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13. ABSTRACT *(Maximum 200 words)*

Density functional methods have been used to compute the optimized geometries, dissociation energies and gas phase heats of formation of several difluoramines (in which the $-NF_2$ is attached to a nitrogen) and the corresponding nitramines. The $-NF_2$ groups are found to be pyramidal, in contrast to the planarity of the $-NO_2$. In each instance, one N–F bond length is at least 0.1 Å longer than the other, while the N–N bonds are anomalously short. For the molecules and properties studied, the effects of $-NO_2$ and $-NF_2$ (on nitrogen) do not differ dramatically. Replacing $>N-NO_2$ by $>N-NF_2$ affects the dissociation energies of other $N-NO_2$ and $C-NO_2$ bonds only slightly (2 - 3 kcal/mole); however the $N-NF_2$ bonds are 3 - 6 kcal/mole stronger than the $N-NO_2$ that were replaced. The difluoramine heats of formation are less positive, by 15 - 17 kcal/mole, than those of the corresponding nitramines.

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Comparative Computational Analysis of Some Nitramine and Difluoramine Structures, Dissociation Energies and Heats of Formation

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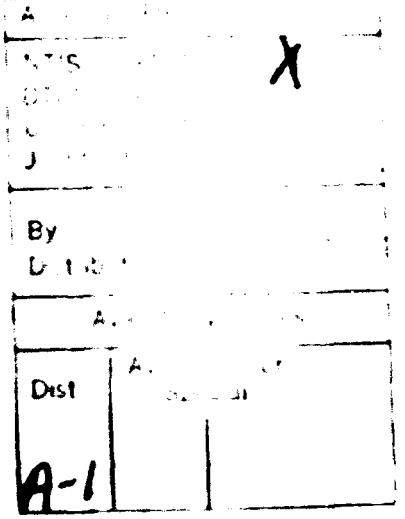
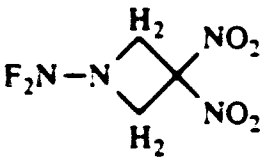
Abstract

Density functional methods have been used to compute the optimized geometries, dissociation energies and gas phase heats of formation of several difluoramines (in which the $-NF_2$ is attached to a nitrogen) and the corresponding nitramines. The $-NF_2$ groups are found to be pyramidal, in contrast to the planarity of the $-NO_2$. In each instance, one N–F bond length is at least 0.1 Å longer than the other, while the N–N bonds are anomalously short. For the molecules and properties studied, the effects of $-NO_2$ and $-NF_2$ (on nitrogen) do not differ dramatically. Replacing $>N-NO_2$ by $>N-NF_2$ affects the dissociation energies of other $N-NO_2$ and $C-NO_2$ bonds only slightly (2 - 3 kcal/mole); however the $N-NF_2$ bonds are 3 - 6 kcal/mole stronger than the $N-NO_2$ that were replaced. The difluoramine heats of formation are less positive, by 15 - 17 kcal/mole, than those of the corresponding nitramines.



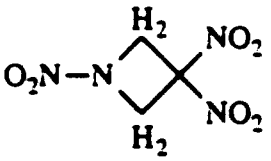
Introduction

It has long been recognized that the judicious introduction of the difluoramino group, $-NF_2$, can significantly improve the propellant properties of energetic materials [1, 2]. One reason for this is that the specific impulse, which is a direct measure of the thrust that a propellant develops, depends in part upon the number of moles of gaseous products obtained per unit weight upon combustion [3, 4]. It is therefore desirable that these gases have low molecular weights. The $-NF_2$ group leads to the formation of HF (provided that hydrogens are present), which is among the lightest of the typical products; these include CO_2, N_2, CO and H_2O. The last of these has a slightly lower molecular weight than does HF, but it makes less efficient use of the hydrogens that are present. For example, **1** and **2** both have four hydrogens, but the stoichiometry of **1** corresponds to three moles of hydrogen-containing products and eight moles total, eq. (1), in contrast to two hydrogen-containing and seven total for **2**, eq. (2). Thus the number of moles in gases obtained per gram of **1** is 0.040, versus 0.036 for **2**.



