-13.5071	-6.11205	73.0298	36.8977	109.927	0.222991	11.283
NO ₂ min	51.1016	12.7431	-13.5071	-6.11205	73.0298	36.8977	109.927	0.222991	11.283

Table A-125. DATB minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.74999	20.60477	0	20.60477	2.72851	0	2.72851	0	1.183788
C max	6.80611	22.5267	0	22.5267	5.40951	0	5.40951	0	1.96176
C min	3.99486	16.3662	0	16.3662	0.420632	0	0.420632	0	0.460164
H avg	5.39709	11.2294	0	11.2294	6.87526	0	6.87526	0	2.15353
H max	5.39709	11.2294	0	11.2294	6.87526	0	6.87526	0	2.15353
H min	5.39709	11.2294	0	11.2294	6.87526	0	6.87526	0	2.15353
N - amino avg	15.6496	19.64435	0	19.64435	41.2359	0	41.2359	0	5.15811
N - amino max	15.6837	19.6501	0	19.6501	41.2791	0	41.2791	0	5.15942
N - amino min	15.6155	19.6386	0	19.6386	41.1927	0	41.1927	0	5.1568
H - amino avg	3.260678	30.01258	0	30.01258	45.36605	0	45.36605	0	5.66171
H - amino max	3.41454	30.7253	0	30.7253	47.1666	0	47.1666	0	5.74535
H - amino min	3.1119	29.3542	0	29.3542	43.5352	0	43.5352	0	5.56648
N - nitro avg	3.96703	20.24437	-5.15681	19.7866	23.47977	25.45803	48.9378	0.158258	4.207477
N - nitro max	4.02531	22.5057	0	22.5057	25.459	45.3315	69.6395	0.247559	4.7422
N - nitro min	3.8601	19.0827	-8.89325	18.2956	20.6723	0	20.6723	0	3.40987
O - nitro avg	20.79207	8.505147	-12.2893	-5.67652	33.0064	42.58367	75.59007	0.236149	9.539945
O - nitro max	22.1218	9.83741	-10.6413	-2.02581	41.8857	47.7533	86.5516	0.249406	10.534
O - nitro min	19.812	6.15372	-14.0203	-10.6923	18.2977	36.695	61.9034	0.208215	8.00844
NH ₂ avg	22.17095	22.70085	0	22.70085	64.99945	0	64.99945	0	7.06741
NH ₂ max	22.1898	22.7025	0	22.7025	65.0415	0	65.0415	0	7.0715
NH ₂ min	22.1521	22.6992	0	22.6992	64.9574	0	64.9574	0	7.06332
NO ₂ avg	45.55113	11.53897	-12.3813	-3.53424	56.7781	42.92237	99.7005	0.243466	11.31243
NO ₂ max	46.5932	12.2036	-10.6582	0.126172	61.9579	46.0626	100.209	0.248373	11.3946
NO ₂ min	43.5415	11.2041	-13.2506	-5.37305	54.1465	36.7797	98.7375	0.233744	11.2703

Table A- 126. Picric acid minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	6.178952	26.49623	0	26.49623	7.659943	0	7.659943	0	2.007713
C max	7.367	30.8191	0	30.8191	11.4647	0	11.4647	0	2.71608
C min	4.32506	23.0023	0	23.0023	2.27097	0	2.27097	0	1.15016
H avg	4.816583	26.00123	0	26.00123	15.68948	0	15.68948	0	3.302267
H max	6.47971	34.9416	0	34.9416	20.7658	0	20.7658	0	3.97315
H min	1.63584	20.644	0	20.644	9.98324	0	9.98324	0	2.51765
O avg	17.4931	17.0825	-6.67025	11.4595	97.4221	18.4914	115.913	0.134078	11.4896
O max	17.4931	17.0825	-6.67025	11.4595	97.4221	18.4914	115.913	0.134078	11.4896
O min	17.4931	17.0825	-6.67025	11.4595	97.4221	18.4914	115.913	0.134078	11.4896
N - nitro avg	3.931607	26.68317	-3.21407	26.46977	35.18083	1.893483	37.0743	0.043379	4.738737
N - nitro max	4.1056	32.5222	-0.62437	32.453	39.5639	3.70702	43.2709	0.078331	5.11697
N - nitro min	3.63347	23.6541	-5.5339	23.4411	31.9481	0	31.9481	0	4.236
O - nitro avg	21.98018	9.730865	-9.79019	-2.96893	48.73178	24.82055	73.55237	0.208062	8.74431
O - nitro max	22.7596	14.3201	-6.30921	6.94774	91.2441	32.8421	103.045	0.249608	10.7942
O - nitro min	20.3182	8.32058	-12.8415	-9.14047	33.1034	11.8008	59.3019	0.101406	7.61324
NO ₂ avg	47.89193	13.41147	-9.78673	-0.57979	95.1452	25.11163	120.2567	0.162404	10.87947
NO ₂ max	49.284	15.4279	-6.3355	6.60269	123.786	32.7446	136.751	0.207771	11.6696
NO ₂ min	46.5428	12.2354	-12.0562	-5.26618	78.4416	12.9655	111.186	0.085822	10.3486

A.14 PBE/6-31G** Test Set Data

Table A-127. BTAT atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	3.00239	24.2545	0	24.2545	7.78602	0	7.78602	0	2.34823	31.1213	17.2245
C	2	3.206	24.7287	0	24.7287	9.86455	0	9.86455	0	2.63691	31.6171	14.476
C	3	1.49411	32.9572	0	32.9572	19.1868	0	19.1868	0	3.57535	38.8579	19.6479
H	4	4.62579	25.4849	0	25.4849	23.8587	0	23.8587	0	3.78427	34.9717	9.55258
H	5	7.52975	35.8043	0	35.8043	14.8039	0	14.8039	0	2.97082	43.3697	21.4564
C	6	0.08627	38.3755	0	38.3755	33.0472	0	33.0472	0	4.75693	44.1886	28.8617
C	7	1.50334	32.1732	0	32.1732	20.5664	0	20.5664	0	3.56664	39.348	20.1318
H	8	7.64329	35.2743	0	35.2743	13.6906	0	13.6906	0	2.86577	42.4234	22.1912
H	9	4.92191	26.2004	0	26.2004	24.4207	0	24.4207	0	3.75972	35.2058	10.652
C	10	0.033097	34.2893	0	34.2893	69.1779	0	69.1779	0	8.31732	42.6066	25.972
N	11	10.8655	12.7658	-7.97704	1.86566	66.4683	15.4448	81.9131	0.153	10.4036	29.9109	-13.0026
N	12	16.7003	11.2408	-9.38452	-0.25663	49.1343	22.5765	71.7109	0.215711	10.179	28.4689	-16.5957
N	13	11.1058	12.6826	-8.36824	2.31728	72.9005	14.8757	87.7762	0.140752	10.7006	30.2403	-13.2549
N	14	16.8077	11.1831	-9.66332	-0.66642	48.2586	23.0349	71.2935	0.218706	10.2367	29.1553	-16.8367
N	15	7.06042	25.5979	0	25.5979	26.7006	0	26.7006	0	4.21315	40.2315	18.002
N	16	6.51338	25.4273	0	25.4273	44.485	0	44.485	0	5.50936	41.1251	15.4129
N - nitro	17	1.69239	31.0184	-3.03213	30.6032	138.738	0	138.738	0	10.2859	45.4311	-3.03213
N - nitro	18	1.61244	21.5288	0	21.5288	54.1129	0	54.1129	0	6.18989	36.6102	3.79769
N - nitro	19	0.995112	14.4288	-5.81137	13.9351	19.322	0	19.322	0	3.53874	22.9097	-5.81137
N - nitro	20	1.52617	29.5112	-0.81263	29.1174	119.598	0	119.598	0	9.06368	43.322	-0.81263
N - nitro	21	0.908297	16.4998	-4.74397	16.017	41.2738	0	41.2738	0	6.28577	26.2908	-4.74397
N - nitro	22	1.54523	24.4659	0	24.4659	87.4543	0	87.4543	0	7.65778	35.9048	1.15022
O - nitro	23	19.6713	11.5662	-4.19367	6.44131	86.0858	6.12021	92.206	0.06197	8.55238	41.9741	-8.66277
O - nitro	24	20.4765	8.7602	-6.06184	-1.39018	62.1523	7.75819	69.9105	0.098658	6.46831	32.6305	-11.3667
O - nitro	25	21.8738	10.4235	-5.71559	2.84377	69.7612	12.4452	82.2064	0.128471	8.36639	40.3583	-11.9095
O - nitro	26	19.674	6.09311	-7.29567	-5.20414	20.8879	9.51237	30.4003	0.214995	4.3603	19.4283	-13.327

Table A-127. BTAT atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
O - nitro	27	17.5319	7.49965	-6.20234	-3.11769	35.8444	6.27094	42.1153	0.126728	5.05248	24.6467	-10.8333
O - nitro	28	20.4189	6.47046	-5.13344	-0.85061	22.8368	8.08844	30.9253	0.193141	5.43725	20.4493	-10.7467
O - nitro	29	19.8673	11.4982	-4.38387	6.16007	85.537	6.12083	91.6578	0.06232	8.61625	40.4712	-8.76443
O - nitro	30	20.2674	7.09934	-5.66788	-1.85394	40.8393	7.72786	48.5671	0.133799	5.46905	29.2426	-11.2199
O - nitro	31	20.6578	7.45944	-5.20925	-0.68842	37.8757	8.18512	46.0608	0.146124	5.83763	25.8979	-11.0329
O - nitro	32	17.1401	7.33497	-5.78467	-2.17008	35.3595	6.2702	41.6297	0.127932	5.3748	23.0403	-10.6827
O - nitro	33	20.2744	6.48818	-6.77997	-4.28161	29.0294	10.3853	39.4146	0.194062	4.73405	22.8144	-13.1965
O - nitro	34	21.2614	9.58935	-5.78711	1.99431	61.7508	12.1064	73.8572	0.137047	7.85414	38.0177	-11.9547
H	35	4.69697	37.8589	0	37.8589	32.384	0	32.384	0	4.79279	47.365	23.386
H	36	5.28211	38.2784	0	38.2784	41.801	0	41.801	0	5.4368	48.1821	21.4439
NO ₂	17,23,24	41.8402	12.285	-5.46383	3.66183	115.147	7.99179	123.138	0.060689	9.29919	45.4311	-11.3667
NO ₂	18,25,26	43.1602	10.6853	-6.69374	-0.15147	74.4833	11.2184	85.7017	0.113766	8.15981	40.3583	-13.327
NO ₂	19,27,28	38.9459	7.35266	-5.67805	-1.52796	30.693	7.44207	38.1351	0.157067	5.73773	24.6467	-10.8333
NO ₂	20,29,30	41.6609	11.6272	-5.24233	3.23499	105.701	7.57648	113.278	0.062411	8.81601	43.322	-11.2199
NO ₂	21,31,32	38.7061	8.05459	-5.48168	-0.92462	42.6535	7.35333	50.0068	0.125424	6.07469	26.2908	-11.0329
NO ₂	22,33,34	43.0811	10.1713	-6.39218	-0.21823	77.8282	11.2921	89.1203	0.110652	7.74619	38.0177	-13.1965

See figure A-16 for corresponding area weighted atom with area weighted atom number.

Table A-128. CL16 atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	4.01799	30.126	0	30.126	11.7768	0	11.7768	0	2.64664	39.8707	22.3688
C	2	3.99417	31.0828	0	31.0828	14.7502	0	14.7502	0	3.18935	40.1399	22.2019
C	3	4.17086	30.1084	0	30.1084	9.94998	0	9.94998	0	2.38283	39.2206	23.3471
N - nitro	4	0.776129	12.8061	-4.98541	11.744	24.7527	2.97068	27.7234	0.095672	4.34338	26.6761	-7.79367
C	5	4.49471	36.7839	0	36.7839	31.2315	0	31.2315	0	4.09434	58.086	23.4469
C	6	3.70026	30.423	0	30.423	13.3762	0	13.3762	0	2.94307	40.1575	23.8297
N - nitro	7	0.931911	20.2275	-2.36822	19.6329	52.7544	3.57707	56.3315	0.059468	6.45346	34.0505	-4.25953
N - nitro	8	1.23421	16.3328	-7.09619	15.8949	36.1424	0.55621	36.6986	0.014927	5.04041	27.8721	-7.84199
O - nitro	9	20.5214	6.80167	-6.19271	-2.07125	31.3412	12.2824	43.6235	0.202281	5.82963	24.6141	-13.044
O - nitro	10	20.7643	7.77051	-6.26705	-1.42265	36.7665	13.0104	49.7769	0.193058	6.43349	25.9544	-13.0616
C	11	4.59395	35.3526	0	35.3526	41.8411	0	41.8411	0	4.88509	58.7142	25.3238
O - nitro	12	21.3714	6.3865	-5.03971	-0.07681	30.1307	9.86511	39.9958	0.185816	5.61488	23.7079	-11.1201
O - nitro	13	20.5277	8.02384	-6.75815	-2.06599	37.9395	14.319	52.2585	0.198926	6.58412	25.6645	-13.9815
O - nitro	14	21.5987	9.35172	-5.4864	0.8398	57.8385	10.2393	68.0778	0.127784	7.28534	31.5223	-11.8706
O - nitro	15	20.3333	7.65396	-6.8522	-2.49615	37.8226	13.6562	51.4789	0.194906	6.33227	24.9203	-14.1183
N - nitro	16	0.410657	12.1645	-2.1853	11.3673	42.6249	0.654762	43.2797	0.0149	5.50655	25.736	-2.99448
N - azide	17	12.3515	21.8114	0	21.8114	65.414	0	65.414	0	6.40329	55.8145	7.83446
N - nitro	18	1.2625	31.6682	-3.52598	31.3482	255.713	0	255.713	0	14.5566	58.0151	-3.52598
O - nitro	19	20.6606	6.83776	-5.93862	-1.55624	34.7663	12.2261	46.9923	0.192482	5.87834	23.4626	-12.7027
O - nitro	20	20.8402	7.29687	-6.0993	-1.46099	37.2241	12.5036	49.7277	0.188218	6.15882	25.6011	-12.8338
N - azide	21	7.61356	36.9233	0	36.9233	49.7042	0	49.7042	0	5.27707	59.3298	19.1409
O - nitro	22	20.4068	11.297	-3.96292	4.28762	116.502	6.69142	123.194	0.051366	8.50659	44.9366	-9.16289
O - nitro	23	18.9043	8.6958	-3.89683	4.48528	45.3669	5.47555	50.8425	0.096098	6.67433	30.2328	-8.02898
N - azide	24	25.3835	14.1457	0	14.1457	80.4794	0	80.4794	0	7.67175	38.5617	1.8179

Table A-128. CL16 atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
NO ₂	4,9,10	42.0618	7.5982	-6.22743	-1.48721	35.4203	12.6308	48.0511	0.193765	6.33143	26.6761	-13.0616
NO ₂	7,12,14	43.902	8.42895	-5.26285	0.783708	53.1085	10.1061	63.2146	0.134311	6.78322	34.0505	-11.8706
NO ₂	8,13,15	42.0952	8.60328	-6.80581	-1.73561	43.6213	13.9759	57.5973	0.18377	6.91787	27.8721	-14.1183
NO ₂	16,19,20	41.9115	7.21104	-6.01617	-1.3763	36.942	12.3749	49.3168	0.187962	6.11273	25.736	-12.8338
NO ₂	18,22,23	40.5735	11.0216	-3.93564	5.24673	112.2	6.19186	118.392	0.049565	8.43004	58.0151	-9.16289

See figure A-17 for corresponding area weighted atom with area weighted atom number.

Table A-129. DNBf atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	5.53793	31.523	0	31.523	1.65719	0	1.65719	0	1.03071	35.2422	28.7161
C	2	4.70085	26.3766	0	26.3766	20.8797	0	20.8797	0	3.7373	33.8541	11.8599
C	3	5.67509	27.0772	0	27.0772	3.8187	0	3.8187	0	1.50888	32.3914	16.5719
C	4	7.68238	25.1712	0	25.1712	5.12199	0	5.12199	0	1.73089	32.6587	17.7447
C	5	5.96439	27.9585	0	27.9585	3.41877	0	3.41877	0	1.52753	32.9587	24.0261
C	6	7.95465	28.1608	0	28.1608	4.41367	0	4.41367	0	1.64423	33.044	19.0261
N - nitro	7	4.21694	26.8632	-6.51399	25.9894	33.4032	8.93166	42.3348	0.166466	5.35767	33.5234	-11.5085
N - nitro	8	3.97943	23.5041	-6.00129	23.037	37.1902	29.2242	66.4144	0.246403	5.25972	30.9224	-17.5213
N	9	15.5383	11.3142	-13.3482	-5.11514	62.8268	59.4312	122.258	0.249807	11.5399	32.3952	-27.7824
N	10	4.88316	30.2589	0	30.2589	15.7613	0	15.7613	0	3.08925	35.8641	12.2264
O - nitro	11	22.7321	9.54985	-9.12091	-2.1312	43.958	25.7494	69.7073	0.232942	8.87198	26.548	-18.0183
O - nitro	12	22.1375	9.84883	-8.10236	-0.61798	50.1515	21.0538	71.2053	0.208252	8.73695	29.1566	-15.9569
O - nitro	13	22.5241	8.88389	-11.5743	-5.58858	38.1676	38.0111	76.1787	0.249999	9.21369	24.5011	-21.9158
O - nitro	14	20.7272	8.211	-17.5624	-13.7605	32.0457	44.2202	76.2659	0.243629	9.10817	20.7361	-27.5797
O	15	15.4735	8.4724	-0.6559	7.10149	68.0547	0.257586	68.3122	0.003756	6.67358	34.3273	-2.61483
O	16	24.4278	10.0702	-4.7619	2.29094	55.5481	6.47201	62.0201	0.093464	7.58439	29.2934	-9.68498
H	17	6.49867	24.1047	0	24.1047	14.458	0	14.458	0	3.15712	30.315	14.0663
H	18	7.78552	29.6048	0	29.6048	17.0954	0	17.0954	0	3.21096	36.2293	17.4435
NO ₂	7,11,12	49.0865	13.057	-8.62998	1.06754	90.7772	23.7424	114.52	0.164339	10.7538	33.5234	-18.0183
NO ₂	8,13,14	47.2308	13.2351	-14.7142	-6.53986	83.4681	50.3358	133.804	0.234671	12.2865	30.9224	-27.5797
NO ₂ *	10,15,16	44.7845	12.8142	-4.11838	7.15555	117.668	7.72622	125.395	0.057819	9.93729	35.8641	-9.68498

See figure A-18 for corresponding area weighted atom with area weighted atom number.

* This "NO₂" is part of a furazan-oxide moiety and should not be considered a formal nitro group.

Table A-130. HNS atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	3.99831	28.2378	0	28.2378	8.6353	0	8.6353	0	2.33445	33.8855	17.8332
C	2	5.71246	28.9368	0	28.9368	4.03037	0	4.03037	0	1.62881	34.5356	25.3777
C	3	7.55091	24.9739	0	24.9739	4.85298	0	4.85298	0	1.52133	30.5923	14.2645
H	4	6.3495	21.83	0	21.83	10.5242	0	10.5242	0	2.65225	26.9678	13.2266
C	5	5.5977	27.8419	0	27.8419	6.84733	0	6.84733	0	2.09111	34.2363	20.1424
C	6	7.37256	25.5495	0	25.5495	22.9647	0	22.9647	0	4.02942	36.7583	12.3412
H	7	7.0639	26.0826	0	26.0826	32.7802	0	32.7802	0	4.91492	34.8782	11.068
C	8	4.37759	26.5235	0	26.5235	12.5148	0	12.5148	0	2.73755	34.4358	15.9632
C	9	1.59547	20.9328	0	20.9328	40.3934	0	40.3934	0	5.46941	34.0769	10.416
H	10	8.30053	27.6262	0	27.6262	26.2781	0	26.2781	0	4.13885	34.9165	13.5962
N - nitro	11	3.82689	27.1336	0	27.1336	42.9858	0	42.9858	0	5.02406	35.3307	0.597389
N - nitro	12	3.96943	27.4988	-10.0832	26.9406	43.688	42.2025	85.8905	0.249925	5.65027	35.2547	-15.3125
N - nitro	13	1.62511	27.4632	-11.127	26.8695	62.9617	0	62.9617	0	6.71828	37.3305	-11.127
O - nitro	14	13.7732	11.6434	-13.685	-3.99141	58.9445	49.3429	108.287	0.248035	12.3252	30.0201	-23.6992
O - nitro	15	22.1175	9.7567	-10.1034	-3.35173	45.7554	32.2124	77.9678	0.242457	9.24105	27.5922	-19.7873
O - nitro	16	22.6678	9.97527	-9.21381	-2.43465	49.3202	25.2864	74.6066	0.224056	8.92646	27.8338	-17.9116
O - nitro	17	22.5897	9.84212	-9.32128	-2.68996	48.2649	26.63	74.8949	0.229139	8.88916	29.0675	-18.1695
O - nitro	18	20.3752	9.31926	-11.5252	-6.01956	44.568	41.164	85.732	0.249606	9.04597	30.6382	-23.514
O - nitro	19	18.8769	7.84475	-8.22961	-2.80786	38.1343	29.8715	68.0058	0.246309	7.50979	25.7768	-18.6427
C	20	1.53223	20.1494	0	20.1494	33.8183	0	33.8183	0	4.87152	30.6193	9.64984
C	21	3.9749	28.0549	0	28.0549	10.157	0	10.157	0	2.4356	33.6157	16.4809
H	22	8.24842	27.683	0	27.683	25.5871	0	25.5871	0	4.04234	34.9404	13.3427
C	23	5.95884	28.895	0	28.895	4.18694	0	4.18694	0	1.6481	33.9778	23.1225
C	24	4.43967	26.5194	0	26.5194	14.108	0	14.108	0	2.87887	36.1006	13.1821
C	25	7.41719	24.9342	0	24.9342	4.67585	0	4.67585	0	1.5209	30.1311	15.0358
N - nitro	26	3.81527	26.8942	0	26.8942	44.1339	0	44.1339	0	5.1963	35.1098	5.95695

Table A-130. HNS atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	27	7.16452	25.4244	0	25.4244	22.4073	0	22.4073	0	3.97219	37.1228	12.3757
N - nitro	28	1.48381	28.5515	-18.4695	27.7266	43.5678	0	43.5678	0	6.13403	37.2295	-18.4695
H	29	6.36286	21.8607	0	21.8607	10.7127	0	10.7127	0	2.62806	26.8869	12.8508
C	30	5.77655	27.9581	0	27.9581	6.91134	0	6.91134	0	2.1416	34.0794	20.6413
O - nitro	31	13.6504	11.5068	-13.846	-4.01293	62.3978	48.1428	110.541	0.245843	12.3498	30.2071	-23.6533
O - nitro	32	22.0415	9.58267	-10.2096	-3.38676	46.6721	32.0343	78.7064	0.241353	9.24472	27.1555	-19.764
H	33	7.06826	26.2219	0	26.2219	30.4807	0	30.4807	0	4.75036	35.069	12.0036
O - nitro	34	20.433	9.69058	-11.6189	-5.72137	52.7468	39.9809	92.7277	0.245262	9.30467	32.3167	-23.3898
O - nitro	35	19.0907	8.03922	-8.41382	-2.75154	39.6396	30.8082	70.4478	0.246071	7.72264	25.7637	-18.6377
N - nitro	36	3.74146	28.1125	-15.6752	27.8821	32.3287	0	32.3287	0	4.64472	35.3589	-15.6752
O - nitro	37	22.7052	9.81347	-9.31414	-2.66186	48.4676	24.6682	73.1359	0.223527	8.86105	28.3145	-17.921
O - nitro	38	22.7178	9.84909	-9.33271	-2.59316	48.6199	26.4058	75.0257	0.228083	8.93729	29.1911	-18.184
NO ₂	11,14,15	39.7176	14.6375	-11.4498	-0.39062	100.984	41.6621	142.647	0.206763	12.7456	35.3307	-23.6992
NO ₂	12,16,17	49.2269	13.7185	-9.26933	0.074246	100.183	25.9984	126.181	0.163588	11.0917	35.2547	-18.1695
NO ₂	13,18,19	40.8772	10.5755	-10.0371	-3.36929	78.5845	38.7214	117.306	0.22113	9.38167	37.3305	-23.514
NO ₂	26,31,32	39.5071	14.4333	-11.5772	-0.42779	102.085	41.1951	143.28	0.20485	12.7446	35.1098	-23.6533
NO ₂	28,34,35	41.0074	10.6196	-10.1568	-3.29888	78.6888	38.3523	117.041	0.220307	9.5084	37.2295	-23.3898
NO ₂	36,37,38	49.1644	13.6116	-9.32809	-0.06711	100.008	25.5449	125.553	0.162063	11.0446	35.3589	-18.184

See figure A-19 for corresponding area weighted atom with area weighted atom number.

Table A-131. Methyl picrate atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	6.08212	24.202	0	24.202	4.28599	0	4.28599	0	1.64893	29.6479	20.2548
C	2	7.25918	21.9255	0	21.9255	15.3091	0	15.3091	0	3.13449	32.1172	8.22853
C	3	5.54737	24.9259	0	24.9259	9.36856	0	9.36856	0	2.25121	32.8225	13.6552
C	4	3.65128	25.7167	0	25.7167	3.65626	0	3.65626	0	1.74744	29.5551	22.1436
C	5	5.61811	24.7986	0	24.7986	10.7468	0	10.7468	0	2.38102	32.9286	12.1473
C	6	7.2794	22.0224	0	22.0224	15.1635	0	15.1635	0	3.09734	31.9158	9.06939
N - nitro	7	3.63801	23.7751	-6.62876	23.2527	45.0734	32.242	77.3154	0.243114	5.82597	33.4519	-16.041
O - nitro	8	22.5385	8.42854	-10.1505	-5.22119	39.3833	25.5673	64.9505	0.238688	7.94783	28.6483	-19.2965
N - nitro	9	3.62628	24.0293	-2.32681	23.6695	39.6325	2.61754	42.2501	0.058115	5.33907	33.4827	-4.88202
O - nitro	10	18.8722	8.45282	-9.23246	-4.09909	45.6426	28.4537	74.0963	0.236546	7.86737	24.7854	-18.2875
N - nitro	11	3.97247	23.6443	-10.1271	23.1687	32.782	34.1774	66.9594	0.249891	4.81444	30.3834	-16.2989
O - nitro	12	22.6545	8.25997	-11.0317	-5.95126	34.7505	32.8402	67.5907	0.2498	8.39897	23.5115	-20.8459
O - nitro	13	18.8223	8.21852	-9.04146	-4.03499	42.5108	27.3813	69.8921	0.238285	7.68065	25.0351	-18.3277
O - nitro	14	22.5451	8.36965	-10.2405	-5.18044	39.3743	26.5829	65.9572	0.240597	8.06729	27.815	-19.2043
O - nitro	15	22.5828	8.25168	-10.9675	-6.07675	32.199	31.9542	64.1532	0.249996	8.22856	23.3797	-20.8415
H	16	6.57764	20.8216	0	20.8216	21.4663	0	21.4663	0	3.98479	29.3844	8.2072
H	17	6.61746	20.8826	0	20.8826	20.4753	0	20.4753	0	3.86922	29.129	8.07354
O	18	10.1692	7.91117	-3.10981	2.48293	43.2193	2.00214	45.2214	0.042314	5.83832	29.1051	-5.19766
C	19	5.56972	16.5142	0	16.5142	43.5814	0	43.5814	0	5.76833	28.8667	2.6619
H	20	8.13057	17.5389	0	17.5389	18.3195	0	18.3195	0	3.22637	27.0306	2.50627
H	21	11.4857	17.4576	0	17.4576	15.4998	0	15.4998	0	3.37059	23.4005	8.4582
H	22	8.14248	17.8252	0	17.8252	18.3733	0	18.3733	0	3.16133	27.2264	2.67633
NO ₂	7,8,13	44.9988	11.8234	-9.64905	-2.55704	83.6075	26.7106	110.318	0.1835	9.66799	33.4519	-19.2965
NO ₂	9,10,14	45.0435	11.9051	-9.78382	-2.54857	84.0881	27.7071	111.795	0.186414	9.81689	33.4827	-19.2043
NO ₂	11,12,15	49.2098	11.6064	-10.998	-4.02693	73.6674	32.3959	106.063	0.212146	10.0127	30.3834	-20.8459

See figure A-20 for corresponding area weighted atom with area weighted atom number.

Table A-132. Picryl azide atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	7.16403	23.5763	0	23.5763	16.8402	0	16.8402	0	3.09336	34.7433	9.83433
C	2	6.111	25.8889	0	25.8889	2.66246	0	2.66246	0	1.35936	30.3294	22.9625
C	3	5.17339	25.2749	0	25.2749	11.9619	0	11.9619	0	2.52386	34.8676	13.9037
H	4	6.88214	23.5989	0	23.5989	22.7484	0	22.7484	0	4.09916	32.264	10.2102
C	5	7.31165	24.224	0	24.224	8.56427	0	8.56427	0	2.14983	32.9028	13.6841
C	6	4.53332	28.8163	0	28.8163	25.5564	0	25.5564	0	3.63203	47.6844	18.5661
N - nitro	7	4.12553	24.2769	-8.67239	23.9517	44.2494	37.6959	81.9452	0.248401	5.40806	31.0611	-17.328
N - nitro	8	3.23628	24.3766	-9.39413	24.1437	49.0921	1.82273	50.9149	0.034518	5.88197	35.2761	-10.7442
C	9	5.65406	29.2237	0	29.2237	31.2698	0	31.2698	0	4.07873	49.2187	18.8742
O - nitro	10	22.5077	8.55964	-10.4644	-5.06659	36.776	30.9115	67.6876	0.248123	8.42699	23.7675	-20.0496
O - nitro	11	22.8911	8.70676	-9.36506	-4.03911	44.1069	21.7419	65.8488	0.221161	7.92737	29.8469	-18.0152
O - nitro	12	22.6346	8.69074	-10.4131	-5.0834	38.7551	29.9353	68.6904	0.245878	8.35529	24.7452	-20.0376
O - nitro	13	21.4611	8.28709	-8.78437	-4.42475	38.8122	20.7088	59.521	0.226873	7.03891	25.1838	-17.5684
N - azide	14	11.7498	13.388	-1.3181	12.845	60.7787	0.739118	61.5178	0.01187	6.32291	46.1364	-3.0453
H	15	6.45615	22.2087	0	22.2087	16.4764	0	16.4764	0	3.39069	29.1754	12.1342
N - nitro	16	3.54368	31.0109	-7.02936	30.633	63.8	24.3708	88.1707	0.200005	6.35248	48.2574	-12.7805
N - azide	17	7.50104	28.2722	0	28.2722	58.5365	0	58.5365	0	6.10409	49.1491	6.7382
O - nitro	18	18.2073	9.14999	-7.88759	-1.51969	50.5527	21.1256	71.6783	0.207863	8.06455	35.657	-15.6175
O - nitro	19	22.4537	10.017	-8.07332	-1.31713	54.4411	19.5563	73.9973	0.194438	8.51277	30.5716	-15.994
N - azide	20	25.905	10.2043	-2.42372	6.48822	52.5263	1.7528	54.2791	0.03125	7.11617	30.748	-4.81363
NO ₂	7,10,12	49.2679	11.9782	-10.4366	-2.98798	80.396	30.4303	110.826	0.199184	10.1535	31.0611	-20.0496
NO ₂	8,11,13	47.5885	11.8748	-9.07288	-2.26063	85.2905	21.2922	106.583	0.159863	9.30699	35.2761	-18.0152
NO ₂	16,18,19	44.2047	13.544	-7.98835	1.09198	123.31	20.2786	143.588	0.121282	10.5319	48.2574	-15.994

See figure A-21 for corresponding area weighted atom with area weighted atom number.

Table A-133. Styphnic acid atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	6.314	27.9173	0	27.9173	8.72453	0	8.72453	0	2.44289	35.005	23.6584
C	2	4.21802	25.483	0	25.483	16.5754	0	16.5754	0	2.94721	34.3806	10.7474
C	3	4.82384	18.9748	0	18.9748	16.662	0	16.662	0	3.2988	27.4529	9.44151
C	4	4.20603	25.4432	0	25.4432	16.1324	0	16.1324	0	2.96762	34.4415	10.7216
C	5	6.3206	27.7378	0	27.7378	8.67266	0	8.67266	0	2.41974	34.9843	23.649
C	6	7.15686	24.3104	0	24.3104	0.724968	0	0.724968	0	0.560934	27.8388	19.9134
N - nitro	7	2.00532	12.8285	-5.9956	11.8632	23.0967	37.4502	60.5469	0.23595	4.79013	21.9528	-18.0277
O - nitro	8	22.6897	6.06515	-12.6386	-10.2154	19.6101	26.2321	45.8422	0.244783	6.30442	18.0597	-21.4947
O	9	18.0073	14.9784	-5.41212	9.4117	89.2938	11.6836	100.977	0.102317	10.528	36.105	-12.4046
N - nitro	10	4.01741	28.3695	-5.32128	28.0403	40.2344	10.2123	50.4467	0.161457	5.02036	34.7314	-9.72263
O - nitro	11	20.4642	12.944	-7.92043	3.59478	76.6569	19.369	96.0259	0.161021	10.6631	34.1403	-14.8525
N- nitro	12	3.95062	28.5534	0	28.5534	33.5665	0	33.5665	0	4.33729	34.8218	1.66729
O - nitro	13	22.3263	9.14837	-7.98558	-1.61192	46.3174	19.8101	66.1275	0.20983	8.08334	26.6698	-15.8114
O - nitro	14	22.6762	6.02275	-12.6448	-10.2198	19.6016	26.1357	45.7373	0.244898	6.30246	18.5837	-21.5041
O - nitro	15	22.3114	9.29691	-7.9076	-1.62296	45.4801	20.2543	65.7344	0.213183	8.07565	26.6579	-15.8076
O - nitro	16	20.5223	12.9473	-7.92515	3.49498	77.0233	19.3609	96.3842	0.160523	10.6557	34.1535	-14.8563
H	17	6.28104	22.3067	0	22.3067	8.02326	0	8.02326	0	2.25148	26.9126	14.9492
O	18	17.9956	14.9099	-5.45115	9.35236	87.5635	11.5376	99.1011	0.102868	10.4446	36.4953	-12.4172
H	19	1.75965	33.7732	0	33.7732	25.8365	0	25.8365	0	4.35119	41.3673	23.573
H	20	1.71787	33.9798	0	33.9798	24.2523	0	24.2523	0	4.19003	41.3077	23.6383
NO ₂	7,8,14	47.3712	7.74007	-12.6239	-9.25497	29.1098	26.3321	55.4418	0.249372	7.22734	21.9528	-21.5041
NO ₂	10,11,15	46.793	13.8916	-7.90904	2.85983	98.7277	19.8997	118.627	0.13961	11.1005	34.7314	-15.8076
NO ₂	12,13,16	46.7993	13.8255	-7.96136	2.82637	99.2485	19.6309	118.879	0.137864	11.0971	34.8218	-15.8114

See figure A-22 for corresponding area weighted atom with area weighted atom number.

Table A-134. Tetryl atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	2.45683	30.5122	0	30.5122	133.237	0	133.237	0	10.4766	42.7152	3.83597
C	2	4.45669	29.7937	0	29.7937	49.255	0	49.255	0	5.79606	43.5228	5.85906
C	3	6.82988	29.3115	0	29.3115	19.7989	0	19.7989	0	3.5672	41.4784	15.9984
C	4	5.61892	29.9431	0	29.9431	14.1147	0	14.1147	0	3.1188	38.1658	20.9262
C	5	7.0639	27.5891	0	27.5891	30.8751	0	30.8751	0	5.29246	37.5815	15.6902
C	6	4.58477	27.9336	0	27.9336	72.9782	0	72.9782	0	8.06105	38.718	9.626
N	7	0.404186	19.1427	0	19.1427	67.3146	0	67.3146	0	6.06798	39.1315	9.1083
N - nitro	8	2.37251	32.2507	-7.6575	31.9572	57.7787	0	57.7787	0	6.27805	42.6154	-7.6575
N - nitro	9	3.86132	30.8037	-1.16905	30.4106	37.6585	0.031052	37.6896	0.000823	5.21758	38.3019	-1.41754
N - nitro	10	2.73934	26.5344	-7.95306	26.1213	128.595	17.2514	145.846	0.104294	10.5667	39.7923	-12.1065
N - nitro	11	1.59332	10.2677	-8.25677	6.10915	16.0586	30.9537	47.0123	0.224904	7.00625	17.6161	-19.0135
O - nitro	12	19.6864	3.76287	-14.6785	-13.093	8.31401	46.229	54.543	0.129195	6.86931	13.1589	-25.694
O - nitro	13	21.7287	5.51831	-15.1015	-12.973	21.7064	42.5126	64.219	0.223758	7.07431	18.1225	-25.7461
C	14	3.59957	29.339	0	29.339	43.7893	0	43.7893	0	4.52797	39.2018	4.67808
O - nitro	15	20.3594	10.0782	-7.81035	-2.11426	64.0452	13.0884	77.1336	0.140892	7.88875	34.1842	-14.0524
O - nitro	16	23.2128	12.4664	-6.30508	2.80811	89.3933	13.9946	103.388	0.117038	9.5975	39.3844	-13.056
O - nitro	17	22.9743	10.7218	-8.52856	-1.06264	60.5092	21.1126	81.6218	0.191757	9.16355	33.2825	-16.6466
O - nitro	18	23.0121	10.525	-8.65743	-1.71083	58.6043	20.9269	79.5312	0.193892	8.9369	32.3374	-16.7595
O - nitro	19	22.2126	9.60836	-8.7561	-2.33292	54.9242	21.8433	76.7675	0.203576	8.50027	33.7588	-16.9321
O - nitro	20	17.4659	11.0475	-9.78252	-2.75603	75.7893	24.4326	100.222	0.184354	9.4951	32.2571	-17.7102
H	21	6.7669	29.6098	0	29.6098	32.0122	0	32.0122	0	4.99189	40.1449	16.0304
H	22	6.23276	25.7466	0	25.7466	24.6503	0	24.6503	0	4.3255	33.6948	13.5831
H	23	8.47547	24.4294	0	24.4294	25.738	0	25.738	0	3.95213	34.0022	7.39959
H	24	8.54085	37.1784	0	37.1784	11.3637	0	11.3637	0	2.88029	43.893	31.265
H	25	8.88565	21.8045	0	21.8045	37.0592	0	37.0592	0	5.02744	30.3275	3.68662
NO ₂	8,15,16	45.9448	14.0351	-7.10218	2.17916	122.969	14.0701	137.039	0.09213	10.5378	42.6154	-14.0524

Table A-134. Tetryl atom specific Politzer parameters using PBE/6-31G** (continuous).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
NO ₂	9,17,18	49.8477	14.57	-8.58126	1.29609	119.33	21.0831	140.413	0.127606	11.3657	38.3019	-16.7595
NO ₂	10,19,20	42.4178	13.0858	-9.21428	-0.54969	114.071	23.258	137.329	0.140677	10.6028	39.7923	-17.7102
NO ₂ *	11,12,13	43.0084	6.16777	-14.832	-12.2618	22.3065	44.6372	66.9437	0.222182	7.57317	18.1225	-25.7461

See figure A-23 for corresponding area weighted atom with area weighted atom number.

* This NO₂ is not connected to the phenyl ring, making its local environment different than the other three nitro groups.

Table A-135. Tri245 atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C	1	5.15432	34.8887	0	34.8887	23.9153	0	23.9153	0	3.81922	44.7031	20.1763
C	2	4.44738	28.4875	0	28.4875	18.3972	0	18.3972	0	3.07155	39.4678	4.12148
N	3	15.331	15.4102	-10.9964	2.55848	93.099	29.5653	122.664	0.182933	13.3119	40.037	-18.3634
C	4	4.26824	36.9116	0	36.9116	23.3427	0	23.3427	0	3.87487	42.692	18.2586
N	5	9.4107	39.8834	0	39.8834	8.17869	0	8.17869	0	2.25054	49.3279	33.7782
N - nitro	6	3.44189	22.2736	-7.98757	21.7319	42.2264	39.2821	81.5085	0.249674	5.81019	32.6048	-15.9569
O - nitro	7	21.2624	8.86538	-11.5394	-7.02656	38.6514	23.905	62.5565	0.236108	8.02298	24.4509	-19.562
O - nitro	8	23.7624	8.28512	-12.122	-8.43997	35.2045	22.4203	57.6249	0.237695	7.4031	24.4591	-19.4591
H	9	5.06744	54.9669	0	54.9669	49.3049	0	49.3049	0	5.95962	67.7679	38.8893
N - nitro	10	4.25004	31.9041	-7.54674	31.6843	66.1748	3.9857	70.1605	0.053581	6.48013	42.547	-9.54316
O - nitro	11	22.956	13.912	-6.40863	5.41426	111.552	13.5469	125.099	0.096563	10.8075	43.4111	-12.8872
O - nitro	12	23.5776	9.73313	-9.08064	-4.62371	52.7965	13.8621	66.6586	0.164711	7.27535	28.1984	-16.4407
N - nitro	13	4.07142	31.7937	-6.32671	31.3748	67.1209	14.0497	81.1706	0.143129	6.8229	44.582	-10.214
O - nitro	14	20.8935	10.9648	-9.03708	-3.44555	65.6065	14.8073	80.4137	0.150232	8.33167	30.0226	-15.0508
O - nitro	15	23.0448	14.1096	-6.78963	5.31955	116.417	15.3563	131.773	0.102956	11.0341	43.4757	-13.3584
NO ₂	6,7,8	48.4667	12.5662	-11.8478	-5.50541	77.2001	23.2428	100.443	0.177856	9.916	32.6048	-19.562
NO ₂	10,11,12	50.7837	15.7046	-8.15373	2.54335	141.894	15.3621	157.256	0.088145	11.9574	43.4111	-16.4407
NO ₂	13,14,15	48.0097	16.0243	-8.14319	3.43945	142.779	16.2353	159.014	0.091676	12.3374	44.582	-15.0508

See figure A-24 for corresponding area weighted atom with area weighted atom number.