$$\longrightarrow \quad 2HF + H_2O + 3CO + 2N_2 \qquad (1)$$

1

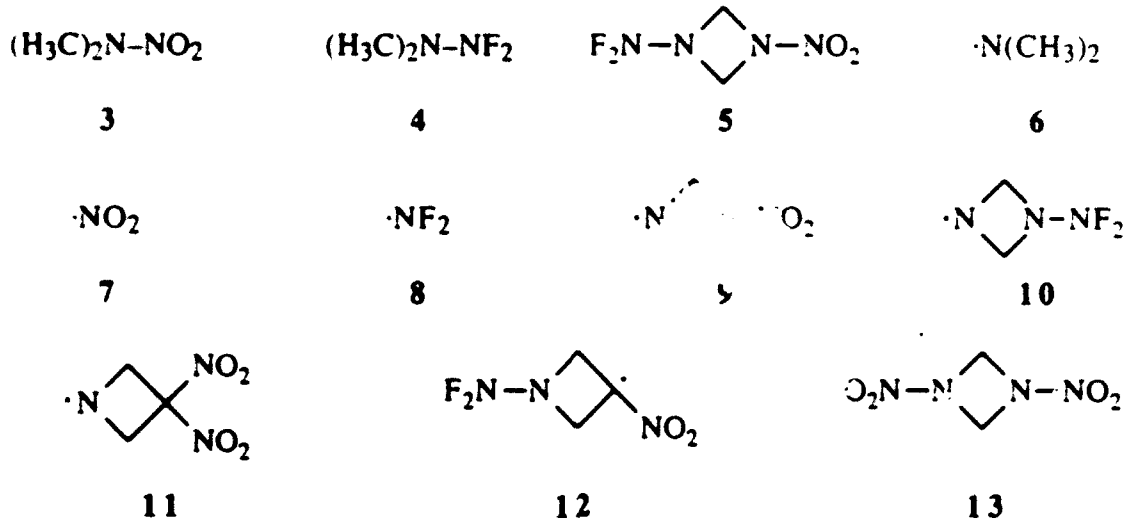


$$\longrightarrow \quad 2H_2O + 2CO + CO_2 + 2N_2 \qquad (2)$$

2

Our present objective is to determine, for several nitramines, how their structures, dissociation energies and heats of formation are affected by replacing $-NO_2$, a group typically associated with energetic molecules, by $-NF_2$. The last of these properties is important because the specific impulse also depends upon the combustion temperature that is achieved, and this tends to be higher as the heat of formation is more positive. As background for this comparison of the effects of these two groups, it may be useful to examine their Hammett and Taft substituent constants [5, 6]. For $-NO_2$, these are [5]: $\sigma_m = 0.71$, $\sigma_p = 0.81$, $\sigma_I = 0.67$ and $\sigma_R = 0.15$. Experimentally-based values are not available for $-NF_2$; earlier, however, we have used correlations with computed quantities to predict that $\sigma_m = 0.54$, $\sigma_p = 0.49$, $\sigma_I = 0.53$ and $\sigma_R = -0.04$ [7, 8]. These data show a general similarity between the two groups, in that they are primarily strong inductive electron withdrawers.

We have carried out computational analyses of 1 and 3 - 5, as well as the various dissociation products 6 - 12. The results for 1 and 5 will be compared to those obtained earlier for 2 [9] and 13 [10].



Methods

The geometries of 1 and 3 - 12 were optimized in two stages, first at the HF/3-21G level and then by means of the non-local density functional (DF) option of Gaussian 92/DFT, revision G.2 [11], using a 6-31G (d,p) basis set and the Becke [12] and Perdew-Wang [13] functionals for exchange and correlation, respectively. Zero-point energies were computed with the HF/3-21G harmonic frequencies, which have been found to be satisfactory for this purpose [14], and were scaled by the recommended 0.89.

Standard gaseous heats of formation were calculated by a separate procedure [15, 16] which involves computing ΔE (using the density functional technique described above) for the formation of each molecule from its elements, incorporating translational, rotational and DF vibrational contributions, and converting the result to $\Delta H°$ at 25°C by means of the ideal gas approximation. The final step is to add empirical atomic correction terms.