A.15 PBE/6-31G** Atom Weighted Test Set Data

Table A-136. BTAT area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.00239	24.2453	0	24.2453	7.83808	0	7.83808	0	2.37849
C	2	3.206	24.9193	0	24.9193	8.72466	0	8.72466	0	2.51001
C	3	1.49411	32.8989	0	32.8989	19.1159	0	19.1159	0	3.49236
H	4	4.62579	25.6805	0	25.6805	24.6715	0	24.6715	0	3.80099
H	5	7.52975	35.874	0	35.874	14.0658	0	14.0658	0	2.86956
C	6	0.08627	36.9868	0	36.9868	44.3753	0	44.3753	0	6.27308
C	7	1.50334	32.2525	0	32.2525	20.8219	0	20.8219	0	3.42915
H	8	7.64329	35.3078	0	35.3078	12.7691	0	12.7691	0	2.74496
H	9	4.92191	26.4626	0	26.4626	23.0606	0	23.0606	0	3.64373
C	10	0.033097	36.6913	0	36.6913	63.4085	0	63.4085	0	7.62366
N	11	10.8655	13.5813	-7.98308	3.00763	67.2595	15.498	82.7575	0.1522	10.9423
N	12	16.7003	11.3751	-9.31356	0.642156	48.6252	22.8674	71.4926	0.217548	10.3435
N	13	11.1058	13.354	-8.34744	3.43817	70.0623	14.9721	85.0344	0.14507	11.0855
N	14	16.8077	11.4474	-9.47595	0.39815	48.9091	23.7298	72.639	0.219961	10.4322
N	15	7.06042	25.6823	0	25.6823	26.2135	0	26.2135	0	4.1599
N	16	6.51338	25.6704	0	25.6704	43.122	0	43.122	0	5.37177
N - nitro	17	1.69239	31.7479	-3.03213	31.0788	131.36	2.67E-15	131.36	2.03E-17	10.0977
N - nitro	18	1.61244	21.8679	0	21.8679	51.7698	0	51.7698	0	6.05021
N - nitro	19	0.995112	15.1526	-5.81137	14.4651	19.6883	0	19.6883	0	3.79613
N - nitro	20	1.52617	29.8519	-0.81263	29.4793	121.811	0	121.811	0	9.11317
N - nitro	21	0.908297	16.2031	-4.74397	15.8786	43.5609	2.67E-15	43.5609	6.13E-17	6.32684
N - nitro	22	1.54523	23.5162	0	23.5162	92.0426	0	92.0426	0	8.03082
O - nitro	23	19.6713	11.7368	-4.42993	6.34358	85.6469	6.24528	91.8921	0.063344	8.7232
O - nitro	24	20.4765	8.60135	-6.00968	-1.5397	59.2866	7.60813	66.8948	0.100798	6.2866
O - nitro	25	21.8738	10.3083	-5.75512	2.90666	67.8437	12.2849	80.1286	0.129809	8.3304
O - nitro	26	19.674	6.05677	-7.23978	-5.08712	21.054	9.28431	30.3383	0.212374	4.39559
O - nitro	27	17.5319	7.57875	-6.17682	-2.9615	36.7117	6.25555	42.9672	0.124393	5.17488
O - nitro	28	20.4189	6.55075	-5.05371	-0.71797	24.7354	8.12196	32.8574	0.186086	5.45421

See figure A-16 for corresponding area weighted atom with area weighted atom number.

Table A-136. BTAT area weighted atom specific Politzer parameters using PBE/6-31G** (continuous).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	29	19.8673	11.6967	-4.45931	6.28275	84.2291	6.0737	90.3028	0.062735	8.7345
O - nitro	30	20.2674	7.26225	-5.61809	-1.86812	42.9395	7.75036	50.6899	0.12952	5.45283
O - nitro	31	20.6578	7.46974	-5.24246	-0.69835	39.2197	8.46427	47.6839	0.145999	5.86173
O - nitro	32	17.1401	7.54129	-5.78665	-2.12532	37.1084	6.08768	43.1961	0.12107	5.44113
O - nitro	33	20.2744	6.30298	-6.75084	-4.2585	28.1735	10.326	38.4996	0.196274	4.71766
O - nitro	34	21.2614	9.60295	-5.77004	2.14926	61.1493	12.158	73.3074	0.138344	7.87155
H	35	4.69697	38.0769	0	38.0769	32.4192	0	32.4192	0	4.7864
H	36	5.28211	38.4677	0	38.4677	42.3461	0	42.3461	0	5.44185

See figure A-16 for corresponding area weighted atom with area weighted atom number.

Table A-137. CL16 area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	4.01799	30.042	0	30.042	11.8742	0	11.8742	0	2.65298
C	2	3.99417	30.8623	0	30.8623	14.761	0	14.761	0	3.18903
C	3	4.17086	30.0268	0	30.0268	9.44897	0	9.44897	0	2.32398
N - nitro	4	0.776129	13.6078	-5.34662	12.3116	30.3897	3.28307	33.6728	0.087993	5.09316
C	5	4.49471	36.562	0	36.562	28.0592	0	28.0592	0	3.78208
C	6	3.70026	30.464	0	30.464	13.0092	0	13.0092	0	2.88581
N - nitro	7	0.931911	20.2144	-1.93238	19.6606	52.5858	3.38711	55.9729	0.056852	6.38173
N - nitro	8	1.23421	16.7846	-7.51283	16.3862	37.3022	0.382621	37.6849	0.01005	5.26824
O - nitro	9	20.5214	6.88345	-6.1917	-2.09943	32.0407	12.4298	44.4705	0.201383	5.82796
O - nitro	10	20.7643	7.87285	-6.21869	-1.52468	38.4122	12.7931	51.2053	0.18742	6.3608
C	11	4.59395	34.791	0	34.791	34.9888	0	34.9888	0	4.44846
O - nitro	12	21.3714	6.49503	-4.95029	-0.0641	31.0465	9.87009	40.9166	0.183035	5.6006
O - nitro	13	20.5277	8.0426	-6.81851	-2.16124	38.7166	14.7992	53.5158	0.200065	6.59164
O - nitro	14	21.5987	9.16047	-5.50491	0.626225	56.5501	10.529	67.0791	0.132326	7.15105
O - nitro	15	20.3333	7.61484	-6.96881	-2.65886	38.7234	14.339	53.0624	0.197205	6.33865
N - nitro	16	0.410657	12.6885	-2.39523	11.7595	44.4707	0.610693	45.0814	0.013363	5.87168
N - azide	17	12.3515	22.3679	0	22.3679	68.1362	0	68.1362	0	6.50546
N - nitro	18	1.2625	32.5603	-3.52598	32.0685	257.034	0	257.034	0	14.6595
O - nitro	19	20.6606	6.76322	-5.94528	-1.66719	35.2648	12.0803	47.3451	0.190051	5.8007
O - nitro	20	20.8402	7.36857	-6.0193	-1.53672	38.6312	12.3266	50.9578	0.183383	6.0684
N - azide	21	7.61356	36.993	0	36.993	50.5783	0.00E+00	50.5783	0.00E+00	5.3778
O - nitro	22	20.4068	11.0518	-4.08734	4.15318	110.624	6.98123	117.605	0.055838	8.37277
O - nitro	23	18.9043	8.47451	-3.92733	4.26033	45.1934	5.38221	50.5756	0.095094	6.58249
N - azide	24	25.3835	14.0766	0	14.0766	78.4346	0	78.4346	0	7.55546

See figure A-17 for corresponding area weighted atom with area weighted atom number.

Table A-138. DNBF area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	5.53793	31.5091	0	31.5091	1.62509	0	1.62509	0	1.02429
C	2	4.70085	26.3235	0	26.3235	21.1612	0	21.1612	0	3.77935
C	3	5.67509	27.1129	0	27.1129	3.63699	0	3.63699	0	1.4871
C	4	7.68238	25.1923	0	25.1923	5.00233	0	5.00233	0	1.71727
C	5	5.96439	28.0165	0	28.0165	3.49505	0	3.49505	0	1.55182
C	6	7.95465	28.2141	0	28.2141	4.32077	0	4.32077	0	1.63489
N - nitro	7	4.21694	26.7748	-6.21978	25.9025	35.7147	11.0755	46.7902	0.180676	5.45257
N - nitro	8	3.97943	23.3782	-7.7792	22.8763	38.5135	41.9375	80.451	0.249547	5.37705
N	9	15.5383	11.1579	-13.4715	-5.74576	62.8824	59.6032	122.486	0.249821	11.3503
N	10	4.88316	30.1613	0	30.1613	16.6797	0	16.6797	0	3.15773
O - nitro	11	22.7321	9.46445	-9.1428	-2.24931	43.5587	25.8231	69.3818	0.233664	8.82553
O - nitro	12	22.1375	9.82963	-8.04735	-0.68735	49.5751	20.8571	70.4322	0.208437	8.67224
O - nitro	13	22.5241	8.8307	-11.5066	-5.77861	36.96	36.7963	73.7563	0.249999	9.03598
O - nitro	14	20.7272	8.12656	-17.5615	-13.9788	32.0217	42.6722	74.6939	0.244917	8.81231
O	15	15.4735	8.13932	-0.64611	6.79543	65.16	0.245105	65.4051	0.003733	6.44059
O	16	24.4278	10.0199	-4.80956	2.30815	55.1595	6.52565	61.6851	0.094598	7.58883
H	17	6.49867	24.0419	0	24.0419	14.1963	0	14.1963	0	3.12022
H	18	7.78552	29.5419	0	29.5419	16.808	0	16.808	0	3.18426

See figure A-18 for corresponding area weighted atom with area weighted atom number.

Table A-139. HNS area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	3.99831	28.2351	0	28.2351	8.52415	0	8.52415	0	2.32008
C	2	5.71246	28.937	0	28.937	3.91372	0	3.91372	0	1.6091
C	3	7.55091	24.9155	0	24.9155	5.08146	0	5.08146	0	1.57581
H	4	6.3495	21.9293	0	21.9293	10.3916	0	10.3916	0	2.61787
C	5	5.5977	27.8938	0	27.8938	6.8184	0	6.8184	0	2.09809
C	6	7.37256	25.7	0	25.7	24.106	0	24.106	0	4.11699
H	7	7.0639	25.9271	0	25.9271	30.6359	0	30.6359	0	4.76878
C	8	4.37759	26.4622	0	26.4622	12.6311	0	12.6311	0	2.74409
C	9	1.59547	20.6427	0	20.6427	40.0832	0	40.0832	0	5.39131
H	10	8.30053	27.5853	0	27.5853	25.5986	0	25.5986	0	4.07621
N - nitro	11	3.82689	27.1423	0	27.1423	43.4048	0	43.4048	0	5.04506
N - nitro	12	3.96943	27.376	-4.67516	26.9647	45.361	37.5672	82.9281	0.247792	5.60712
N - nitro	13	1.62511	27.72	-11.127	27.4729	50.3698	0	50.3698	0	5.70298
O - nitro	14	13.7732	11.3631	-13.6302	-4.36806	58.8684	47.8076	106.676	0.247312	12.0492
O - nitro	15	22.1175	9.51441	-10.1435	-3.66921	45.4693	30.9956	76.4648	0.241043	9.04847
O - nitro	16	22.6678	9.73235	-9.20891	-2.76436	48.8525	24.5334	73.3859	0.222546	8.71063
O - nitro	17	22.5897	9.72366	-9.3139	-2.99855	47.5816	25.5737	73.1552	0.227374	8.7004
O - nitro	18	20.3752	9.58757	-11.6469	-5.94233	47.9074	40.2729	88.1803	0.248126	9.21378
O - nitro	19	18.8769	8.06444	-8.37437	-2.6285	39.4147	30.2951	69.7098	0.245721	7.75892
C	20	1.53223	20.1313	0	20.1313	35.0135	0	35.0135	0	4.98556
C	21	3.9749	28.032	0	28.032	9.76175	0.00E+00	9.76175	0.00E+00	2.40873
H	22	8.24842	27.636	0	27.636	25.4297	0	25.4297	0	4.04337
C	23	5.95884	28.9109	0	28.9109	4.14412	0	4.14412	0	1.64369
C	24	4.43967	26.4774	0	26.4774	14.7021	0	14.7021	0	2.92034
C	25	7.41719	24.8804	0	24.8804	4.50846	0	4.50846	0	1.52156
N - nitro	26	3.81527	26.7561	0	26.7561	45.4823	0	45.4823	0	5.31032
C	27	7.16452	25.5244	0	25.5244	23.1307	0	23.1307	0	4.03975
N - nitro	28	1.48381	28.6492	-18.4695	28.0852	43.1128	0	43.1128	0	5.73389
H	29	6.36286	21.8932	0	21.8932	10.9475	0	10.9475	0	2.64993
C	30	5.77655	27.9967	0	27.9967	7.02393	0	7.02393	0	2.16318

See figure A-19 for corresponding area weighted atom with area weighted atom number.

Table A-139. HNS area weighted atom specific Politzer parameters using PBE/6-31G** (continued).

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
O - nitro	31	13.6504	11.5263	-13.5383	-4.32986	59.8006	48.6527	108.453	0.247359	12.0586
O - nitro	32	22.0415	9.32302	-10.1725	-3.84206	45.3645	30.9703	76.3348	0.241111	8.94069
H	33	7.06826	25.9733	0	25.9733	30.3574	0	30.3574	0	4.75862
O - nitro	34	20.433	9.80759	-11.7014	-5.71317	55.5168	39.3588	94.8756	0.242749	9.37242
O - nitro	35	19.0907	8.24	-8.43699	-2.46899	40.6856	30.3783	71.0639	0.244741	7.89562
N - nitro	36	3.74146	28.0167	-15.6752	27.8144	32.8538	0	32.8538	0	4.66996
O - nitro	37	22.7052	9.61331	-9.16743	-2.8432	46.5476	24.7666	71.3142	0.226679	8.62509
O - nitro	38	22.7178	9.74569	-9.35289	-2.85638	48.3479	25.4113	73.7591	0.225825	8.79616

See figure A-19 for corresponding area weighted atom with area weighted atom number.

Table A-140. Methyl picrate area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.08212	24.2548	0	24.2548	4.50754	0	4.50754	0	1.69435
C	2	7.25918	21.9098	0	21.9098	14.0829	0	14.0829	0	2.98946
C	3	5.54737	24.764	0	24.764	9.2214	0	9.2214	0	2.25324
C	4	3.65128	25.7276	0	25.7276	3.76078	0	3.76078	0	1.78226
C	5	5.61811	24.6345	0	24.6345	10.0146	0	10.0146	0	2.31053
C	6	7.2794	21.9258	0	21.9258	14.1533	0	14.1533	0	2.99635
N - nitro	7	3.63801	24.0606	-7.30314	23.5489	41.7889	40.0837	81.8726	0.249892	5.61823
O - nitro	8	22.5385	8.55045	-10.2477	-5.13648	39.9813	26.3293	66.3106	0.239403	8.10923
N - nitro	9	3.62628	24.1523	-2.63427	23.8189	38.7436	2.76491	41.5085	0.062174	5.24057
O - nitro	10	18.8722	8.51088	-9.22212	-3.68623	43.4437	28.4689	71.9127	0.239159	8.06776
N - nitro	11	3.97247	23.6456	-9.64975	23.2541	32.2523	34.9286	67.1809	0.249603	4.66091
O - nitro	12	22.6545	8.44236	-10.9894	-5.62269	34.9953	32.5764	67.5717	0.24968	8.55871
O - nitro	13	18.8223	8.54559	-9.26714	-3.7305	44.1291	28.2339	72.363	0.237938	8.07981
O - nitro	14	22.5451	8.4704	-10.2273	-5.20938	39.172	26.4026	65.5746	0.24052	8.04359
O - nitro	15	22.5828	8.36455	-10.9613	-5.72835	33.4108	32.8877	66.2986	0.249984	8.48506
H	16	6.57764	20.8612	0	20.8612	20.8179	0	20.8179	0	3.91282
H	17	6.61746	20.7842	0	20.7842	20.8549	0	20.8549	0	3.90211
O	18	10.1692	8.15887	-3.12515	2.60829	45.2059	1.97796	47.1838	0.040163	5.99719
C	19	5.56972	16.4311	0	16.4311	43.1393	0	43.1393	0	5.71119
H	20	8.13057	17.5384	0	17.5384	17.6259	0	17.6259	0	3.17438
H	21	11.4857	17.4311	0	17.4311	15.1493	0.00E+00	15.1493	0.00E+00	3.32993
H	22	8.14248	17.7195	0	17.7195	18.8384	0	18.8384	0	3.25639

See figure A-20 for corresponding area weighted atom with area weighted atom number.

Table A-141. Picryl azide area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	7.16403	23.4372	0	23.4372	15.2485	0	15.2485	0	2.92253
C	2	6.111	25.8732	0	25.8732	2.80602	0	2.80602	0	1.38651
C	3	5.17339	24.9043	0	24.9043	11.7285	0	11.7285	0	2.49154
H	4	6.88214	23.5451	0	23.5451	22.6386	0	22.6386	0	4.08273
C	5	7.31165	24.1965	0	24.1965	8.14225	0	8.14225	0	2.08945
C	6	4.53332	28.5875	0	28.5875	22.6868	0	22.6868	0	3.39173
N - nitro	7	4.12553	24.3804	-11.0349	24.1181	39.4788	42.0528	81.5316	0.249751	5.04734
N - nitro	8	3.23628	24.7786	-9.51382	24.4118	46.0572	1.80841	47.8656	0.036354	5.79911
C	9	5.65406	28.8919	0	28.8919	27.5324	0	27.5324	0	3.74975
O - nitro	10	22.5077	8.79253	-10.428	-4.82807	37.5383	31.0346	68.5729	0.247751	8.57304
O - nitro	11	22.8911	8.7947	-9.43964	-4.05891	44.1648	22.6271	66.7919	0.224005	8.00484
O - nitro	12	22.6346	8.875	-10.4972	-4.61245	39.7513	30.6153	70.3666	0.245786	8.72622
O - nitro	13	21.4611	8.30671	-8.93034	-4.61431	39.5922	21.6937	61.2859	0.228677	7.06123
N - azide	14	11.7498	13.7188	-1.37968	13.2269	63.8054	0.721922	64.5273	0.011063	6.42238
H	15	6.45615	22.2484	0	22.2484	16.6647	0	16.6647	0	3.41644
N - nitro	16	3.54368	30.9514	-6.95488	30.5685	66.3566	20.7573	87.114	0.181502	6.45267
N - azide	17	7.50104	28.094	0	28.094	59.3763	0	59.3763	0	6.10872
O - nitro	18	18.2073	9.06382	-7.83067	-1.64249	50.8899	20.8545	71.7444	0.206184	7.94552
O - nitro	19	22.4537	10.0177	-8.00187	-1.28373	54.8408	19.4163	74.2571	0.193105	8.47517
N - azide	20	25.905	10.4261	-2.47913	6.63452	52.0638	1.81457	53.8783	0.032545	7.20681

See figure A-21 for corresponding area weighted atom with area weighted atom number.

Table A-142. Styphnic acid area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	6.314	27.6971	0	27.6971	8.50405	0	8.50405	0	2.39485
C	2	4.21802	25.3633	0	25.3633	15.6903	0	15.6903	0	2.87371
C	3	4.82384	18.8896	0	18.8896	16.5513	0	16.5513	0	3.30194
C	4	4.20603	25.4595	0	25.4595	15.2987	0	15.2987	0	2.84126
C	5	6.3206	27.7052	0	27.7052	8.55844	0	8.55844	0	2.40248
C	6	7.15686	24.2996	0	24.2996	0.72009	0	0.72009	0	0.551797
N - nitro	7	2.00532	12.9431	-7.04527	12.1061	22.6463	44.4546	67.1009	0.223593	4.64267
O - nitro	8	22.6897	6.12117	-12.7306	-10.387	19.55	26.2666	45.8166	0.244627	6.21992
O	9	18.0073	15.1381	-5.39629	9.67276	85.9677	11.3848	97.3525	0.103268	10.4476
N - nitro	10	4.01741	28.649	-6.196	28.3509	32.8215	10.001	42.8225	0.179001	4.54807
O - nitro	11	20.4642	13.2543	-7.90787	3.96614	77.1513	19.3234	96.4747	0.160177	10.8207
N- nitro	12	3.95062	28.7373	0	28.7373	31.1025	0	31.1025	0	4.12306
O - nitro	13	22.3263	9.64632	-7.93937	-1.14313	48.5055	19.7769	68.2823	0.205746	8.37783
O - nitro	14	22.6762	5.97501	-12.7615	-10.4092	19.1892	26.0983	45.2875	0.244181	6.21244
O - nitro	15	22.3114	9.71042	-7.9003	-1.14246	47.4833	20.0271	67.5105	0.20865	8.37606
O - nitro	16	20.5223	13.2963	-7.91251	4.00107	77.7686	19.3141	97.0827	0.159366	10.8462
H	17	6.28104	22.3804	0	22.3804	8.13229	0	8.13229	0	2.25554
O	18	17.9956	15.1907	-5.43389	9.76842	86.8278	11.3667	98.1945	0.102357	10.4846
H	19	1.75965	34.028	0	34.028	25.8465	0	25.8465	0	4.34112
H	20	1.71787	34.1338	0	34.1338	25.1334	0	25.1334	0	4.27623

See figure A-22 for corresponding area weighted atom with area weighted atom number.

Table A-143. Tetryl area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	2.45683	30.5404	0	30.5404	135.297	0	135.297	0	10.539
C	2	4.45669	29.8163	0	29.8163	47.7387	0	47.7387	0	5.73142
C	3	6.82988	29.2716	0	29.2716	20.738	0	20.738	0	3.67749
C	4	5.61892	29.9665	0	29.9665	14.3395	0	14.3395	0	3.15075
C	5	7.0639	27.646	0	27.646	31.0443	0	31.0443	0	5.31695
C	6	4.58477	27.7902	0	27.7902	74.2164	0	74.2164	0	8.1329
N	7	0.404186	19.0472	0	19.0472	77.7527	0	77.7527	0	6.61818
N - nitro	8	2.37251	31.9812	-7.6575	31.5561	63.0695	0	63.0695	0	6.65314
N - nitro	9	3.86132	30.5287	-1.12523	30.2835	42.3813	0.024484	42.4058	0.000577	5.33063
N - nitro	10	2.73934	26.7924	-7.72343	26.3808	127.236	17.1987	144.435	0.104897	10.4817
N - nitro	11	1.59332	10.1679	-8.7918	5.67384	16.2332	33.9922	50.2254	0.218744	7.33434
O - nitro	12	19.6864	3.98971	-14.6502	-12.9951	9.48262	46.0499	55.5326	0.1416	6.90017
O - nitro	13	21.7287	5.38943	-15.0249	-12.9546	21.0624	42.7801	63.8425	0.22107	7.04089
C	14	3.59957	29.5025	0	29.5025	40.3781	0	40.3781	0	4.29493
O - nitro	15	20.3594	9.99318	-7.76529	-2.02551	60.9629	12.4002	73.3631	0.140456	7.87179
O - nitro	16	23.2128	12.2298	-6.17997	2.70057	89.7635	13.8036	103.567	0.115518	9.41758
O - nitro	17	22.9743	10.528	-8.45011	-1.23205	60.3664	20.9292	81.2955	0.191167	8.97485
O - nitro	18	23.0121	10.2954	-8.65454	-1.89836	56.8324	20.4301	77.2625	0.194504	8.78607
O - nitro	19	22.2126	9.59528	-8.70817	-2.4044	55.1078	21.574	76.6818	0.20219	8.42548
O - nitro	20	17.4659	11.4743	-9.94078	-2.74921	78.486	24.4436	102.93	0.181082	9.73042
H	21	6.7669	29.9624	0	29.9624	31.0685	0.00E+00	31.0685	0.00E+00	4.87963
H	22	6.23276	25.4825	0	25.4825	25.2387	0	25.2387	0	4.40761
H	23	8.47547	24.6583	0	24.6583	25.8404	0	25.8404	0	3.96314
H	24	8.54085	37.2853	0	37.2853	11.7038	0	11.7038	0	2.93897
H	25	8.88565	21.8713	0	21.8713	35.0313	0	35.0313	0	4.83751

See figure A-23 for corresponding area weighted atom with area weighted atom number.

Table A-144. Tri245 area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C	1	5.15432	34.8673	0	34.8673	23.4316	0	23.4316	0	3.7995
C	2	4.44738	28.3638	0	28.3638	19.4965	0	19.4965	0	3.1296
N	3	15.331	15.8522	-11.2065	2.97945	92.791	29.3327	122.124	0.182498	13.6508
C	4	4.26824	37.0733	0	37.0733	22.0836	0	22.0836	0	3.72293
N	5	9.4107	39.6534	0	39.6534	8.05356	0	8.05356	0	2.20076
N - nitro	6	3.44189	22.1368	-9.24453	21.6312	44.0176	39.7581	83.7757	0.249354	5.88311
O - nitro	7	21.2624	8.78482	-11.5143	-7.19848	38.8707	24.3637	63.2344	0.236842	7.8722
O - nitro	8	23.7624	8.31779	-12.1317	-8.62779	36.1519	21.7179	57.8697	0.234447	7.19476
H	9	5.06744	55.0434	0	55.0434	50.2511	0	50.2511	0	6.03119
N - nitro	10	4.25004	32.4296	-8.86737	32.2585	61.775	2.24164	64.0167	0.03379	6.21773
O - nitro	11	22.956	14.1653	-6.63902	5.78945	111.069	14.1246	125.194	0.100093	11.0069
O - nitro	12	23.5776	10.192	-9.15419	-4.18752	55.0845	14.2684	69.3529	0.163409	7.76761
N - nitro	13	4.07142	32.1321	-6.35656	31.707	58.6437	13.7475	72.3912	0.153842	6.45158
O - nitro	14	20.8935	11.1387	-9.08187	-3.01007	64.2941	14.9727	79.2668	0.15321	8.70799
O - nitro	15	23.0448	14.2569	-6.81496	5.51136	115.973	15.2879	131.261	0.102904	11.1315

See figure A-24 for corresponding area weighted atom with area weighted atom number.

A.15 PBE/6-31G** Test Set Statistics

Table A-145. BTAT minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	1.554201	31.12973	0	31.12973	26.60481	0	26.60481	0	4.20023	37.95658	21.05232
C max	3.206	38.3755	0	38.3755	69.1779	0	69.1779	0	8.31732	44.1886	28.8617
C min	0.033097	24.2545	0	24.2545	7.78602	0	7.78602	0	2.34823	31.1213	14.476
H avg	5.783303	33.1502	0	33.1502	25.15982	0	25.15982	0	3.935028	41.91962	18.11368
H max	7.64329	38.2784	0	38.2784	41.801	0	41.801	0	5.4368	48.1821	23.386
H min	4.62579	25.4849	0	25.4849	13.6906	0	13.6906	0	2.86577	34.9717	9.55258
N	11.50885	16.48292	-5.89885	9.047515	51.32455	12.65532	63.97988	0.121362	8.540402	33.18867	-4.37917
N	16.8077	25.5979	0	25.5979	72.9005	23.0349	87.7762	0.218706	10.7006	41.1251	18.002
N	6.51338	11.1831	-9.66332	-0.66642	26.7006	0	26.7006	0	4.21315	28.4689	-16.8367
N - nitro avg	1.37994	22.90882	-2.40002	22.61123	76.74983	0	76.74983	0	7.170293	35.0781	-1.57536
N - nitro max	1.69239	31.0184	0	30.6032	138.738	0	138.738	0	10.2859	45.4311	3.79769
N - nitro min	0.908297	14.4288	-5.81137	13.9351	19.322	0	19.322	0	3.53874	22.9097	-5.81137
O - nitro avg	19.92623	8.356883	-5.68461	-0.17643	48.99668	8.415922	57.41258	0.135437	6.343586	29.91428	-11.1414
O - nitro max	21.8738	11.5662	-4.19367	6.44131	86.0858	12.4452	92.206	0.214995	8.61625	41.9741	-8.66277
O - nitro min	17.1401	6.09311	-7.29567	-5.20414	20.8879	6.12021	30.4003	0.06197	4.3603	19.4283	-13.327
NO ₂ avg	41.2324	10.02934	-5.8253	0.679089	74.41767	8.812362	83.22998	0.105001	7.638937	36.34443	-11.8294
NO ₂ max	43.1602	12.285	-5.24233	3.66183	115.147	11.2921	123.138	0.157067	9.29919	45.4311	-10.8333
NO ₂ min	38.7061	7.35266	-6.69374	-1.52796	30.693	7.35333	38.1351	0.060689	5.73773	24.6467	-13.327

Table A-146. CL16 minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	4.16199	32.31278	0	32.31278	20.48763	0	20.48763	0	3.356887	46.03148	23.4197
C max	4.59395	36.7839	0	36.7839	41.8411	0	41.8411	0	4.88509	58.7142	25.3238
C min	3.70026	30.1084	0	30.1084	9.94998	0	9.94998	0	2.38283	39.2206	22.2019
N - azide avg	15.11619	24.29347	0	24.29347	65.1992	0	65.1992	0	6.450703	51.23533	9.597753
N - azide max	25.3835	36.9233	0	36.9233	80.4794	0	80.4794	0	7.67175	59.3298	19.1409
N - azide min	7.61356	14.1457	0	14.1457	49.7042	0	49.7042	0	5.27707	38.5617	1.8179
N - nitro avg	0.923081	18.63982	-4.03222	17.99746	82.39748	1.551744	83.94924	0.036993	7.18008	34.46996	-5.28313
N - nitro max	1.2625	31.6682	-2.1853	31.3482	255.713	3.57707	255.713	0.095672	14.5566	58.0151	-2.99448
N - nitro min	0.410657	12.1645	-7.09619	11.3673	24.7527	0	27.7234	0	4.34338	25.736	-7.84199
O - nitro avg	20.59287	8.011563	-5.64939	-0.15374	46.56983	11.02691	57.59679	0.163093	6.529781	28.06166	-11.9924
O - nitro max	21.5987	11.297	-3.89683	4.48528	116.502	14.319	123.194	0.202281	8.50659	44.9366	-8.02898
O - nitro min	18.9043	6.3865	-6.8522	-2.49615	30.1307	5.47555	39.9958	0.051366	5.61488	23.4626	-14.1183
NO ₂ avg	42.1088	8.572614	-5.64958	0.286264	56.25842	11.05591	67.31436	0.149875	6.915058	34.46996	-12.2094
NO ₂ max	43.902	11.0216	-3.93564	5.24673	112.2	13.9759	118.392	0.193765	8.43004	58.0151	-9.16289
NO ₂ min	40.5735	7.21104	-6.80581	-1.73561	35.4203	6.19186	48.0511	0.049565	6.11273	25.736	-14.1183

Table A-147. DNBf minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	6.252548	27.71122	0	27.71122	6.55167	0	6.55167	0	1.863257	33.35818	19.65747
C max	7.95465	31.523	0	31.523	20.8797	0	20.8797	0	3.7373	35.2422	28.7161
C min	4.70085	25.1712	0	25.1712	1.65719	0	1.65719	0	1.03071	32.3914	11.8599
H avg	7.142095	26.85475	0	26.85475	15.7767	0	15.7767	0	3.18404	33.27215	15.7549
H max	7.78552	29.6048	0	29.6048	17.0954	0	17.0954	0	3.21096	36.2293	17.4435
H min	6.49867	24.1047	0	24.1047	14.458	0	14.458	0	3.15712	30.315	14.0663
N avg	10.21073	20.78655	-6.6741	12.57188	39.29405	29.7156	69.00965	0.124904	7.314575	34.12965	-7.778
N max	15.5383	30.2589	0	30.2589	62.8268	59.4312	122.258	0.249807	11.5399	35.8641	12.2264
N min	4.88316	11.3142	-13.3482	-5.11514	15.7613	0	15.7613	0	3.08925	32.3952	-27.7824
O avg	19.95065	9.2713	-2.7089	4.696215	61.8014	3.364798	65.16615	0.04861	7.128985	31.81035	-6.14991
O max	24.4278	10.0702	-0.6559	7.10149	68.0547	6.47201	68.3122	0.093464	7.58439	34.3273	-2.61483
O min	15.4735	8.4724	-4.7619	2.29094	55.5481	0.257586	62.0201	0.003756	6.67358	29.2934	-9.68498
N - nitro avg	4.098185	25.18365	-6.25764	24.5132	35.2967	19.07793	54.3746	0.206435	5.308695	32.2229	-14.5149
N - nitro max	4.21694	26.8632	-6.00129	25.9894	37.1902	29.2242	66.4144	0.246403	5.35767	33.5234	-11.5085
N - nitro min	3.97943	23.5041	-6.51399	23.037	33.4032	8.93166	42.3348	0.166466	5.25972	30.9224	-17.5213
O - nitro avg	22.03023	9.123393	-11.59	-5.52456	41.0807	32.25863	73.3393	0.233706	8.982698	25.23545	-20.8677
O - nitro max	22.7321	9.84883	-8.10236	-0.61798	50.1515	44.2202	76.2659	0.249999	9.21369	29.1566	-15.9569
O - nitro min	20.7272	8.211	-17.5624	-13.7605	32.0457	21.0538	69.7073	0.208252	8.73695	20.7361	-27.5797
NO ₂ avg*	48.15865	13.14605	-11.6721	-2.73616	87.12265	37.0391	124.162	0.199505	11.52015	32.2229	-22.799
NO ₂ max*	49.0865	13.2351	-8.62998	1.06754	90.7772	50.3358	133.804	0.234671	12.2865	33.5234	-18.0183
NO ₂ min*	47.2308	13.057	-14.7142	-6.53986	83.4681	23.7424	114.52	0.164339	10.7538	30.9224	-27.5797
NO ₂ avg	47.03393	13.03543	-9.15419	0.561077	97.30443	27.26814	124.573	0.152276	10.99253	33.43663	-18.4277
NO ₂ max	49.0865	13.2351	-4.11838	7.15555	117.668	50.3358	133.804	0.234671	12.2865	35.8641	-9.68498
NO ₂ min	44.7845	12.8142	-14.7142	-6.53986	83.4681	7.72622	114.52	0.057819	9.93729	30.9224	-27.5797

* These statistics do not include the “NO₂” part of the furazan-oxide moiety.

Table A-148. HNS minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.17635	26.06654	0	26.06654	14.03597	0	14.03597	0	2.805776	33.8691	16.20188
C max	7.55091	28.9368	0	28.9368	40.3934	0	40.3934	0	5.46941	37.1228	25.3777
C min	1.53223	20.1494	0	20.1494	4.03037	0	4.03037	0	1.5209	30.1311	9.64984
H avg	7.232245	25.2174	0	25.2174	22.72717	0	22.72717	0	3.854463	32.27647	12.68132
H max	8.30053	27.683	0	27.683	32.7802	0	32.7802	0	4.91492	35.069	13.5962
H min	6.3495	21.83	0	21.83	10.5242	0	10.5242	0	2.62806	26.8869	11.068
N - nitro avg	3.076995	27.60897	-9.22582	27.2411	44.94432	7.03375	51.97807	0.041654	5.561277	35.93568	-9.00498
N - nitro max	3.96943	28.5515	0	27.8821	62.9617	42.2025	85.8905	0.249925	6.71828	37.3305	5.95695
N - nitro min	1.48381	26.8942	-18.4695	26.8695	32.3287	0	32.3287	0	4.64472	35.1098	-18.4695
O - nitro avg	20.08658	9.738611	-10.4011	-3.53523	48.62759	33.87895	82.50655	0.239145	9.36315	28.65643	-20.2728
O - nitro max	22.7178	11.6434	-8.22961	-2.43465	62.3978	49.3429	110.541	0.249606	12.3498	32.3167	-17.9116
O - nitro min	13.6504	7.84475	-13.846	-6.01956	38.1343	24.6682	68.0058	0.223527	7.50979	25.7637	-23.6992
NO ₂ avg	43.2501	12.93267	-10.3031	-1.24657	93.42222	35.2457	128.668	0.19645	11.0861	35.93568	-21.7683
NO ₂ max	49.2269	14.6375	-9.26933	0.074246	102.085	41.6621	143.28	0.22113	12.7456	37.3305	-18.1695
NO ₂ min	39.5071	10.5755	-11.5772	-3.36929	78.5845	25.5449	117.041	0.162063	9.38167	35.1098	-23.6992

Table A-149. Methyl picrate minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.906243	23.93185	0	23.93185	9.755035	0	9.755035	0	2.376738	31.49785	14.2498
C max	7.2794	25.7167	0	25.7167	15.3091	0	15.3091	0	3.13449	32.9286	22.1436
C min	3.65128	21.9255	0	21.9255	3.65626	0	3.65626	0	1.64893	29.5551	8.22853
H avg	8.19077	18.90518	0	18.90518	18.82684	0	18.82684	0	3.52246	27.23418	5.984308
H max	11.4857	20.8826	0	20.8826	21.4663	0	21.4663	0	3.98479	29.3844	8.4582
H min	6.57764	17.4576	0	17.4576	15.4998	0	15.4998	0	3.16133	23.4005	2.50627
O avg	10.1692	7.91117	-3.10981	2.48293	43.2193	2.00214	45.2214	0.042314	5.83832	29.1051	-5.19766
O max	10.1692	7.91117	-3.10981	2.48293	43.2193	2.00214	45.2214	0.042314	5.83832	29.1051	-5.19766
O min	10.1692	7.91117	-3.10981	2.48293	43.2193	2.00214	45.2214	0.042314	5.83832	29.1051	-5.19766
N - nitro avg	3.745587	23.81623	-6.36089	23.36363	39.16263	23.01231	62.17497	0.183707	5.326493	32.43933	-12.4073
N - nitro max	3.97247	24.0293	-2.32681	23.6695	45.0734	34.1774	77.3154	0.249891	5.82597	33.4827	-4.88202
N - nitro min	3.62628	23.6443	-10.1271	23.1687	32.782	2.61754	42.2501	0.058115	4.81444	30.3834	-16.2989
O - nitro avg	21.3359	8.330197	-10.1107	-5.09395	38.97675	28.7966	67.77333	0.242319	8.031778	25.52917	-19.4672
O - nitro max	22.6545	8.45282	-9.04146	-4.03499	45.6426	32.8402	74.0963	0.249996	8.39897	28.6483	-18.2875
O - nitro min	18.8223	8.21852	-11.0317	-6.07675	32.199	25.5673	64.1532	0.236546	7.68065	23.3797	-20.8459
NO ₂ avg	46.41737	11.7783	-10.1436	-3.04418	80.45433	28.93787	109.392	0.19402	9.832527	32.43933	-19.7822
NO ₂ max	49.2098	11.9051	-9.64905	-2.54857	84.0881	32.3959	111.795	0.212146	10.0127	33.4827	-19.2043
NO ₂ min	44.9988	11.6064	-10.998	-4.02693	73.6674	26.7106	106.063	0.1835	9.66799	30.3834	-20.8459

Table A-150. Picryl azide minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.991242	26.16735	0	26.16735	16.14251	0	16.14251	0	2.806195	38.29103	16.30416
C max	7.31165	29.2237	0	29.2237	31.2698	0	31.2698	0	4.07873	49.2187	22.9625
C min	4.53332	23.5763	0	23.5763	2.66246	0	2.66246	0	1.35936	30.3294	9.83433
H avg	6.669145	22.9038	0	22.9038	19.6124	0	19.6124	0	3.744925	30.7197	11.1722
H max	6.88214	23.5989	0	23.5989	22.7484	0	22.7484	0	4.09916	32.264	12.1342
H min	6.45615	22.2087	0	22.2087	16.4764	0	16.4764	0	3.39069	29.1754	10.2102
N - azide avg	15.05195	17.28817	-1.24727	15.86847	57.2805	0.830639	58.11113	0.014373	6.51439	42.01117	-0.37358
N - azide max	25.905	28.2722	0	28.2722	60.7787	1.7528	61.5178	0.03125	7.11617	49.1491	6.7382
N - azide min	7.50104	10.2043	-2.42372	6.48822	52.5263	0	54.2791	0	6.10409	30.748	-4.81363
N - nitro avg	3.635163	26.5548	-8.36529	26.2428	52.3805	21.29648	73.67693	0.160975	5.880837	38.1982	-13.6176
N - nitro max	4.12553	31.0109	-7.02936	30.633	63.8	37.6959	88.1707	0.248401	6.35248	48.2574	-10.7442
N - nitro min	3.23628	24.2769	-9.39413	23.9517	44.2494	1.82273	50.9149	0.034518	5.40806	31.0611	-17.328
O - nitro avg	21.69258	8.90187	-9.16464	-3.57511	43.90733	23.99657	67.9039	0.224056	8.054313	28.29533	-17.8804
O - nitro max	22.8911	10.017	-7.88759	-1.31713	54.4411	30.9115	73.9973	0.248123	8.51277	35.657	-15.6175
O - nitro min	18.2073	8.28709	-10.4644	-5.0834	36.776	19.5563	59.521	0.194438	7.03891	23.7675	-20.0496
NO ₂ avg	47.02037	12.46567	-9.16594	-1.38554	96.33217	24.00037	120.3323	0.16011	9.997463	38.1982	-18.0196
NO ₂ max	49.2679	13.544	-7.98835	1.09198	123.31	30.4303	143.588	0.199184	10.5319	48.2574	-15.994
NO ₂ min	44.2047	11.8748	-10.4366	-2.98798	80.396	20.2786	106.583	0.121282	9.30699	31.0611	-20.0496

Table A-151. Styphnic acid minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	5.506558	24.97775	0	24.97775	11.24866	0	11.24866	0	2.439532	32.35052	16.35522
C max	7.15686	27.9173	0	27.9173	16.662	0	16.662	0	3.2988	35.005	23.6584
C min	4.20603	18.9748	0	18.9748	0.724968	0	0.724968	0	0.560934	27.4529	9.44151
H avg	3.252853	30.0199	0	30.0199	19.37069	0	19.37069	0	3.597567	36.5292	20.72017
H max	6.28104	33.9798	0	33.9798	25.8365	0	25.8365	0	4.35119	41.3673	23.6383
H min	1.71787	22.3067	0	22.3067	8.02326	0	8.02326	0	2.25148	26.9126	14.9492
O avg	18.00145	14.94415	-5.43164	9.38203	88.42865	11.6106	100.0391	0.102593	10.4863	36.30015	-12.4109
O max	18.0073	14.9784	-5.41212	9.4117	89.2938	11.6836	100.977	0.102868	10.528	36.4953	-12.4046
O min	17.9956	14.9099	-5.45115	9.35236	87.5635	11.5376	99.1011	0.102317	10.4446	36.105	-12.4172
N - nitro avg	3.32445	23.25047	-3.77229	22.81897	32.2992	15.8875	48.1867	0.132469	4.715927	30.502	-8.69435
N - nitro max	4.01741	28.5534	0	28.5534	40.2344	37.4502	60.5469	0.23595	5.02036	34.8218	1.66729
N - nitro min	2.00532	12.8285	-5.9956	11.8632	23.0967	0	33.5665	0	4.33729	21.9528	-18.0277
O - nitro avg	21.83168	9.40408	-9.50369	-2.76339	47.44823	21.86035	69.30858	0.205706	8.347445	26.37748	-17.3878
O - nitro max	22.6897	12.9473	-7.9076	3.59478	77.0233	26.2321	96.3842	0.244898	10.6631	34.1535	-14.8525
O - nitro min	20.4642	6.02275	-12.6448	-10.2198	19.6016	19.3609	45.7373	0.160523	6.30246	18.0597	-21.5041
NO ₂ avg	46.98783	11.81906	-9.4981	-1.18959	75.69533	21.95423	97.64927	0.175615	9.808313	30.502	-17.7077
NO ₂ max	47.3712	13.8916	-7.90904	2.85983	99.2485	26.3321	118.879	0.249372	11.1005	34.8218	-15.8076
NO ₂ min	46.793	7.74007	-12.6239	-9.25497	29.1098	19.6309	55.4418	0.137864	7.22734	21.9528	-21.5041

Table A-152. Tetryl minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	4.944366	29.20317	0	29.20317	52.00689	0	52.00689	0	5.834306	40.19764	10.94484
C max	7.0639	30.5122	0	30.5122	133.237	0	133.237	0	10.4766	43.5228	20.9262
C min	2.45683	27.5891	0	27.5891	14.1147	0	14.1147	0	3.1188	37.5815	3.83597
H avg	7.780326	27.75374	0	27.75374	26.16468	0	26.16468	0	4.23545	36.41248	14.39294
H max	8.88565	37.1784	0	37.1784	37.0592	0	37.0592	0	5.02744	43.893	31.265
H min	6.23276	21.8045	0	21.8045	11.3637	0	11.3637	0	2.88029	30.3275	3.68662
N avg	0.404186	19.1427	0	19.1427	67.3146	0	67.3146	0	6.06798	39.1315	9.1083
N max	0.404186	19.1427	0	19.1427	67.3146	0	67.3146	0	6.06798	39.1315	9.1083
N min	0.404186	19.1427	0	19.1427	67.3146	0	67.3146	0	6.06798	39.1315	9.1083
N - nitro avg	2.641623	24.96413	-6.2591	23.64956	60.0227	12.05904	72.08165	0.082505	7.267145	34.58143	-10.0488
N - nitro max	3.86132	32.2507	-1.16905	31.9572	128.595	30.9537	145.846	0.224904	10.5667	42.6154	-1.41754
N - nitro min	1.59332	10.2677	-8.25677	6.10915	16.0586	0	37.6896	0	5.21758	17.6161	-19.0135
O - nitro avg	21.33153	9.216055	-9.95251	-4.15432	54.16074	25.5175	79.67826	0.173058	8.440711	29.56073	-18.3246
O - nitro max	23.2128	12.4664	-6.30508	2.80811	89.3933	46.229	103.388	0.223758	9.5975	39.3844	-13.056
O - nitro min	17.4659	3.76287	-15.1015	-13.093	8.31401	13.0884	54.543	0.117038	6.86931	13.1589	-25.7461
NO ₂ avg*	46.0701	13.89697	-8.29924	0.975188	118.79	19.4704	138.2603	0.120138	10.83543	40.23653	-16.174
NO ₂ max*	49.8477	14.57	-7.10218	2.17916	122.969	23.258	140.413	0.140677	11.3657	42.6154	-14.0524
NO ₂ min*	42.4178	13.0858	-9.21428	-0.54969	114.071	14.0701	137.039	0.09213	10.5378	38.3019	-17.7102
NO ₂ avg	45.30468	11.96467	-9.93243	-2.33406	94.66913	25.7621	120.4312	0.145649	10.01987	34.70803	-18.5671
NO ₂ max	49.8477	14.57	-7.10218	2.17916	122.969	44.6372	140.413	0.222182	11.3657	42.6154	-14.0524
NO ₂ min	42.4178	6.16777	-14.832	-12.2618	22.3065	14.0701	66.9437	0.09213	7.57317	18.1225	-25.7461

* These statistics do not include the nitrate ester moiety.