Results and Discussion

1. Structures

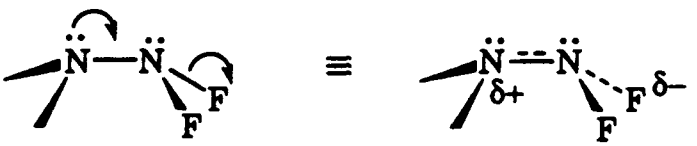
Our calculated DF optimized geometries for 1 and 3 - 12 are presented in Table 1. Some experimentally-determined structural data are also included; the agreement with these is good.

In each difluoramine, the arrangements of the bonds around the two nitrogens in the >N–NF_2 portion are roughly pyramidal; the lone pairs can be regarded as occupying the approximate

fourth tetrahedral directions. This is in marked contrast to the $-NO_2$ groups, which are invariably planar.

A striking feature of the difluoramine structures involves the N–F and N–N bond lengths. To put these in perspective, we computed the DF optimized geometries of H_3C-NF_2 (**14**) and $(H_3C)_2N-NH_2$ (**15**). The N–F distances in **14** were found to be 1.436 Å, and the calculated N–N bond length in **15** is 1.492 Å. (These will be taken as reference points.) In the difluoramines **1**, **4**, **5**, **10** and **12**, one N–F distance is approximately the same as in **14**, between 1.417 and 1.431 Å, but the other is considerably longer, ranging from 1.530 to 1.563 Å. In addition, the N–N bonds are much shorter than in **15**, by about 0.13 Å.

In seeking an interpretation of these observations, it is tempting to recall the three-dimensional nature of $>N-NF_2$ and to suggest that the negative hyperconjugation shown in **16** can occur preferentially with the N–F bond that is more nearly coplanar with the N–N bond and the lone pair. The anticipated result would be a lengthening of the former and a



16

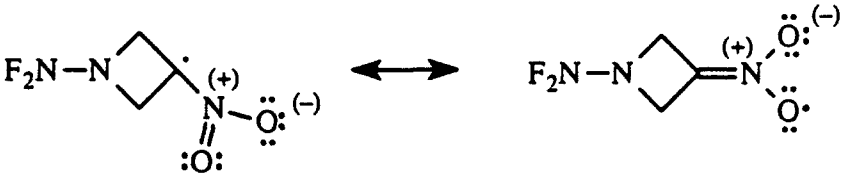
shortening of the latter, as has been found. However it has recently been pointed out that the lengths of the N–F bonds in NH_2F, NHF_2 and NF_3 *increase* in the same order as their dissociation energies [17-19], instead of the inverse correlation that is customarily found for bonds of all kinds. If this anomalous behavior also occurs in the present difluoramines, then the delocalization shown in **16** would not explain our observed N–F bond lengths. These points are being investigated.

2. Dissociation Energies

Using the total energies in Table 1, and adding zero-point corrections, the $N-NO_2$, $C-NO_2$ and $N-NF_2$ dissociation energies were calculated for **1** and **3** - **5**. They are listed in Table 2.

The results are quite reasonable, when compared to those of earlier work. Our 43.8 kcal/mole for $(H_3C)_2N-NO_2$ is very close to the experimental value, 43.3 kcal/mole [20]. The $N-NO_2$ dissociation energy of **5** is somewhat below the 40 - 50 kcal/mole range that is typical of $N-NO_2$ bonds [20-24], but is very similar to the 36.6 kcal/mole that we have obtained for **13** [10]. We suggested at that time that the low magnitude may reflect some release of strain upon breaking the bond. Our finding the $C-NO_2$ dissociation energy of **1** to be the same as the $N-NO_2$ of **5** may well seem surprising, since $C-NO_2$ bonds are normally stronger than $N-NO_2$ [25]. We have already encountered an analogous situation in the case of **2** [9], and following our earlier

interpretation, we suggest now that the product **12** is stabilized by delocalization of the unpaired electron:



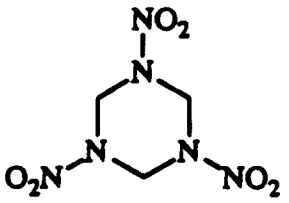
12A **12B**

Indeed Table 1 shows the C–NO_2 bond to be about 0.13 Å shorter in **12** than in **1**, while the N–O distances are 0.02 Å longer. A second factor may be that the destabilizing effect of two –NO_2 groups on the same carbon has been eliminated [26].