Table A-153. Tri245 minimum, maximum and average atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
C avg	4.623313	33.42927	0	33.42927	21.88507	0	21.88507	0	3.588547	42.28763	14.18546
C max	5.15432	36.9116	0	36.9116	23.9153	0	23.9153	0	3.87487	44.7031	20.1763
C min	4.26824	28.4875	0	28.4875	18.3972	0	18.3972	0	3.07155	39.4678	4.12148
H avg	5.06744	54.9669	0	54.9669	49.3049	0	49.3049	0	5.95962	67.7679	38.8893
H max	5.06744	54.9669	0	54.9669	49.3049	0	49.3049	0	5.95962	67.7679	38.8893
H min	5.06744	54.9669	0	54.9669	49.3049	0	49.3049	0	5.95962	67.7679	38.8893
N avg	12.37085	27.6468	-5.4982	21.22094	50.63885	14.78265	65.42135	0.091467	7.78122	44.68245	7.7074
N max	15.331	39.8834	0	39.8834	93.099	29.5653	122.664	0.182933	13.3119	49.3279	33.7782
N min	9.4107	15.4102	-10.9964	2.55848	8.17869	0	8.17869	0	2.25054	40.037	-18.3634
N - nitro avg	3.921117	28.65713	-7.28701	28.26367	58.50737	19.10583	77.6132	0.148795	6.371073	39.91127	-11.9047
N - nitro max	4.25004	31.9041	-6.32671	31.6843	67.1209	39.2821	81.5085	0.249674	6.8229	44.582	-9.54316
N - nitro min	3.44189	22.2736	-7.98757	21.7319	42.2264	3.9857	70.1605	0.053581	5.81019	32.6048	-15.9569
O - nitro avg	22.58278	10.97834	-9.1629	-2.13366	70.03798	17.31632	87.35428	0.164711	8.81245	32.3363	-16.1264
O - nitro max	23.7624	14.1096	-6.40863	5.41426	116.417	23.905	131.773	0.237695	11.0341	43.4757	-12.8872
O - nitro min	20.8935	8.28512	-12.122	-8.43997	35.2045	13.5469	57.6249	0.096563	7.27535	24.4509	-19.562
NO ₂ avg	49.0867	14.76503	-9.38157	0.15913	120.6244	18.28007	138.9043	0.119226	11.4036	40.1993	-17.0178
NO ₂ max	50.7837	16.0243	-8.14319	3.43945	142.779	23.2428	159.014	0.177856	12.3374	44.582	-15.0508
NO ₂ min	48.0097	12.5662	-11.8478	-5.50541	77.2001	15.3621	100.443	0.088145	9.916	32.6048	-19.562

Table A-154. BTAT minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	1.554201	31.33235	0	31.33235	27.38072	0	27.38072	0	4.284458
C max	3.206	36.9868	0	36.9868	63.4085	0	63.4085	0	7.62366
C min	0.033097	24.2453	0	24.2453	7.83808	0	7.83808	0	2.37849
H avg	5.783303	33.31158	0	33.31158	24.88872	0	24.88872	0	3.881248
H max	7.64329	38.4677	0	38.4677	42.3461	0	42.3461	0	5.44185
H min	4.62579	25.6805	0	25.6805	12.7691	0	12.7691	0	2.74496
N	11.50885	16.85175	-5.85334	9.806468	50.6986	12.84455	63.54317	0.122463	8.722528
N	16.8077	25.6823	0	25.6823	70.0623	23.7298	85.0344	0.219961	11.0855
N	6.51338	11.3751	-9.47595	0.39815	26.2135	0	26.2135	0	4.1599
N - nitro avg	1.37994	23.0566	-2.40002	22.71432	76.70543	8.89E-16	76.70543	1.36E-17	7.235812
N - nitro max	1.69239	31.7479	0	31.0788	131.36	2.67E-15	131.36	6.13E-17	10.0977
N - nitro min	0.908297	15.1526	-5.81137	14.4651	19.6883	0	19.6883	0	3.79613
O - nitro avg	19.92623	8.392386	-5.69104	-0.13119	49.00815	8.388345	57.39651	0.134229	6.370357
O - nitro max	21.8738	11.7368	-4.42993	6.34358	85.6469	12.2849	91.8921	0.212374	8.7345
O - nitro min	17.1401	6.05677	-7.23978	-5.08712	21.054	6.0737	30.3383	0.062735	4.39559

Table A-155. CL16 minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	4.16199	32.12468	0	32.12468	18.69023	0	18.69023	0	3.213723
C max	4.59395	36.562	0	36.562	34.9888	0	34.9888	0	4.44846
C min	3.70026	30.0268	0	30.0268	9.44897	0	9.44897	0	2.32398
N - azide avg	15.11619	24.47917	0	24.47917	65.71637	0	65.71637	0	6.479573
N - azide max	25.3835	36.993	0	36.993	78.4346	0	78.4346	0	7.55546
N - azide min	7.61356	14.0766	0	14.0766	50.5783	0	50.5783	0	5.3778
N - nitro avg	0.923081	19.17112	-4.14261	18.43728	84.35648	1.532699	85.8892	0.033652	7.454862
N - nitro max	1.2625	32.5603	-1.93238	32.0685	257.034	3.38711	257.034	0.087993	14.6595
N - nitro min	0.410657	12.6885	-7.51283	11.7595	30.3897	0	33.6728	0	5.09316
O - nitro avg	20.59287	7.972734	-5.66322	-0.26725	46.52029	11.15305	57.67332	0.16258	6.469506
O - nitro max	21.5987	11.0518	-3.92733	4.26033	110.624	14.7992	117.605	0.201383	8.37277
O - nitro min	18.9043	6.49503	-6.96881	-2.65886	31.0465	5.38221	40.9166	0.055838	5.6006

Table A-156. DNBf minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	6.252548	27.72807	0	27.72807	6.540238	0	6.540238	0	1.865787
C max	7.95465	31.5091	0	31.5091	21.1612	0	21.1612	0	3.77935
C min	4.70085	25.1923	0	25.1923	1.62509	0	1.62509	0	1.02429
H avg	7.142095	26.7919	0	26.7919	15.50215	0	15.50215	0	3.15224
H max	7.78552	29.5419	0	29.5419	16.808	0	16.808	0	3.18426
H min	6.49867	24.0419	0	24.0419	14.1963	0	14.1963	0	3.12022
N avg	10.21073	20.6596	-6.73575	12.20777	39.78105	29.8016	69.58285	0.124911	7.254015
N max	15.5383	30.1613	0	30.1613	62.8824	59.6032	122.486	0.249821	11.3503
N min	4.88316	11.1579	-13.4715	-5.74576	16.6797	0	16.6797	0	3.15773
O avg	19.95065	9.07961	-2.72784	4.55179	60.15975	3.385378	63.5451	0.049166	7.01471
O max	24.4278	10.0199	-0.64611	6.79543	65.16	6.52565	65.4051	0.094598	7.58883
O min	15.4735	8.13932	-4.80956	2.30815	55.1595	0.245105	61.6851	0.003733	6.44059
N - nitro avg	4.098185	25.0765	-6.99949	24.3894	37.1141	26.5065	63.6206	0.215112	5.41481
N - nitro max	4.21694	26.7748	-6.21978	25.9025	38.5135	41.9375	80.451	0.249547	5.45257
N - nitro min	3.97943	23.3782	-7.7792	22.8763	35.7147	11.0755	46.7902	0.180676	5.37705
O - nitro avg	22.03023	9.062835	-11.5646	-5.67352	40.52888	31.53718	72.06605	0.234254	8.836515
O - nitro max	22.7321	9.82963	-8.04735	-0.68735	49.5751	42.6722	74.6939	0.249999	9.03598
O - nitro min	20.7272	8.12656	-17.5615	-13.9788	32.0217	20.8571	69.3818	0.208437	8.67224

Table A-157. HNS minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.17635	26.05281	0	26.05281	14.2459	0	14.2459	0	2.824163
C max	7.55091	28.937	0	28.937	40.0832	0	40.0832	0	5.39131
C min	1.53223	20.1313	0	20.1313	3.91372	0	3.91372	0	1.52156
H avg	7.232245	25.15737	0	25.15737	22.22678	0	22.22678	0	3.81913
H max	8.30053	27.636	0	27.636	30.6359	0	30.6359	0	4.76878
H min	6.3495	21.8932	0	21.8932	10.3916	0	10.3916	0	2.61787
N - nitro avg	3.076995	27.61005	-8.32448	27.3726	43.43075	6.2612	49.69193	0.041299	5.344888
N - nitro max	3.96943	28.6492	0	28.0852	50.3698	37.5672	82.9281	0.247792	5.73389
N - nitro min	1.48381	26.7561	-18.4695	26.7561	32.8538	0	32.8538	0	4.66996
O - nitro avg	20.08658	9.686787	-10.3906	-3.70206	48.69641	33.25136	81.94772	0.238382	9.264165
O - nitro max	22.7178	11.5263	-8.37437	-2.46899	59.8006	48.6527	108.453	0.248126	12.0586
O - nitro min	13.6504	8.06444	-13.6302	-5.94233	39.4147	24.5334	69.7098	0.222546	7.75892

Table A-158. Methyl picrate minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.906243	23.86942	0	23.86942	9.290087	0	9.290087	0	2.337698
C max	7.2794	25.7276	0	25.7276	14.1533	0	14.1533	0	2.99635
C min	3.65128	21.9098	0	21.9098	3.76078	0	3.76078	0	1.69435
H avg	8.19077	18.86688	0	18.86688	18.65728	0	18.65728	0	3.515126
H max	11.4857	20.8612	0	20.8612	20.8549	0	20.8549	0	3.91282
H min	6.57764	17.4311	0	17.4311	15.1493	0	15.1493	0	3.17438
O avg	10.1692	8.15887	-3.12515	2.60829	45.2059	1.97796	47.1838	0.040163	5.99719
O max	10.1692	8.15887	-3.12515	2.60829	45.2059	1.97796	47.1838	0.040163	5.99719
O min	10.1692	8.15887	-3.12515	2.60829	45.2059	1.97796	47.1838	0.040163	5.99719
N - nitro avg	3.745587	23.95283	-6.52905	23.54063	37.59493	25.92574	63.52067	0.187223	5.173237
N - nitro max	3.97247	24.1523	-2.63427	23.8189	41.7889	40.0837	81.8726	0.249892	5.61823
N - nitro min	3.62628	23.6456	-9.64975	23.2541	32.2523	2.76491	41.5085	0.062174	4.66091
O - nitro avg	21.3359	8.480705	-10.1525	-4.85227	39.1887	29.1498	68.33853	0.242781	8.224027
O - nitro max	22.6545	8.55045	-9.22212	-3.68623	44.1291	32.8877	72.363	0.249984	8.55871
O - nitro min	18.8223	8.36455	-10.9894	-5.72835	33.4108	26.3293	65.5746	0.237938	8.04359

Table A-159. Picryl azide minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.991242	25.98177	0	25.98177	14.69075	0	14.69075	0	2.671918
C max	7.31165	28.8919	0	28.8919	27.5324	0	27.5324	0	3.74975
C min	4.53332	23.4372	0	23.4372	2.80602	0	2.80602	0	1.38651
H avg	6.669145	22.89675	0	22.89675	19.65165	0	19.65165	0	3.749585
H max	6.88214	23.5451	0	23.5451	22.6386	0	22.6386	0	4.08273
H min	6.45615	22.2484	0	22.2484	16.6647	0	16.6647	0	3.41644
N - azide avg	15.05195	17.41297	-1.28627	15.98514	58.41517	0.845497	59.26063	0.014536	6.579303
N - azide max	25.905	28.094	0	28.094	63.8054	1.81457	64.5273	0.032545	7.20681
N - azide min	7.50104	10.4261	-2.47913	6.63452	52.0638	0	53.8783	0	6.10872
N - nitro avg	3.635163	26.70347	-9.16787	26.36613	50.63087	21.5395	72.1704	0.155869	5.766373
N - nitro max	4.12553	30.9514	-6.95488	30.5685	66.3566	42.0528	87.114	0.249751	6.45267
N - nitro min	3.23628	24.3804	-11.0349	24.1181	39.4788	1.80841	47.8656	0.036354	5.04734
O - nitro avg	21.69258	8.975077	-9.18795	-3.50666	44.46288	24.37358	68.83647	0.224251	8.131003
O - nitro max	22.8911	10.0177	-7.83067	-1.28373	54.8408	31.0346	74.2571	0.247751	8.72622
O - nitro min	18.2073	8.30671	-10.4972	-4.82807	37.5383	19.4163	61.2859	0.193105	7.06123

Table A-160. Styphnic acid minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² ₊ ([kcal/mol] ²)	σ ² ₋ ([kcal/mol] ²)	σ ² _{total} ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	5.506558	24.90238	0	24.90238	10.88715	0	10.88715	0	2.39434
C max	7.15686	27.7052	0	27.7052	16.5513	0	16.5513	0	3.30194
C min	4.20603	18.8896	0	18.8896	0.72009	0	0.72009	0	0.551797
H avg	3.252853	30.18073	0	30.18073	19.70406	0	19.70406	0	3.624297
H max	6.28104	34.1338	0	34.1338	25.8465	0	25.8465	0	4.34112
H min	1.71787	22.3804	0	22.3804	8.13229	0	8.13229	0	2.25554
O avg	18.00145	15.1644	-5.41509	9.72059	86.39775	11.37575	97.7735	0.102813	10.4661
O max	18.0073	15.1907	-5.39629	9.76842	86.8278	11.3848	98.1945	0.103268	10.4846
O min	17.9956	15.1381	-5.43389	9.67276	85.9677	11.3667	97.3525	0.102357	10.4476
N - nitro avg	3.32445	23.44313	-4.41376	23.06477	28.85677	18.15187	47.00863	0.134198	4.437933
N - nitro max	4.01741	28.7373	0	28.7373	32.8215	44.4546	67.1009	0.223593	4.64267
N - nitro min	2.00532	12.9431	-7.04527	12.1061	22.6463	0	31.1025	0	4.12306
O - nitro avg	21.83168	9.667253	-9.52536	-2.5191	48.27465	21.80107	70.07572	0.203791	8.475525
O - nitro max	22.6897	13.2963	-7.9003	4.00107	77.7686	26.2666	97.0827	0.244627	10.8462
O - nitro min	20.4642	5.97501	-12.7615	-10.4092	19.1892	19.3141	45.2875	0.159366	6.21244

Table A-161. Tetryl minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ ⁺ ESP (kcal/mol)	Σ ⁻ ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	4.944366	29.21907	0	29.21907	51.96457	0	51.96457	0	5.834777
C max	7.0639	30.5404	0	30.5404	135.297	0	135.297	0	10.539
C min	2.45683	27.646	0	27.646	14.3395	0	14.3395	0	3.15075
H avg	7.780326	27.85196	0	27.85196	25.77654	0	25.77654	0	4.205372
H max	8.88565	37.2853	0	37.2853	35.0313	0	35.0313	0	4.87963
H min	6.23276	21.8713	0	21.8713	11.7038	0	11.7038	0	2.93897
N avg	0.404186	19.0472	0	19.0472	77.7527	0	77.7527	0	6.61818
N max	0.404186	19.0472	0	19.0472	77.7527	0	77.7527	0	6.61818
N min	0.404186	19.0472	0	19.0472	77.7527	0	77.7527	0	6.61818
N - nitro avg	2.641623	24.86755	-6.32449	23.47356	62.23	12.80385	75.03393	0.081055	7.449953
N - nitro max	3.86132	31.9812	-1.12523	31.5561	127.236	33.9922	144.435	0.218744	10.4817
N - nitro min	1.59332	10.1679	-8.7918	5.67384	16.2332	0	42.4058	0	5.33063
O - nitro avg	21.33153	9.186888	-9.92175	-4.19483	54.008	25.30134	79.30938	0.173448	8.393406
O - nitro max	23.2128	12.2298	-6.17997	2.70057	89.7635	46.0499	103.567	0.22107	9.73042
O - nitro min	17.4659	3.98971	-15.0249	-12.9951	9.48262	12.4002	55.5326	0.115518	6.90017

Table A-162. Tri245 minimum, maximum and average area weighted atom specific Politzer parameters using PBE/6-31G**.

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)
C avg	4.623313	33.4348	0	33.4348	21.67057	0	21.67057	0	3.550677
C max	5.15432	37.0733	0	37.0733	23.4316	0	23.4316	0	3.7995
C min	4.26824	28.3638	0	28.3638	19.4965	0	19.4965	0	3.1296
H avg	5.06744	55.0434	0	55.0434	50.2511	0	50.2511	0	6.03119
H max	5.06744	55.0434	0	55.0434	50.2511	0	50.2511	0	6.03119
H min	5.06744	55.0434	0	55.0434	50.2511	0	50.2511	0	6.03119
N avg	12.37085	27.7528	-5.60325	21.31643	50.42228	14.66635	65.08878	0.091249	7.92578
N max	15.331	39.6534	0	39.6534	92.791	29.3327	122.124	0.182498	13.6508
N min	9.4107	15.8522	-11.2065	2.97945	8.05356	0	8.05356	0	2.20076
N - nitro avg	3.921117	28.8995	-8.15615	28.53223	54.8121	18.58241	73.39453	0.145662	6.18414
N - nitro max	4.25004	32.4296	-6.35656	32.2585	61.775	39.7581	83.7757	0.249354	6.45158
N - nitro min	3.44189	22.1368	-9.24453	21.6312	44.0176	2.24164	64.0167	0.03379	5.88311
O - nitro avg	22.58278	11.14259	-9.22267	-1.95384	70.24053	17.45587	87.69647	0.165151	8.946827
O - nitro max	23.7624	14.2569	-6.63902	5.78945	115.973	24.3637	131.261	0.236842	11.1315
O - nitro min	20.8935	8.31779	-12.1317	-8.62779	36.1519	14.1246	57.8697	0.100093	7.19476

A.16 PBE/6-31G** Explicit X-N_{nitro} Fitting And Test Set Data

Table A-163. Non-aromatic fitting set Politzer parameters for explicit X-N subgroups of the X-NO₂ nitro groups using PBE/6-31G**.

Molecule	X	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
FOX7 ^a	C	8,9,12	12.9597	10.61	-5.57915	8.54582	28.4908	29.8147	58.3055	2.50E-01	5.70068	25.1223	-30.8277
HMX ^b	N	7,8	5.36656	16.8504	-6.02867	15.8756	36.8927	30.9556	67.8483	0.248086	5.64632	31.4677	-22.8715
HMX	N	9,10	5.00453	36.2632	-7.28288	36.1532	53.1659	0	53.1659	0	5.06045	50.7881	-7.28288
HMX	N	15,18	4.89504	36.3971	-5.18909	36.0764	48.4685	10.3445	58.813	0.144951	5.11257	50.202	-9.00915
HMX	N	21,,26	5.33175	17.4638	-7.94754	16.57	35.6958	48.5929	84.2886	0.244147	5.4524	34.8437	-22.7604
PETN ^c	O	5,6	12.6436	19.3678	-3.14905	19.1357	107.916	9.08018	116.996	0.071588	9.19064	37.1661	-8.02961
PETN	O	18,21	12.6409	19.4197	-0.53721	19.1916	106.632	0.160036	106.792	0.001496	9.11681	37.185	-1.09375
PETN	O	19,22	12.5037	19.5361	-0.40275	19.2831	106.01	0.188618	106.199	0.001773	9.10194	37.2025	-1.41252
PETN	O	20,23	12.4559	19.4895	-0.49354	19.3045	107.341	0.125283	107.466	0.001164	9.11127	37.323	-1.27384
EDNA ^d	N	5,6	12.5115	27.2438	-6.34031	26.8035	101.531	26.8703	128.401	0.165475	8.01311	56.7476	-17.7271
EDNA	N	12,14	12.52	27.089	-8.53075	26.6559	94.1576	57.8669	152.025	0.235754	7.77917	56.5901	-28.6502
NQ ^e	N	5,6	19.5432	3.62982	-16.8243	-13.1422	5.85882	126.382	132.241	0.042341	10.9345	9.42457	-45.4944
RDX ^f	N	10,13	6.99763	22.9387	-7.81245	22.3199	116.426	45.16	161.586	0.201371	9.85532	46.6585	-22.9179
RDX	N	11,14	8.68465	20.7576	-5.32611	20.4347	38.6784	20.9645	59.6429	0.227948	5.04591	40.2133	-15.0088
RDX	N	12,15	8.87226	21.2107	-9.81845	20.8291	39.3372	31.14	70.4772	0.246618	5.08611	40.2497	-19.5607
CL20 ^g	N	13,19	6.82375	29.3003	-1.90637	29.2329	27.4084	0	27.4084	0	3.94027	47.1642	-1.90637
CL20	N	14,20	7.16198	29.347	-9.7515	29.2646	29.9235	0	29.9235	0	4.13893	45.234	-9.7515
CL20	N	15,21	5.02623	34.561	-3.84695	34.3032	73.5512	9.81469	83.3659	0.10387	5.85233	49.033	-6.97979
CL20	N	16,22	3.95464	33.8899	0	33.8899	227.767	0	227.767	0	13.1172	65.1367	4.35241
CL20	N	17,23	4.91959	33.3521	-6.76957	33.233	87.6927	0	87.6927	0	7.49525	51.8348	-6.76957
CL20	N	18,24	4.59973	32.5326	-1.4326	32.2838	168.692	0.137071	168.83	0.000811	9.96122	64.9598	-1.80283

^a See figure A-1 for corresponding atom numbers.

^b See figure A-2 for corresponding atom numbers.

^c See figure A-3 for corresponding atom numbers.

^d See figure A-4 for corresponding atom numbers.

^e See figure A-5 for corresponding atom numbers.

^f See figure A-6 figure A-9 for corresponding atom numbers.

^g See figure A-7for corresponding atom numbers.

Table A-164. Aromatic fitting set Politzer parameters for explicit X-N subgroups of the X-NO₂ nitro groups using PBE/6-31G**.

Molecule	X	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
HNB ^a	C	1,4	4.70787	37.7858	0	37.7858	77.6575	0	77.6575	0	6.08709	51.88	7.76982
HNB	C	2,5	4.70906	37.8229	-0.9946	37.7049	75.6725	0	75.6725	0	6.01489	51.8605	-0.9946
HNB	C	3,6	4.55999	37.9925	0	37.9925	69.6134	0	69.6134	0	5.56262	51.4539	4.86132
HNB	C	13,16	4.59325	37.3519	0	37.3519	87.5985	0	87.5985	0	6.50948	50.9519	2.59914
HNB	C	14,17	4.74429	37.4058	-0.49009	37.294	78.5898	0	78.5898	0	6.16364	51.479	-0.49009
HNB	C	15,18	4.72262	37.8058	0	37.8058	71.7006	0	71.7006	0	5.673	51.4213	0.062123
TATB ^b	C	1,13	10.4085	20.7783	-3.01727	20.689	12.4721	1.60459	14.0767	0.100996	2.35502	28.5548	-4.59149
TATB	C	3,15	10.4104	19.1422	-6.61646	18.778	10.9279	21.9977	32.9257	0.221742	2.43878	24.5212	-15.7423
TATB	C	5,17	10.4456	20.3131	-10.0442	20.0811	10.068	56.7443	66.8124	0.127983	2.23711	23.8278	-21.5669
PNA ^c	C	2,7	7.8488	33.6238	0	33.6238	51.4415	0	51.4415	0	5.50641	49.6774	7.73782
PNA	C	3,8	3.77692	27.1878	-3.21614	26.7071	42.1105	6.97422	49.0847	0.121897	4.77647	38.583	-6.28639
PNA	C	4,9	6.40724	24.9541	-2.64725	24.7713	41.6268	0.53618	42.163	0.012555	4.92955	37.7805	-3.2756
PNA	C	15,18	7.84199	33.4657	-7.69138	33.3915	54.59	0	54.59	0	5.67926	49.8594	-7.69138
PNA	C	16,19	3.78049	27.006	-5.25727	26.628	45.4114	18.9632	64.3746	0.207801	4.83921	38.6671	-11.2575
TNT ^d	C	10,7	8.39856	24.7712	-4.35856	24.4309	32.6099	18.3914	51.0014	0.23057	4.80385	37.0231	-12.5289
TNT	C	12,8	9.00302	23.735	-6.87813	23.5345	28.2619	24.9028	53.1647	0.249002	4.264	35.3256	-13.243
TNT	C	14,9	6.37213	22.9486	-5.23719	22.8576	35.8999	0	35.8999	0	4.55568	39.7151	-5.23719
TNA ^e	C	2,11	8.73642	28.2615	-11.8555	28.2615	34.0609	0	34.0609	0	4.30835	41.9327	-11.8555
TNA	C	3,12	3.74133	22.3919	-5.3184	20.8964	14.7579	7.57574	22.3336	0.224146	4.55744	32.3268	-11.6949
TNA	C	4,13	9.26348	23.7935	-9.42896	23.5302	22.7094	17.1309	39.8402	0.245098	3.72909	32.0789	-12.4642
TNA	C	6,14	10.3252	30.1952	-6.68078	30.0223	19.3649	19.6307	38.9957	0.249988	3.2904	37.0544	-13.1796
NTOf	C	1,8	8.39283	22.5202	-4.48293	22.2418	31.104	12.7579	43.8618	0.206262	4.65917	29.7509	-12.4994
DATB ^g	C	3,7	10.4943	19.7174	-7.68936	19.4195	13.0899	43.9435	57.0334	0.176837	2.97709	24.9818	-17.3682
DATB	C	5,8	10.5009	19.6585	-6.70852	19.3358	14.0147	34.2154	48.2302	0.206143	3.04087	24.9561	-18.4877
DATB	C	16,6	10.5779	22.6161	0	22.6161	9.18094	0	9.18094	0	2.07705	26.2945	5.71285

Table A-164. Aromatic fitting set Politzer parameters for explicit X-N subgroups of the X-NO₂ nitro groups using PBE/6-31G** (continued).

Molecule	X	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
Picric acid ^h	C	2,7	10.2987	31.4261	-0.62437	31.3869	21.4658	0	21.4658	0	3.59609	38.8861	-0.62437
Picric acid	C	4,8	10.2093	24.6921	-3.3486	24.4903	16.5183	1.90505	18.4233	0.092712	2.68883	30.1035	-5.50263
Picric acid	C	6,9	9.45199	24.6306	-4.21624	24.5589	23.9735	5.44326	29.4168	0.1508	3.63729	32.0369	-6.54932

^a See figure A-8 for corresponding atom numbers.

^b See figure A-9 for corresponding atom numbers.

^c See figure A-10 for corresponding atom numbers.

^d See figure A-11 for corresponding atom numbers.

^e See figure A-12 for corresponding atom numbers.

^f See figure A-13 figure A-9 for corresponding atom numbers.

^g See figure A-14 for corresponding atom numbers.

^h See figure A-15 for corresponding atom numbers.

Table A-165. Test set Politzer parameters for explicit X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	X	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
Non-aromatic													
BTAT ^a	C	6,17,18,19	4.38621	24.3169	-4.42175	24.0295	126.262	1.93104	128.193	0.014837	9.91268	45.4311	-5.81137
BTAT	C	10,20,21,22	4.01279	24.7897	-2.7783	24.4979	115.568	3.86387	119.432	0.031305	9.22733	43.322	-4.74397
Aromatic													
CL16 ^b	C	1,4	4.79412	26.9815	-4.98541	26.6172	58.7073	2.97068	61.678	0.045845	5.99418	39.8707	-7.79367
CL16	C	2,7	4.92608	28.8263	-2.36822	28.6521	42.0527	3.57707	45.6297	0.072248	5.05996	40.1399	-4.25953
CL16	C	3,8	5.40507	26.4832	-7.09619	26.3158	53.6397	0.55621	54.1959	0.010158	5.75715	39.2206	-7.84199
CL16	C	6,16	4.11092	28.2524	-2.1853	28.041	51.7734	0.654762	52.4282	0.012333	5.01953	40.1575	-2.99448
CL16	C	11,18	5.85645	34.3682	-3.52598	34.2756	101.636	0	101.636	0	7.46263	58.7142	-3.52598
CL16*	C	5,17	16.8462	25.2474	0	25.2474	97.2084	0	97.2084	0	8.09469	58.086	7.83446
DNBF ^c	C	3,8	9.65451	25.5963	-6.00129	25.3871	20.7475	29.2242	49.9717	0.242806	3.34964	32.3914	-17.5213
DNBF	C	5,7	10.1813	27.5156	-6.51399	27.1497	15.8318	8.93166	24.7635	0.230589	2.96101	33.5234	-11.5085
DNBF†	C	1,10	10.4211	30.9375	0	30.9375	8.58658	0	8.58658	0	1.97657	35.8641	12.2264
HNS ^d	C	2,11	9.53935	28.2177	0	28.2177	20.3437	0	20.3437	0	2.91358	35.3307	0.597389
HNS	C	5,12	9.56713	27.7002	-10.0832	27.4665	22.086	42.2025	64.2885	0.225522	3.48817	35.2547	-15.3125
HNS	C	8,13	6.0027	26.7338	-11.127	26.6019	23.957	0	23.957	0	3.65606	37.3305	-11.127
HNS	C	23,26	9.77411	28.1174	0	28.1174	20.6641	0	20.6641	0	2.98002	35.1098	5.95695
HNS	C	24,28	5.92348	26.9258	-18.4695	26.7643	20.6607	0	20.6607	0	3.59976	37.2295	-18.4695
HNS	C	30,36	9.51801	28.0191	-15.6752	27.9279	16.967	0	16.967	0	3.12854	35.3589	-15.6752
Methyl picrate ^e	C	1,11	10.0546	23.9863	-10.1271	23.7989	15.3803	34.1774	49.5577	0.214033	2.83302	30.3834	-16.2989
Methyl picrate	C	3,7	9.18537	24.4517	-6.62876	24.2293	24.4035	32.242	56.6455	0.245213	3.79026	33.4519	-16.041
Methyl picrate	C	5,9	9.24439	24.4773	-2.32681	24.3233	22.9543	2.61754	25.5718	0.091883	3.6615	33.4827	-4.88202
Picryl azide ^f	C	2,7	10.2365	25.2471	-8.67239	25.113	19.8429	37.6959	57.5388	0.225932	2.86552	31.0611	-17.328
Picryl azide	C	3,8	8.40968	24.8817	-9.39413	24.7779	28.412	1.82273	30.2348	0.056652	4.00019	35.2761	-10.7442
Picryl azide	C	9,16	9.19774	29.9838	-7.02936	29.8265	45.8863	24.3708	70.2571	0.226554	5.21998	49.2187	-12.7805
Picryl azide*	C	6,14	16.2831	17.3003	-1.3181	16.7823	96.901	0.739118	97.6402	0.007513	8.49832	47.6844	-3.0453

Table A-165. Test set Politzer parameters for explicit X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	X	Atom(s) number	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
Styphnic acid ^g	C	1,12	10.2646	28.1604	0	28.1604	18.3166	0	18.3166	0	3.2371	35.005	1.66729
Styphnic acid	C	3,7	11.1049	20.9454	0	20.9454	14.2352	0	14.2352	0	3.0265	27.4529	9.44151
Styphnic acid	C	5,10	10.338	27.9723	-5.32128	27.8508	20.481	10.2123	30.6933	0.222018	3.43178	34.9843	-9.72263
Tetryl ^h	C	2,8	6.8292	30.576	-7.6575	30.486	53.279	0	53.279	0	6.08332	43.5228	-7.6575
Tetryl	C	4,9	9.48025	30.2911	-1.16905	30.1335	23.8133	0.031052	23.8444	0.001301	3.99527	38.3019	-1.41754
Tetryl	C	6,10	7.32411	27.4262	-7.95306	27.2713	93.5993	17.2514	110.851	0.131408	8.94729	39.7923	-12.1065
Tetryl [†]	N	7,11	1.99751	12.53	-8.25677	8.84199	44.0835	30.9537	75.0373	0.242346	7.44609	39.1315	-19.0135
tri245 ⁱ	C	1,13	9.22574	33.5199	-6.32671	33.3251	45.3862	14.0497	59.4359	0.180506	5.26515	44.7031	-10.214
tri245	C	2,6	7.88928	25.4007	-7.98757	25.101	39.8874	39.2821	79.1695	0.249985	5.22588	39.4678	-15.9569
tri245	C	4,10	8.51828	34.4694	-7.54674	34.3549	50.497	3.9857	54.4827	0.067804	5.63004	42.692	-9.54316

^a See figure A-16 for corresponding atom numbers.^b See figure A-17 for corresponding atom numbers.^c See figure A-18 for corresponding atom numbers.^d See figure A-19 for corresponding atom numbers.^e See figure A-20 for corresponding atom numbers.^f See figure A-21 figure A-9 for corresponding atom numbers.^g See figure A-22 for corresponding atom numbers.^h See figure A-23 for corresponding atom numbers.ⁱ See figure A-24 for corresponding atom numbers.

* Azide nitrogen.

[†] "NO₂" portion of the furazan-oxide moiety.[‡] Nitrate ester moiety

Table A-166. Fitting set average differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
FOX7	126	8.54582	58.3055	25.1223
HMX	29	26.1688	66.02895	41.82538
PETN	13	19.22873	109.3633	37.21915
EDNA	34	26.7297	140.213	56.66885
NQ	320	-13.1422	132.241	9.42457
RDX	28	21.19457	97.23537	42.37383
CL20	12	32.03457	104.1646	53.89375
Aromatic				
HNB	11	37.65582	76.80538	51.50777
TATB	490	19.84937	37.93827	25.6346
PNA	22	29.02434	52.33076	42.91348
TNT	98	23.60767	46.68867	37.3546
TNA	141	25.6776	33.8076	35.8482
NTO	291	22.2418	43.8618	29.7509
DATB	320	20.45713	38.14818	25.4108
Picric acid	64	26.81203	23.10197	33.6755

167. Test set average differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
BTAT	22	24.2637	123.8125	44.37655
Aromatic				
CL16	17	28.78034	63.11356	43.62058
DNBF	76	26.2684	37.3676	32.9574
HNS	54	27.51595	27.8135	35.93568
Methyl picrate	192	24.11717	43.925	32.43933
Picryl azide	19	26.57247	52.6769	38.51863
Stylphic acid	43	25.6522	21.0817	32.48073
Tetryl	25	29.29693	62.65813	40.539
tri245	68	30.927	64.3627	42.28763
Alternative set of X-N groups				
CL16*	17	28.19152	68.79603	46.03148
DNBF†	76	27.82477	27.77393	33.9263
Picryl azide*	19	24.12493	63.91773	40.81008
Tetryl‡	25	24.1832	65.75293	40.18713

* Includes azide nitrogen.

† Includes “NO₂” portion of the furazan-oxide moiety.

‡ Includes nitrate ester moiety.

Table A-168. Fitting set maximum differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
FOX7	126	8.54582	58.3055	25.1223
HMX	29	36.1532	84.2886	50.7881
PETN	13	19.3045	116.996	37.323
EDNA	34	26.8035	152.025	56.7476
NQ	320	-13.1422	132.241	9.42457
RDX	28	22.3199	161.586	46.6585
CL20	12	34.3032	227.767	65.1367
Aromatic				
HNB	11	37.9925	87.5985	51.88
TATB	490	20.689	66.8124	28.5548
PNA	22	33.6238	64.3746	49.8594
TNT	98	24.4309	53.1647	39.7151
TNA	141	30.0223	39.8402	41.9327
NT0	291	22.2418	43.8618	29.7509
DATB	320	22.6161	57.0334	26.2945
Picric acid	64	31.3869	29.4168	38.8861

Table A-169. Test set maximum differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
BTAT	22	24.4979	128.193	45.4311
Aromatic				
CL16	17	34.2756	101.636	58.7142
DNBF	76	27.1497	49.9717	33.5234
HNS	54	28.2177	64.2885	37.3305
Methyl picrate	192	24.3233	56.6455	33.4827
Picryl azide	19	29.8265	70.2571	49.2187
Stylphic acid	43	28.1604	30.6933	35.005
Tetryl	25	30.486	110.851	43.5228
tri245	68	34.3549	79.1695	44.7031
Alternative set of X-N groups				
CL16*	17	34.2756	101.636	58.7142
DNBF†	76	30.9375	49.9717	35.8641
Picryl azide*	19	29.8265	97.6402	49.2187
Tetryl‡	25	30.486	110.851	43.5228

* Includes azide nitrogen.

† Includes "NO₂" portion of the furazan-oxide moiety.

‡ Includes nitrate ester moiety.

Table A-170. Fitting set minimum differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
FOX7	126	8.54582	58.3055	25.1223
HMX	29	15.8756	53.1659	31.4677
PETN	13	19.1357	106.199	37.1661
EDNA	34	26.6559	128.401	56.5901
NQ	320	-13.1422	132.241	9.42457
RDX	28	20.4347	59.6429	40.2133
CL20	12	29.2329	27.4084	45.234
Aromatic				
HNB	11	37.294	69.6134	50.9519
TATB	490	18.778	14.0767	23.8278
PNA	22	24.7713	42.163	37.7805
TNT	98	22.8576	35.8999	35.3256
TNA	141	20.8964	22.3336	32.0789
NT0	291	22.2418	43.8618	29.7509
DATB	320	19.3358	9.18094	24.9561
Picric acid	64	24.4903	18.4233	30.1035

Table A-171. Test set minimum differences in Σ total, σ^2 total and V+ for explicit X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
BTAT	22	24.0295	119.432	43.322
Aromatic				
CL16	17	26.3158	45.6297	39.2206
DNBF	76	25.3871	24.7635	32.3914
HNS	54	26.6019	16.967	35.1098
Methyl picrate	192	23.7989	25.5718	30.3834
Picryl azide	19	24.7779	30.2348	31.0611
Stylphic acid	43	20.9454	14.2352	27.4529
Tetryl	25	27.2713	23.8444	38.3019
tri245	68	25.101	54.4827	39.4678
Alternative set of X-N groups				
CL16*	17	25.2474	45.6297	39.2206
DNBF†	76	25.3871	8.58658	32.3914
Picryl azide*	19	16.7823	30.2348	31.0611
Tetryl‡	25	8.84199	23.8444	38.3019

* Includes azide nitrogen.

† Includes “NO₂” portion of the furazan-oxide moiety.