It is interesting to note, by comparing our results in Table 2 for **1** and **5** to those obtained earlier for **2** [9] and for **13** [10], that replacing >N–NO_2 by >N–NF_2 has only a very small effect (2 - 3 kcal/mole) upon the dissociation energies of other N–NO_2 and C–NO_2 bonds in the molecule. However the N–NF_2 bond is in each instance somewhat stronger than the N–NO_2 that it replaced. The difference is 3.5 kcal/mole for **3** and **4** (Table 2), about 5 kcal/mole for **1** and **2** [9], and 6.1 kcal/mole for **5** and **13** [10].

3. Heats of Formation

Our calculated standard gas phase heats of formation of the difluoramine derivatives **1**, **4** and **5** are given in Table 3, where they are compared with those of their nitramine analogs (**2**, **3** and **13**). In each instance, $\Delta H^{\circ}_{f,298^{\circ}K}$ is lower (less positive) for the difluoramine compound. (An analogous observation was reported by Leroy *et al* for groups of –NO_2 and –NF_2 derivatives in which these substituents are attached to carbons [27].) However the lower heats of formation of difluoramines do not necessarily preclude their having higher specific impulse values than the corresponding nitramines. For example, the specific impulse of **18** is predicted to be higher than that of **17**, even though the heat of formation of the latter has been estimated to be double that of the former [4]. **18** produces more moles of gases per gram than does **17**, 0.044 vs 0.041.



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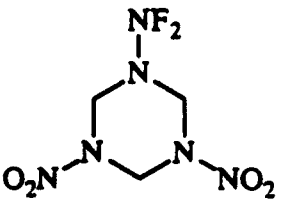

18

Conclusions

In the particular molecules that we have studied, and for the properties of present interest, the effects of $-NO_2$ and $-NF_2$ subsituted on nitrogens are not dramatically different. This conclusion is consistent with that of Leroy *et al*, for $-NO_2$ and $-NF_2$ on carbon, that they "generally have similar destabilizing effects" [28]. We do find the $N-NF_2$ bonds to be somewhat stronger than the $N-NO_2$. Since the cleavage of the $N-NO_2$ bond is believed to play a key role in the decomposition of many nitramines [20, 21, 29-32], it may be that the replacement of $>N-NO_2$ by $>N-NF_2$ will improve shock/impact sensitivity.

Acknowledgement

We greatly appreciate discussions with Dr. Jane S. Murray and Dr. Mark L. Trudell, and the support of this work by the Office of Naval Research through contract no. N00014-91-J-4057.

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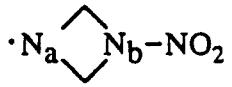
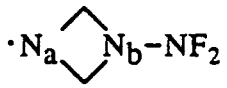
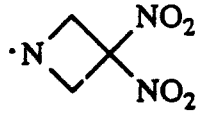
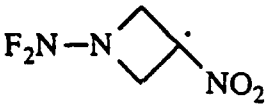
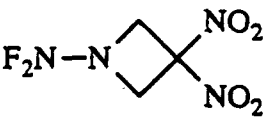
Table 1. Computed (DF) energies and structural properties.[a]