‡ Includes nitrate ester moiety

A.17 PBE/6-31G** Additive X+N_{nitro} Fitting And Test Set Data

Table A-172. Non-aromatic fitting set Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
FOX7	126	8+(9+12)	23.46058	146.1792	65.9242
FOX7*	126	8+(9+12)/2	17.57779	82.73145	45.4712
HMX	29	8+7	31.1549	110.0711	59.1114
HMX	29	9+10	72.4568	88.01551	96.3673
HMX	29	15+18	72.2008	91.3287	100.0746
HMX	29	21+26	32.4025	124.916	60.8019
PETN	13	5+6	42.7695	140.4606	74.2463
PETN	13	18+21	42.9982	141.9923	74.2319
PETN	13	19+22	43.5648	133.9251	74.2494
PETN	13	20+23	43.656	135.4674	74.1785
EDNA	34	5+6	46.835	169.1005	89.3015
EDNA	34	12+14	47.1199	189.8812	89.5638
NQ	320	5+6	-21.0144	188.8102	17.13478
RDX	28	10+13	44.4141	268.067	84.2865
RDX	28	11+14	40.8818	106.3543	78.9463
RDX	28	12+15	41.5608	119.9612	79.4069
CL20	12	13+19	57.2716	58.1902	80.9016
CL20	12	14+20	57.5848	65.8444	79.8117
CL20	12	15+21	66.4002	148.9139	90.8578
CL20	12	16+22	69.1111	514.733	127.936
CL20	12	17+23	68.9728	126.6271	97.6148
CL20	12	18+24	64.2971	314.82	125.1166

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-173. Aromatic fitting set Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
HNB	11	1+4	62.146	83.6517	89.486
HNB	11	2+5	62.2139	91.7839	88.049
HNB	11	3+6	62.1819	94.9629	86.5235
HNB	11	13+16	60.8463	89.01	88.049
HNB	11	14+17	61.5925	100.6122	86.6622
HNB	11	15+18	62.005	80.9159	86.8768
TATB	490	1+13	40.8417	32.39041	56.2405
TATB	490	3+15	36.6618	47.59672	48.3346
TATB	490	5+17	39.4904	80.77266	47.5979
PNA	22	2+7	67.2151	125.1233	98.8239
PNA	22	3+8	32.20583	85.7968	59.3454
PNA	22	4+9	45.1162	48.93441	64.4358
PNA	22	15+18	66.6131	135.4349	98.696
PNA	22	16+19	30.19577	61.3408	54.2783
TNT	98	10+7	49.547	82.7068	73.9288
TNT	98	12+8	47.4347	83.1474	70.4743
TNT	98	14+9	48.5088	74.4265	76.1414
TNA	141	2+11	56.3903	82.8178	83.5159
TNA	141	3+12	20.15715	25.963	48.8203
TNA	141	4+13	46.3576	67.91159	63.6941
TNA	141	6+14	59.8598	64.70598	74.0517
NTO	291	1+8	44.4805	72.9519	59.4817
DATB	320	3+7	38.4465	74.74311	49.7829
DATB	320	5+8	38.1672	67.60924	49.7741
DATB	320	16+6	45.2083	23.94623	51.9891
Picric acid	64	2+7	63.0561	48.8836	77.5482
Picric acid	64	4+8	48.4909	40.76533	59.3404
Picric acid	64	6+9	48.7832	56.40815	63.8629

Table A-174. Test set Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic					
BTAT	22	6+(17+18+19)	104.4426	245.2201	149.1396
BTAT	22	10+(20+21+22)	103.8896	317.504	148.1242
BTAT ^a	22	6+(17+18+19)/3	60.39787	103.7715	79.17227
BTAT ^a	22	10+(20+21+22)/3	57.4894	151.9533	77.77913
Aromatic					
CL16	17	1+4	41.87	39.5002	66.5468
CL16	17	2+7	50.7157	71.0817	74.1904
CL16	17	3+8	46.0033	46.64858	67.0927
CL16	17	6+16	41.7903	56.6559	65.8935
CL16	17	11+18	66.7008	297.5541	116.7293
CL16 ^b	17	5+17	58.5953	96.6455	113.9005
DNBF	76	3+8	50.1142	70.2331	63.3138
DNBF	76	5+7	53.9479	45.75357	66.4821
DNBF ^c	76	1+10	61.7819	17.41849	71.1063
HNS	54	2+11	56.0704	47.01617	69.8663
HNS	54	5+12	54.7825	92.73783	69.491
HNS	54	8+13	53.393	75.4765	71.7663
HNS	54	23+26	55.7892	48.32084	69.0876
HNS	54	24+28	54.246	57.6758	73.3301
HNS	54	30+36	55.8402	39.24004	69.4383
Methyl picrate	192	1+11	47.3707	71.24539	60.0313
Methyl picrate	192	3+7	48.1786	86.68396	66.2744
Methyl picrate	192	5+9	48.4681	52.9969	66.4113
Picryl azide	19	2+7	49.8406	84.60766	61.3905
Picryl azide	19	3+8	49.4186	62.8768	70.1437
Picryl azide	19	9+16	59.8567	119.4405	97.4761
Picryl azide ^b	19	6+14	41.6613	87.0742	93.8208
Stylphic acid	43	1+12	56.4707	42.29103	69.8268
Stylphic acid	43	3+7	30.838	77.2089	49.4057
Stylphic acid	43	5+10	55.7781	59.11936	69.7157
Tetryl	25	2+8	61.7509	107.0337	86.1382
Tetryl	25	4+9	60.3537	51.8043	76.4677
Tetryl	25	6+10	54.0549	218.8242	78.5103
Tetryl ^d	25	7+11	25.25185	114.3269	56.7476
tri245	68	1+13	66.2635	105.0859	89.2851
tri245	68	2+6	50.2194	99.9057	72.0726
tri245	68	4+10	68.5959	93.5032	85.239

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes “NO₂” portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-175. Fitting set average differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
FOX7	126	23.46058	146.1792	65.9242
FOX7*	126	17.57779	82.73145	45.4712
HMX	29	52.05375	103.5828	79.0888
PETN	13	43.24713	137.9614	74.22653
EDNA	34	46.97745	179.4909	89.43265
NQ	320	-21.0144	188.8102	17.13478
RDX	28	42.28557	164.7942	80.8799
CL20	12	63.9396	204.8548	100.3731
Aromatic				
HNB	11	61.83093	90.1561	87.60775
TATB	490	38.99797	53.5866	50.72433
PNA	22	48.2692	91.32604	75.11588
TNT	98	48.49683	80.09357	73.51483
TNA	141	45.69121	60.34959	67.5205
NTO	291	44.4805	72.9519	59.4817
DATB	320	40.60733	55.43286	50.51537
Picric acid	64	53.4434	48.68569	66.91717

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-176. Test set average differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
BTAT	22	104.1661	281.3621	148.6319
BTAT ^a	22	58.94363	127.8624	78.4757
Aromatic				
CL16	17	49.41602	102.2881	78.09054
DNBF	76	52.03105	57.99334	64.89795
HNS	54	55.02022	60.07786	70.4966
Methyl picrate	192	53.57027	64.11607	68.85743
Picryl azide	19	53.03863	88.97499	76.33677
Stylphic acid	43	47.6956	59.53976	62.98273
Tetryl	25	58.71983	125.8874	80.37207
tri245	68	61.69293	99.49827	82.1989
Alternative set of X-N groups				
CL16 ^b	17	50.9459	101.3477	84.05887
DNBF ^c	76	55.28133	44.46839	66.9674
Picryl azide ^b	19	50.1943	88.49979	80.70778
Tetryl ^d	25	50.35284	122.9973	74.46595

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes “NO₂” portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-177. Fitting set maximum differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
FOX7	126	23.46058	146.1792
FOX7*	126	17.57779	82.73145
HMX	29	72.4568	124.916
PETN	13	43.656	141.9923
EDNA	34	47.1199	189.8812
NQ	320	-21.0144	188.8102
RDX	28	44.4141	268.067
CL20	12	69.1111	514.733
Aromatic			
HNB	11	62.2139	100.6122
TATB	490	40.8417	80.77266
PNA	22	67.2151	135.4349
TNT	98	49.547	83.1474
TNA	141	59.8598	82.8178
NTO	291	44.4805	72.9519
DATB	320	45.2083	74.74311
Picric acid	64	63.0561	56.40815

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-178. Test set maximum differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
BTAT	22	104.4426	317.504
BTAT ^a	22	60.39787	151.9533
Aromatic			
CL16	17	66.7008	297.5541
DNBF	76	53.9479	70.2331
HNS	54	56.0704	92.73783
Methyl picrate	192	48.4681	86.68396
Picryl azide	19	59.8567	119.4405
Stylphic acid	43	56.4707	77.2089
Tetryl	25	61.7509	218.8242
tri245	68	68.5959	105.0859
Alternative set of X-N groups			
CL16 ^b	17	66.7008	297.5541
DNBF ^c	76	61.7819	70.2331
Picryl azide ^b	19	59.8567	119.4405
Tetryl ^d	25	61.7509	218.8242

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes “NO₂” portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-179. Fitting set minimum differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
FOX7	126	23.46058	146.1792
FOX7*	126	17.57779	82.73145
HMX	29	31.1549	88.01551
PETN	13	42.7695	133.9251
EDNA	34	46.835	169.1005
NQ	320	-21.0144	188.8102
RDX	28	40.8818	106.3543
CL20	12	57.2716	58.1902
Aromatic			
HNB	11	60.8463	80.9159
TATB	490	36.6618	32.39041
PNA	22	30.19577	48.93441
TNT	98	47.4347	74.4265
TNA	141	20.15715	25.963
NTO	291	44.4805	72.9519
DATB	320	38.1672	23.94623
Picric acid	64	48.4909	40.76533

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-180. Test set minimum differences in Σ total, σ^2 total and V+ for additive X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
BTAT	22	103.8896	245.2201
BTAT ^a	22	57.4894	103.7715
Aromatic			
CL16	17	41.7903	39.5002
DNBF	76	50.1142	45.75357
HNS	54	53.393	39.24004
Methyl picrate	192	47.3707	52.9969
Picryl azide	19	49.4186	62.8768
Stylphic acid	43	30.838	42.29103
Tetryl	25	54.0549	51.8043
tri245	68	50.2194	93.5032
Alternative set of X-N groups			
CL16 ^b	17	41.7903	39.5002
DNBF ^c	76	50.1142	17.41849
Picryl azide ^b	19	41.6613	62.8768
Tetryl ^d	25	25.25185	51.8043

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes “NO₂” portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

A.18 PBE/6-31G** Difference X-N_{nitro} Fitting and Test Set Data

Table A-181. Non-aromatic fitting set Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
FOX7	126	8-(9+12)	-0.07058	-107.612	-15.8878
FOX7*	126	8-(9+12)/2	5.81221	-44.1641	4.5652
HMX	29	8-7	4.0325	-66.0603	3.824
HMX	29	9-10	5.954	-77.8785	-5.2089
HMX	29	15-18	6.2418	-79.5559	-0.3294
HMX	29	21-26	3.5793	-72.0228	8.8855
PETN	13	5-6	-11.2517	50.197	0.0859
PETN	13	18-21	-11.248	49.1209	0.1381
PETN	13	19-22	-11.939	53.5889	0.1556
PETN	13	20-23	-11.9144	54.8296	0.4675
EDNA	34	5-6	12.5132	6.5059	24.1937
EDNA	34	12-14	11.7569	-23.4568	23.6164
NQ	320	5-6	-8.09023	74.9918	1.71436
RDX	28	10-13	5.2069	-14.771	9.0305
RDX	28	11-14	-0.0332	-42.9413	1.4803
RDX	28	12-15	0.2736	-59.4024	1.0925
CL20	12	13-19	2.751	-13.62	13.4268
CL20	12	14-20	2.0724	-15.7974	10.6563
CL20	12	15-21	8.8846	-103.704	7.2082
CL20	12	16-22	2.5645	118.673	2.3374
CL20	12	17-23	8.533	-57.4855	6.0548
CL20	12	18-24	-1.0399	-85.486	4.803

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-182. Aromatic fitting set Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
HNB	11	1-4	19.7504	-48.9215	14.274
HNB	11	2-5	19.6445	-59.9463	15.672
HNB	11	3-6	19.1579	-61.0465	16.3843
HNB	11	13-16	21.0139	-58.5194	13.8548
HNB	11	14-17	19.5799	-67.7562	16.2958
HNB	11	15-18	19.5224	-50.9457	15.9658
TATB	490	1-13	1.8031	-24.5782	0.8691
TATB	490	3-15	3.2816	-43.4859	0.7078
TATB	490	5-17	2.5726	-77.7551	0.0577
PNA	22	2-7	0.1121	-76.8107	-0.5309
PNA	22	3-8	24.27937	-49.6316	17.8206
PNA	22	4-9	11.0782	-30.4658	11.1252
PNA	22	15-18	0.5933	-91.1451	-1.0228
PNA	22	16-19	26.12123	-24.379	23.0559
TNT	98	10-7	-3.259	-51.5994	-0.1174
TNT	98	12-8	-2.1481	-53.7564	0.1769
TNT	98	14-9	-6.0984	-41.4417	-3.2888
TNA	141	2-11	0.0717	-50.5996	-0.3495
TNA	141	3-12	24.78265	2.5596	15.8333
TNA	141	4-13	2.9718	-49.0892	0.4637
TNA	141	6-14	0.89	-49.8618	0.0571
NTO	291	1-8	2.6545	-32.7385	-0.0201
DATB	320	3-7	1.6417	-63.6377	0.1807
DATB	320	5-8	2.01	-56.7478	0.1381
DATB	320	16-6	0.0817	-19.071	-0.5999
Picric acid	64	2-7	-1.1477	-27.0266	0.224
Picric acid	64	4-8	2.3477	-36.2625	-0.8666
Picric acid	64	6-9	2.1556	-36.7633	-0.2109

Table A-183. Test set Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	sensitivity	Atom numbers	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic					
BTAT	22	6-(17+18+19)	-27.6916	-179.126	-60.7624
BTAT	22	10-(20+21+22)	-35.311	-179.148	-62.911
BTAT ^a	22	6-(17+18+19)/3	16.35313	-37.6771	9.204933
BTAT ^a	22	10-(20+21+22)/3	11.0892	-13.5975	7.434067
Aromatic					
CL16	17	1-4	18.382	-15.9466	13.1946
CL16	17	2-7	11.4499	-41.5813	6.0894
CL16	17	3-8	14.2135	-26.7486	11.3485
CL16	17	6-16	19.0557	-29.9035	14.4215
CL16	17	11-18	4.0044	-213.872	0.6991
CL16 ^b	17	5-17	14.9725	-34.1825	2.2715
DNBF	76	3-8	4.0402	-62.5957	1.469
DNBF	76	5-7	1.9691	-38.916	-0.5647
DNBF ^c	76	1-10	1.2641	-14.1041	-0.6219
HNS	54	2-11	1.8032	-38.9554	-0.7951
HNS	54	5-12	0.9013	-79.0432	-1.0184
HNS	54	8-13	-0.346	-50.4469	-2.8947
HNS	54	23-26	2.0008	-39.947	-1.132
HNS	54	24-28	-1.2072	-29.4598	-1.1289
HNS	54	30-36	0.076	-25.4174	-1.2795
Methyl picrate	192	1-11	1.0333	-62.6734	-0.7355
Methyl picrate	192	3-7	1.6732	-67.9468	-0.6294
Methyl picrate	192	5-9	1.1291	-31.5033	-0.5541
Picryl azide	19	2-7	1.9372	-79.2827	-0.7317
Picryl azide	19	3-8	1.1312	-38.953	-0.4085
Picryl azide	19	9-16	-1.4093	-56.9009	0.9613
Picryl azide ^b	19	6-14	15.9713	-35.9614	1.548
Stylphic acid	43	1-12	-0.6361	-24.842	0.1832
Stylphic acid	43	3-7	7.1116	-43.8849	5.5001
Stylphic acid	43	5-10	-0.3025	-41.774	0.2529
Tetryl	25	2-8	-2.1635	-8.5237	0.9074
Tetryl	25	4-9	-0.4675	-23.5749	-0.1361
Tetryl	25	6-10	1.8123	-72.8678	-1.0743
Tetryl ^d	25	7-11	13.03355	20.3023	21.5154
tri245	68	1-13	3.5139	-57.2553	0.1211
tri245	68	2-6	6.7556	-63.1113	6.863
tri245	68	4-10	5.2273	-46.8178	0.145

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes "NO₂" portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-184. Fitting set average differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
FOX7	126	-0.07058	-107.612	-15.8878
FOX7*	126	5.81221	-44.1641	4.5652
HMX	29	4.9519	-73.8794	1.7928
PETN	13	-11.5883	51.9341	0.211775
EDNA	34	12.13505	-8.47545	23.90505
NQ	320	-8.09023	74.9918	1.71436
RDX	28	1.815767	-39.0382	3.867767
CL20	12	3.960933	-26.2367	7.414417
Aromatic				
HNB	11	19.77817	-57.8559	15.40778
TATB	490	2.552433	-48.6064	0.544867
PNA	22	12.43684	-54.4864	10.0896
TNT	98	-3.83517	-48.9325	-1.07643
TNA	141	7.179038	-36.7478	4.00115
NTO	291	2.6545	-32.7385	-0.0201
DATB	320	1.244467	-46.4855	-0.0937
Picric acid	64	1.118533	-33.3508	-0.2845

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-185. Test set average differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)	V+ (kcal/mol)
Non-aromatic				
BTAT	22	-31.5013	-179.137	-61.8367
BTAT ^a	22	13.72117	-25.6373	8.3195
Aromatic				
CL16	17	13.4211	-65.6104	9.15062
DNBF	76	3.00465	-50.7559	0.45215
HNS	54	0.538017	-43.8783	-1.37477
Methyl picrate	192	0.4097	-47.8313	-1.36483
Picryl azide	19	0.553033	-58.3789	-0.05963
Stylphic acid	43	2.057667	-36.8336	1.978733
Tetryl	25	-0.2729	-34.9888	-0.101
tri245	68	5.1656	-55.7281	2.376367
Alternative set of X-N groups				
CL16 ^b	17	13.67967	-60.3724	8.0041
DNBF ^c	76	2.424467	-38.5386	0.094133
Picryl azide ^b	19	4.4076	-52.7745	0.342275
Tetryl ^d	25	3.053713	-21.166	5.3031

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes “NO₂” portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-186. Fitting set maximum differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
FOX7	126	-0.07058	-107.612
FOX7*	126	5.81221	-44.1641
HMX	29	6.2418	-66.0603
PETN	13	-11.248	54.8296
EDNA	34	12.5132	6.5059
NQ	320	-8.09023	74.9918
RDX	28	5.2069	-14.771
CL20	12	8.8846	118.673
Aromatic			
HNB	11	21.0139	-48.9215
TATB	490	3.2816	-24.5782
PNA	22	26.12123	-24.379
TNT	98	-2.1481	-41.4417
TNA	141	24.78265	2.5596
NTO	291	2.6545	-32.7385
DATB	320	2.01	-19.071
Picric acid	64	2.3477	-27.0266

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-187. Test set maximum differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
BTAT	22	-27.6916	-179.126
BTAT ^a	22	16.35313	-13.5975
Aromatic			
CL16	17	19.0557	-15.9466
DNBF	76	4.0402	-38.916
HNS	54	2.0008	-25.4174
Methyl picrate	192	1.6732	-31.5033
Picryl azide	19	1.9372	-38.953
Stylphic acid	43	7.1116	-24.842
Tetryl	25	1.8123	-8.5237
tri245	68	6.7556	-46.8178
Alternative set of X-N groups			
CL16 ^b	17	19.0557	-15.9466
DNBF ^c	76	4.0402	-14.1041
Picryl azide ^b	19	15.9713	-35.9614
Tetryl ^d	25	13.03355	20.3023

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes "NO₂" portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

Table A-188. Fitting set minimum differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
FOX7	126	-0.07058	-107.612
FOX7*	126	5.81221	-44.1641
HMX	29	3.5793	-79.5559
PETN	13	-11.939	49.1209
EDNA	34	11.7569	-23.4568
NQ	320	-8.09023	74.9918
RDX	28	-0.0332	-59.4024
CL20	12	-1.0399	-103.704
Aromatic			
HNB	11	19.1579	-67.7562
TATB	490	1.8031	-77.7551
PNA	22	0.1121	-91.1451
TNT	98	-6.0984	-53.7564
TNA	141	0.0717	-50.5996
NTO	291	2.6545	-32.7385
DATB	320	0.0817	-63.6377
Picric acid	64	-1.1477	-36.7633

* Averaged nitrogens as both NO₂ are on the same carbon.

Table A-189. Test set minimum differences in Σ total, σ^2 total and V+ for difference X-N subgroups of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Σ tot ESP (kcal/mol)	σ^2 tot ([kcal/mol] ²)
Non-aromatic			
BTAT	22	-35.311	-179.148
BTAT ^a	22	11.0892	-37.6771
Aromatic			
CL16	17	4.0044	-213.872
DNBF	76	1.9691	-62.5957
HNS	54	-1.2072	-79.0432
Methyl picrate	192	1.0333	-67.9468
Picryl azide	19	-1.4093	-79.2827
Stylphic acid	43	-0.6361	-43.8849
Tetryl	25	-2.1635	-72.8678
tri245	68	3.5139	-63.1113
Alternative set of X-N groups			
CL16 ^b	17	4.0044	-213.872
DNBF ^c	76	1.2641	-62.5957
Picryl azide ^b	19	-1.4093	-79.2827
Tetryl ^d	25	-2.1635	-72.8678

^a Averaged nitrogens as the three NO₂ are on the same carbon.

^b Includes azide nitrogen.

^c Includes "NO₂" portion of the furazan-oxide moiety.

^d Includes nitrate ester moiety.

A-19. PBE/6-31G** X of the X-N_{nitro} Fitting and Test Set Data

Table A-190. Aromatic fitting set averages Σ total, σ^2 total and V+ as well as maximum Σ total and V+ for the carbon of the X-NO₂ nitro group using PBE/6-31G**.

Molecule	Sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Average σ^2 tot ([kcal/mol] ²)	Average V+ (kcal/mol)	Maximum V+ (kcal/mol)	Maximum Σ tot ESP (kcal/mol)
HNB	11	40.80455	16.15008	51.50777	51.88	40.9482
TATB	490	20.7752	2.490097	25.6346	28.5548	21.3224
PNA	22	30.35302	18.4198	42.60274	49.1465	33.6636
TNT	98	22.33083	15.58053	36.2192	36.9057	23.144
TNA	141	26.43513	11.80092	35.76083	41.5832	30.3749
NTO	291	23.5675	20.1067	29.7308	29.7308	23.5675
DATB	320	20.9259	4.473693	25.21083	25.6946	22.645
Picric acid	64	27.28097	7.66746	33.31633	38.8861	30.9542

Table A-191. Aromatic test set averages and maximum Σ total, σ^2 total and V+ for the carbon of the X-NO₂ nitro or X-N₃ azide groups using PBE/6-31G**.

Molecule	Sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Average σ^2 tot ([kcal/mol] ²)	Average V+ (kcal/mol)	Maximum V+ (kcal/mol)	Maximum Σ tot ESP (kcal/mol)
CL16	17	31.41856	18.33886	43.62058	58.7142	35.3526
CL16 ^a	17	32.31278	20.48763	46.03148	58.7142	36.7839
DNBF	76	28.8529	2.964887	33.53077	35.2422	31.523
HNS	54	27.77912	8.099797	34.56092	36.1006	28.9368
Methyl picrate	192	24.64217	8.133783	31.79967	32.9286	24.9259
Picryl azide	19	26.79583	15.29805	38.13857	49.2187	29.2237
Picryl azide ^a	19	27.30095	17.86264	40.52503	49.2187	29.2237
Stylphic acid	43	24.87663	11.35306	32.48073	35.005	27.9173
Tetryl	25	29.22347	45.4493	40.13553	43.5228	29.9431
tri245	68	33.42927	21.88507	42.28763	44.7031	36.9116

^a Includes azide nitrogen.

Table A-192. Fitting and test set Politzer parameters for the aggregate aromatic carbons for aromatic species using PBE/6-31G** (figure A-155).