Molecule		Energy (hartrees)	Distance (Å)	Angle (deg)
$\cdot N(CH_3)_2$	**6**	−134.50899	N–C: 1.445	C–N–C: 111
$\cdot NO_2$	**7**	−205.09815	N–O: 1.218 (1.200)	O–N–O: 133 (133.8)
$\cdot NF_2$	**8**	−254.27515	N–F: 1.378 (1.353)	F–N–F: 104 (103.2)
$(H_3C)_2N–NO_2$	**3**	−339.68569	N–N: 1.409 (1.382) C–N: 1.462 (1.460) N–O: 1.243 (1.223)	C–N–N: 115 (116.2) N–N–O: 117 (114.8) C–N–C: 119 O–N–O: 126 (130.4) C–N–N–O: 19, 164
$(H_3C)_2N–NF_2$	**4**	−388.86799	N–N: 1.358 C_a,C_b–N: 1.469, 1.474 N–F_a,F_b: 1.431, 1.542	N–N–C_a,C_b: 109, 118 N–N–F_a,F_b: 105, 108 C–N–C: 116 F–N–F: 98 C_a–N–N–F_a,F_b: 171, 85 C_b–N–N–F_a,F_b: 54, 49
	**9**	−393.13891	N–N: 1.416 C–N_a,N_b: 1.470, 1.490 N–O: 1.240	C–N_a,N_b–C: 89, 87 N–C–N: 92 C–N–N: 118 N–N–O: 116 O–N–C: 128 C–N–C–N: 8 N–C–N–N: 129 C–N–N–O: 38, 142
	**10**	−442.32215	N–N: 1.357 C_a,C_b–N_a: 1.465, 1.466 C_a,C_b-N_b: 1.507, 1.500 N–F_a,F_b: 1.422, 1.563	C–N_a,N_b–C: 89, 86 N–C–N: 92 C_a,C_b–N–N: 121, 115 N–N–F_a,F_b: 103, 107 F–N–F: 99 C–N–C–N: 9 N–C_a,C_b–N–N: 126, 132 C_a–N–N–F_a,F_b: 64, 40 C_b–N–N–F_a,F_b: 165, 62
	**11**	−581.62276	C_a,C_b–N: 1.487, 1.483 C_a,C_b–C: 1.539, 1.537 C–NO_2: 1.532 N–O: 1.235, 1.237	C–C–C: 86 C_a–C–$(NO_2)_a,(NO_2)_b$: 115,118 C_b–C–$(NO_2)_a,(NO_2)_b$: 118,115 C–C–N: 92 C–N–C: 90 N–C–N: 105 C–N–O: 115-118 O–N–O: 127 C–C–N–C: 1 C–C–C–N: 1 N–C–N–O: 57-60, 123-126 N–C_a,C_b–$(NO_2)_a$: 119,117 N–C_a,C_b–$(NO_2)_b$: 116,118

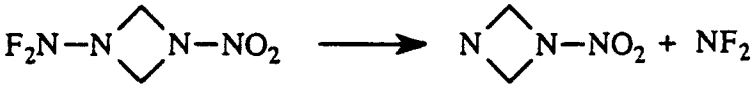
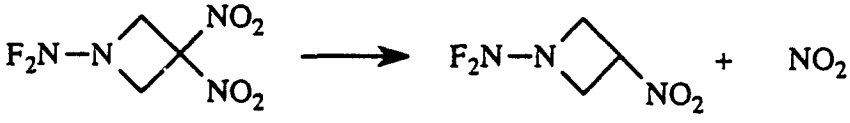
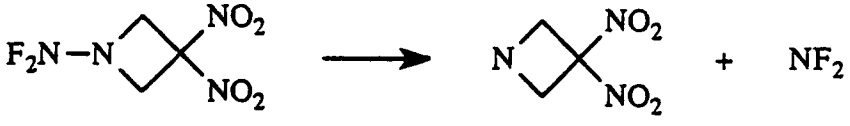
(continued)

Table 1. Computed (DF) energies and structural properties (continued).