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
Training set											
HNB	23.6862	40.8031	0	40.8031	16.1747	0	16.1747	0	3.13985	51.88	31.4721
TATB	31.5023	21.0651	0	21.0651	2.60097	0	2.60097	0	1.25625	28.5548	16.9679
PNA	25.9533	31.93	0	31.93	30.0811	0	30.0811	0	4.53291	49.1465	20.155
TNT	33.796	22.0661	0	22.0661	24.1956	0	24.1956	0	3.78787	40.074	8.5699
TNA	32.1794	27.2467	0	27.2467	18.7099	0	18.7099	0	3.45259	41.5832	13.4664
NTO	7.14697	21.4704	0	21.4704	23.1762	0	23.1762	0	4.08072	29.7308	0.251004
DATB	34.4999	20.3194	0	20.3194	8.45494	0	8.45494	0	2.5087	25.6946	11.7865
Picric acid	37.0737	26.1898	0	26.1898	15.1299	0	15.1299	0	2.92859	38.8861	11.5951
Test set											
CL16	24.9719	32.4102	0	32.4102	28.3945	0	28.3945	0	3.95251	58.7142	22.2019
DNBF	37.5153	27.6339	0	27.6339	9.81834	0	9.81834	0	2.46614	35.2422	11.8599
HNS	69.3412	26.8103	0	26.8103	12.5702	0	12.5702	0	2.69056	37.1228	12.3412
Methyl picrate	35.4375	23.5708	0	23.5708	12.8724	0	12.8724	0	2.69737	32.9286	8.22853
Picryl azide	35.9474	25.8272	0	25.8272	19.6556	0	19.6556	0	2.97226	49.2187	9.83433
Styphnic acid	33.0393	25.1579	0	25.1579	18.3928	0	18.3928	0	2.99417	35.005	9.44151
Tetryl	31.011	29.0049	0	29.0049	43.7782	0	43.7782	0	5.44514	43.5228	3.83597
Tri245	13.8699	33.4671	0	33.4671	34.3022	0	34.3022	0	4.86649	44.7031	4.12148

Table A-193. Fitting and test set Politzer parameters for the aggregate aromatic members (carbon and nitrogen) for aromatic species using PBE/6-31G** (figure A-156).

Atom / group	Surface Area (Å ²)	Σ+ ESP (kcal/mol)	Σ- ESP (kcal/mol)	Σ total ESP (kcal/mol)	σ ² + ([kcal/mol] ²)	σ ² - ([kcal/mol] ²)	σ ² total ([kcal/mol] ²)	balance	Π (kcal/mol)	V+ (kcal/mol)	V- (kcal/mol)
Training set											
HNB	23.6862	40.8031	0	40.8031	16.1747	0	16.1747	0	3.13985	51.88	31.4721
TATB	31.5023	21.0651	0	21.0651	2.60097	0	2.60097	0	1.25625	28.5548	16.9679
PNA	25.9533	31.93	0	31.93	30.0811	0	30.0811	0	4.53291	49.1465	20.155
TNT	33.796	22.0661	0	22.0661	24.1956	0	24.1956	0	3.78787	40.074	8.5699
TNA	32.1794	27.2467	0	27.2467	18.7099	0	18.7099	0	3.45259	41.5832	13.4664
NTO	47.0102	19.6101	-10.5447	13.8022	50.9204	37.9212	88.8416	0.244648	11.1052	35.4066	-21.8718
DATB	34.4999	20.3194	0	20.3194	8.45494	0	8.45494	0	2.5087	25.6946	11.7865
Picric acid	37.0737	26.1898	0	26.1898	15.1299	0	15.1299	0	2.92859	38.8861	11.5951
Test set											
CL16	24.9719	32.4102	0	32.4102	28.3945	0	28.3945	0	3.95251	58.7142	22.2019
DNBF	37.5153	27.6339	0	27.6339	9.81834	0	9.81834	0	2.46614	35.2422	11.8599
HNS	69.3412	26.8103	0	26.8103	12.5702	0	12.5702	0	2.69056	37.1228	12.3412
Methyl picrate	35.4375	23.5708	0	23.5708	12.8724	0	12.8724	0	2.69737	32.9286	8.22853
Picryl azide	35.9474	25.8272	0	25.8272	19.6556	0	19.6556	0	2.97226	49.2187	9.83433
Styphnic acid	33.0393	25.1579	0	25.1579	18.3928	0	18.3928	0	2.99417	35.005	9.44151
Tetryl	31.011	29.0049	0	29.0049	43.7782	0	43.7782	0	5.44514	43.5228	3.83597
Tri245	38.6117	30.5923	-10.9964	22.1545	133.978	29.5653	163.543	0.148098	17.0667	49.3279	-18.3634

A.19 PBE/6-31G** Correlations From Fitting Set With Predictions of Test Set Data

Table A-194. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total (figure A-125) for the nitro nitrogens in nonaromatic species for both the training and test sets using PBE/6-31G**.

Molecule	Average Σ tot ESP (kcal/mol) for N	Predicted sensitivity (cm)	Experimental sensitivity (cm)	error	% error
Training set					
FOX7	5.88279	110.3	126	-15.66	-12.43
HMX	23.55093	21.7	29	-7.28	-25.12
PETN	27.4177	15.2	13	2.22	17.04
EDNA	17.4212	38.2	34	4.17	12.26
NQ	-6.46207	343.5	320	23.53	7.35
RDX	20.2349	29.5	28	1.46	5.23
CL20	29.98933	12.0	12	0.01	0.08
Test set					
BTAT	22.61123	26.9	22.1	4.78	21.62

Table A-195. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total (figure A-125) for the nitro nitrogens plus the associated aromatic carbon (the X-NO₂ nitrogen and carbon) for aromatic species for both the training and test sets using PBE/6-31G**.

Molecule	Average Σ tot ESP (kcal/mol) for C	Average Σ tot ESP (kcal/mol) for N	Total average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Experimental sensitivity (cm)	error	% error
Training set							
HNB	21.02638	40.80455	61.83093	9.3	11	-1.68	-15.25
TATB	18.22277	21.17005	39.39282	395.3	490	-94.72	-19.33
PNA	17.91618	31.61855	49.53473	72.7	22	50.67	230.30
TNT	26.166	22.20726	48.37326	88.2	98	-9.78	-9.98
TNA	19.25609	27.14712	46.4032	122.6	141	-18.41	-13.06
NT0	20.913	21.10035	42.01335	255.2	291	-35.82	-12.31
DATB	19.68143	20.65057	40.332	337.9	320	17.90	5.59
Picric acid	26.16243	26.54357	52.706	42.8	64	-21.21	-33.14
Test set							
CL16	32.31278	17.99746	50.31024	74.9	17	57.92	340.69
DNBF	27.71122	24.5132	52.22442	54.5	76	-21.48	-28.26
HNS	26.06654	27.2411	53.30764	45.5	54	-8.45	-15.65
Methyl picrate	23.93185	23.36363	47.29548	123.6	192	-68.43	-35.64
Picryl azide	26.16735	26.2428	52.41015	52.9	19	33.87	178.25
Styphnic acid	24.97775	22.81897	47.79672	113.7	43	70.71	164.43
Tetryl	29.20317	23.64956	52.85273	49.1	25	24.12	96.49
Tri245	33.42927	28.26367	61.69293	11.3	68	-56.68	-83.35

Table A-196. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total (figure A-126) for the groups in nonaromatic species for both the training and test sets using PBE/6-31G**.

Molecule	Average Σ tot ESP (kcal/mol) for NO ₂	Predicted sensitivity (cm)	Experimental sensitivity (cm)	error	% error
Training set					
FOX7	-18.5528	106.6582	126	-19.34	-15.35
HMX	-3.83427	21.44122	29	-7.56	-26.06
PETN	1.005616	12.6514	13	-0.35	-2.68
EDNA	-10.6115	44.88184	34	10.88	32.01
NQ	-28.3166	309.1693	320	-10.83	-3.38
RDX	-8.73759	36.59008	28	8.59	30.68
CL20	1.582096	11.88089	12	-0.12	-0.99
Test set					
BTAT	0.679089	13.10979	22.1	-8.99	-40.68

Table A-197. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total (figure A-126) for the nitro groups plus the associated aromatic carbon (the C-NO₂ group) for aromatic species for both the training and test sets using PBE/6-31G**.

Molecule	Average Σ tot ESP (kcal/mol) for C	Average Σ tot ESP (kcal/mol) for NO ₂	Total average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Experimental sensitivity (cm)	error	% error
Training set							
HNB	21.02638	3.533863	24.56025	34.04134	11	23.04	209.47
TATB	18.22277	-5.80814	12.41463	325.9228	490	-164.08	-33.49
PNA	17.91618	-0.84781	17.06837	137.1485	22	115.15	523.40
TNT	26.166	-2.38476	23.78124	39.34899	98	-58.65	-59.85
TNA	19.25609	-1.76303	17.49306	126.7317	141	-14.27	-10.12
NTD	20.913	-6.58316	14.32984	228.2477	291	-62.75	-21.56
DATB	19.68143	-4.19909	15.48234	184.2081	320	-135.79	-42.43
Picric acid	26.16243	-1.15916	25.00327	31.34872	64	-32.65	-51.02
Test set							
CL16	32.31278	0.286264	32.59905	7.632068	17	-9.37	-55.11
DNBF	27.71122	-2.73616	24.97506	31.51366	76	-44.49	-58.53
HNS	26.06654	-1.24657	24.81997	32.43595	54	-21.56	-39.93
Methyl picrate	23.93185	-3.04418	20.88767	67.40202	192	-124.60	-64.89
Picryl azide	26.16735	-1.38554	24.78181	32.66701	19	13.67	71.93
Styphnic acid	24.97775	-1.18959	23.78816	39.2984	43	-3.70	-8.61
Tetryl	29.20317	0.975188	30.17836	11.97243	25	-13.03	-52.11
Tri245	33.42927	0.15913	33.5884	6.34927	68	-61.65	-90.66

Table A-198. Comparison of predicted impact sensitivities to experiment using fit of average Σ total for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = a \cdot \exp(-b \cdot x)]$ as the form of the equation and with $a = 106086.8513$ and $b = 0.2749$ with an $R^2 = 0.9248$. Test set yielded an $R^2 = 0.5503$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set					
HNB	11	37.65582	3.39	-7.61	-69.19
PNA	22	29.02434	36.35	14.35	65.23
Picric acid	64	26.81203	66.78	2.78	4.34
TNT	98	23.60767	161.14	63.14	64.43
TNA	141	25.6776	91.22	-49.78	-35.31
NTO	291	22.2418	234.57	-56.43	-19.39
DATB	320	20.45713	383.12	63.12	19.72
TATB	490	19.84937	452.79	-37.21	-7.59
Test set					
CL16	17	28.78034	38.87	21.87	128.66
Picryl azide	19	26.57247	71.32	52.32	275.39
Tetryl	25	29.29693	33.73	8.73	34.91
Stylphic acid	43	25.6522	91.86	48.86	113.62
HNS	54	27.51595	55.03	1.03	1.91
tri245	68	30.927	21.55	-46.45	-68.31
DNBF	76	26.2684	77.54	1.54	2.03
Methyl picrate	192	24.11717	140.08	-51.92	-27.04

Table A-199. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = y_0 + a \cdot \exp(-b \cdot x)]$ as the form of the equation and with $y_0 = 7.8043$, $a = 134622.3047$ and $b = 0.2876$ with an $R^2 = 0.9251$. Test set yielded an $R^2 = 0.5607$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set					
HNB	11	37.65582	10.47	-0.53	-4.82
PNA	22	29.02434	39.71	17.71	80.51
Picric acid	64	26.81203	68.09	4.09	6.39
TNT	98	23.60767	159.32	61.32	62.57
TNA	141	25.6776	91.35	-49.65	-35.22
NT0	291	22.2418	232.22	-58.78	-20.20
DATB	320	20.45713	382.74	62.74	19.61
TATB	490	19.84937	454.35	-35.65	-7.27
Test set					
CL16	17	28.78034	42.03	25.03	147.24
Picryl azide	19	26.57247	72.39	53.39	281.00
Tetryl	25	29.29693	37.31	12.31	49.22
Stylphic acid	43	25.6522	91.96	48.96	113.86
HNS	54	27.51595	57.04	3.04	5.63
tri245	68	30.927	26.26	-41.74	-61.38
DNBF	76	26.2684	78.29	2.29	3.02
Methyl picrate	192	24.11717	138.66	-53.34	-27.78

Table A-200. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = a*b/(b+x)]$ as the form of the equation and with $a = -42.9343$ and $b = -18.2317$ with an $R^2 = 0.9118$. Test set yielded an $R^2 = 0.5179$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set					
HNB	11	37.65582	40.30	29.30	266.35
PNA	22	29.02434	72.53	50.53	229.67
Picric acid	64	26.81203	91.23	27.23	42.54
TNT	98	23.60767	145.60	47.60	48.58
TNA	141	25.6776	105.13	-35.87	-25.44
NT0	291	22.2418	195.20	-95.80	-32.92
DATB	320	20.45713	351.74	31.74	9.92
TATB	490	19.84937	483.89	-6.11	-1.25
Test set					
CL16	17	28.78034	74.21	57.21	336.50
Picryl azide	19	26.57247	93.85	74.85	393.94
Tetryl	25	29.29693	70.74	45.74	182.96
Stylphic acid	43	25.6522	105.49	62.49	145.32
HNS	54	27.51595	84.31	30.31	56.13
tri245	68	30.927	61.66	-6.34	-9.33
DNBF	76	26.2684	97.40	21.40	28.16
Methyl picrate	192	24.11717	133.00	-59.00	-30.73

Table A-201. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = y_0 + a*b/(b+x)]$ as the form of the equation and with $y_0 = -73.5168$, $a = -86.1842$ and $b = -17.1309$ with an $R^2 = 0.9272$. Test set yielded an $R^2 = 0.4928$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set					
HNB	11	37.65582	-1.58	-12.58	-114.40
PNA	22	29.02434	50.62	28.62	130.09
Picric acid	64	26.81203	78.99	14.99	23.42
TNT	98	23.60767	154.44	56.44	57.59
TNA	141	25.6776	99.23	-41.77	-29.62
NT0	291	22.2418	215.36	-75.64	-25.99
DATB	320	20.45713	370.35	50.35	15.74
TATB	490	19.84937	469.59	-20.41	-4.17
Test set					
CL16	17	28.78034	53.22	36.22	213.06
Picryl azide	19	26.57247	82.86	63.86	336.09
Tetryl	25	29.29693	47.84	22.84	91.35
Stylphic acid	43	25.6522	99.74	56.74	131.96
HNS	54	27.51595	68.65	14.65	27.13
tri245	68	30.927	33.50	-34.50	-50.74
DNBF	76	26.2684	88.06	12.06	15.87
Methyl picrate	192	24.11717	137.81	-54.19	-28.22

Table A-202. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total and maximum V+ for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = y_0 + a*\exp(-b*x) + c*\exp(-d*z)]$ as the form of the equation and with $y_0 = -4643.0357$, $a = 57070071804.3329$, $b = 0.9694$, $c = 5124.2966$ and $d = 0.0019$ with an $R^2 = 0.9338$. In the preceding equation, x is the average Σ total and z is the maximum V+. Test set yielded an $R^2 = 0.3825$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Maximum V+ (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set						
HNB	11	37.65582	51.88	0.25	-10.75	-97.77
PNA	22	29.02434	49.8594	18.14	-3.86	-17.54
Picric acid	64	26.81203	38.8861	116.60	52.60	82.19
TNT	98	23.60767	39.7151	115.39	17.39	17.74
TNA	141	25.6776	41.9327	89.72	-51.28	-36.37
NT0	291	22.2418	29.7509	224.32	-66.68	-22.91
DATB	320	20.45713	26.2945	370.81	50.81	15.88
TATB	490	19.84937	28.5548	461.68	-28.32	-5.78
Test set						
CL16	17	28.78034	58.7142	-59.61	-76.61	-450.67
Picryl azide	19	26.57247	49.2187	24.15	5.15	27.13
Tetryl	25	29.29693	43.5228	74.59	49.59	198.36
Stylphic acid	43	25.6522	35.005	152.44	109.44	254.51
HNS	54	27.51595	37.3305	130.54	76.54	141.75
tri245	68	30.927	44.7031	64.00	-4.00	-5.88
DNBF	76	26.2684	33.5234	165.55	89.55	117.83
Methyl picrate	192	24.11717	33.4827	169.43	-22.57	-11.76

Table A-203. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total and maximum V+ for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = y_0 + a*b/(b+x) + c*d/(d+z)]$ as the form of the equation and with $y_0 = -14.28$, $a = -35.9446$, $b = -18.5189$, $c = 0.0001$ and $d = -29.7509$ with an $R^2 = 0.9747$ excluding NTO. In the preceding equation, x is the average Σ total and z is the maximum V+. Test set yielded an $R^2 = 0.5256$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Maximum V+ (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set						
HNB	11	37.65582	51.88	20.50	9.50	86.40
PNA	22	29.02434	49.8594	49.08	27.08	123.10
Picric acid	64	26.81203	38.8861	65.99	1.99	3.10
TNT	98	23.60767	39.7151	116.53	18.53	18.91
TNA	141	25.6776	41.9327	78.71	-62.29	-44.18
NTO	291	22.2418	29.7509	#DIV/0!	#DIV/0!	#DIV/0!
DATB	320	20.45713	26.2945	329.15	9.15	2.86
TATB	490	19.84937	28.5548	486.04	-3.96	-0.81
Test set						
CL16	17	28.78034	58.7142	50.59	33.59	197.58
Picryl azide	19	26.57247	49.2187	68.37	49.37	259.86
Tetryl	25	29.29693	43.5228	47.48	22.48	89.92
Stylphic acid	43	25.6522	35.005	79.04	36.04	83.80
HNS	54	27.51595	37.3305	59.71	5.71	10.57
tri245	68	30.927	44.7031	39.37	-28.63	-42.11
DNBF	76	26.2684	33.5234	71.62	-4.38	-5.77
Methyl picrate	192	24.11717	33.4827	104.62	-87.38	-45.51

Table A-204. Comparison of predicted impact sensitivities to experiment using fit of average average Σ total and maximum V+ for the explicit X-N subgroups of the X-NO₂ for aromatic species for both the training and test sets using PBE/6-31G**. Fit used $[y = a*b/(b+x) + c*d/(d+z)]$ as the form of the equation and with $a = -30.2474$, $b = -18.6947$, $c = 0.0003$ and $d = -29.751$ with an $R^2 = 0.9737$. In the preceding equation, x is the average Σ total and z is the maximum V+. Test set yielded an $R^2 = 0.5305$.

Molecule	Experimental sensitivity (cm)	Average Σ tot ESP (kcal/mol)	Maximum V+ (kcal/mol)	Predicted sensitivity (cm)	Error	% Error
Training set						
HNB	11	37.65582	51.88	29.82	18.82	171.11
PNA	22	29.02434	49.8594	54.74	32.74	148.83
Picric acid	64	26.81203	38.8861	69.66	5.66	8.84
TNT	98	23.60767	39.7151	115.10	17.10	17.44
TNA	141	25.6776	41.9327	80.98	-60.02	-42.57
NTO	291	22.2418	29.7509	248.67	-42.33	-14.55
DATB	320	20.45713	26.2945	320.85	0.85	0.26
TATB	490	19.84937	28.5548	489.73	-0.27	-0.06
Test set						
CL16	17	28.78034	58.7142	56.07	39.07	229.80
Picryl azide	19	26.57247	49.2187	71.78	52.78	277.79
Tetryl	25	29.29693	43.5228	53.33	28.33	113.34
Stylphic acid	43	25.6522	35.005	81.27	38.27	89.01
HNS	54	27.51595	37.3305	64.10	10.10	18.71
tri245	68	30.927	44.7031	46.23	-21.77	-32.02
DNBF	76	26.2684	33.5234	74.66	-1.34	-1.76
Methyl picrate	192	24.11717	33.4827	104.28	-87.72	-45.69

List of Symbols, Abbreviation, and Acronyms

6-31G*	Pople's gaussian double-zeta polarized basis set with d polarization functions on each of the atoms Li–Ca
6-31G**	Pople's gaussian double-zeta polarized basis set with d polarization functions on each of the atoms Li–Ca and p polarization functions on H and He
Å	Ångstrom
ν	balance parameter
Π	average deviation of electrostatic surface potential
Σ	average electrostatic surface potential
σ^2	variance of electrostatic surface potential
$\nabla\rho$	gradient of the electronic density
ρ	electronic density
C	carbon
H	hydrogen
$h_{50\%}$	measure of impact sensitivity; value of the height with the likelihood of 50% of drops yielding an initiation event
N	nitrogen
N_3	azide group
NO_2	nitro group
O	oxygen
R^2	coefficient of determination
V	electrostatic potential
X	unknown/unassigned atom type
AIM	atoms in molecules
ARL	U.S. Army Research Laboratory
B3LYP	Becke 3-parameter exchange with Lee-Yang-Parr correlation density functional theory functional

BTAT	N^3 , N^6 -bis(2,2,2-trinitroethyl-1,2,4,5-tetrazine-3,6-diamine
CL16	azidopentanitrobenzene
CL20	2,4,6,8,10,12-hexanitrohexa-azaisowurtzitane
cm	centimeter
DATB	1,3-diamino-2,4,6-trinitrobenzene
DFT	density functional theory
DNBF	2,2',3,3',4,4',5,5',6,6'-decanitro biphenyl
EDNA	N,N'-dinitro-1,2-ethanediamine
EM	energetic materials
ESP	electrostatic surface potential
FOX-7	1,1-diamino-2,2-dinitro-ethylene
HMX	1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane
HNB	hexanitrobenzene
HNS	2,2',4,4',6,6'-hexanitrostilbene
kcal/mol	kilocalories per mole (unit of energy)
KS-DFT	Kohn-Sham density functional theory
Methyl picrate	2-methoxy-1,3,5-trinitrobenzene
NQ	nitroguanidine
NTO	3-nitro-1,2,4-triazole-5-one
PBE	Perdew, Burke, and Ernzerhof density functional theory
PETN	tetranitrate pentaerythritol
Picric acid	2,4,6-trinitrophenol
Picryl azide	2-azido-1,3,5-trinitrobenzene
PNA	pentanitroaniline
RDX	hexahydro-1,3,5-trinitro-1,3,5-triazine
Styphnic acid	2,4,6-trinitroresorcinol
TATB	1,3,5-triamino-2,4,6-trinitrobenzene

Tetryl	<i>N</i> -methyl- <i>N</i> ,2,4,6-tetranitroaniline
TNA	2,4,6-trinitroaniline
TNT	2,4,6-trinitrotoluene
Tri245	2,4,5-trinitroimidazole

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