Molecule	Energy (hartrees)	Distance (Å)	Angle (deg)
 **12**	–630.80980	N–N: 1.367 C_a,C_b–C: 1.489, 1.493 C–NO_2: 1.403 C_a,C_b–N: 1.525, 1.513 N–O: 1.257, 1.258 N–F_a,F_b: 1.418, 1.538	C–C–C: 95 C_a,C_b–C–NO_2: 132, 131 C–C–N: 86 C–N–O: 117 C–N–C: 92 C_a,C_b–N–N: 119, 114 N–N–F_a,F_b: 103, 108 O–N–O: 126 F–N–F: 99 C–C–C–N: 7 C–C–N–C: 7 N–C–C–NO_2: 155 C–C_a,C_b–N–N: 126, 131 C–C–N–O: 13, 167 C_a–N–N–F_a,F_b: 61, 43 C_b–N–N–F_a,F_b: 169, 65
 **5**	–647.48986	C_a,C_b–N(NO_2): 1.485, 1.487 C_a,C_b–N(NF_2): 1.507, 1.498 N–NO_2: 1.423 N–NF_2: 1.368 N–O: 1.237, 1.238 N–F_a,F_b: 1.418, 1.536	C–N(NO_2)–C: 92 C–N(NF_2)–C: 91 N–C–N: 89 C–N–NO_2: 117 C_a,C_b–N–NF_2: 119, 114 N–N–O: 116 N–N–F_a,F_b: 103, 107 O–N–O: 128 F–N–F: 99 C–N–C–N: 1 N–C_a,C_b–N–NO_2: 120, 121 N–C_a,C_b–N–NF_2: 119, 124 C–N–N–O: 38, 145 C_a–N–N–F_a,F_b: 63, 42 C_b–N–N–F_a,F_b: 168, 64
 **1**	–835.97709	C_a,C_b–C: 1.536, 1.534 C–(NO_2)$_a$,(NO_2)$_b$: 1.540, 1.534 C_a,C_b–N(NF_2): 1.501, 1.511 N–N: 1.366 N–O: 1.233-1.236 N–F_a,F_b: 1.417, 1.538	C–C–C: 90 C_a–C–(NO_2)$_a$,(NO_2)$_b$: 114, 117 C_b–C–(NO_2)$_a$,(NO_2)$_b$: 116, 116 C–C–N: 88 NO_2–C–NO_2: 105 C–N–O: 114-118 C–N–C: 92 C_a,C_b–N–NF_2: 114, 120 N–N–F_a,F_b: 103, 107 O–N–O: 128 F–N–F: 99 C–C–C–N: 12 C–C–N–C: 12 N–C–C–(NO_2)$_a$,(NO_2)$_b$: 105, 131 C–C_a,C_b–N–NF_2: 136, 132 C_a–N–N–F_a,F_b: 169, 65 C_b–N–N–F_a,F_b: 61, 43

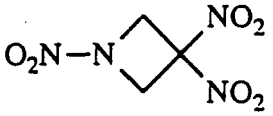
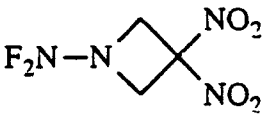
[a]Experimentally-determined data are in parentheses. NO_2, NF_2: M. D. Harmony, V. W. Laurie, R. L. Kuczkowski, R. H. Schwendeman, D. A. Ramsay, F. J. Lovas, W. J. Lafferty and A. G. Maki, J. Phys. Chem. Ref. Data 8 (1979) 619; $(H_3C)_2N$-NO_2: R. Stolevik and P. Rademacher, Acta Chem. Scand. 23 (1969) 672.

Table 2. Calculated dissociation energies, including zero-point corrections.

Process	Dissociation energy, kcal/mole
$(H_3C)_2N{-}NO_2 \longrightarrow (H_3C)_2N + NO_2$ **3** **6** **7**	43.8 (43.3)[a]
$(H_3C)_2N{-}NF_2 \longrightarrow (H_3C)_2N + NF_2$ **4** **6** **8**	47.3
 **5** **10** **7**	38.7
 **5** **9** **8**	42.7
 **1** **12** **7**	38.5
 **1** **11** **8**	44.7

[a]Experimentally-determined value, from ref. 20.

Table 3. Calculated gas phase heats of formation.

Compound		$\Delta H^{\circ}_{f,298°K}$, kcal/mole
3	$(H_3C)_2N-NO_2$	-2.7 (-1.1)[a]
4	$(H_3C)_2N-NF_2$	-19.8
13		43.9
5		28.6
2		30.7
1		15.7

[a]Experimentally-determined value, from J. B. Pedley, R. D. Naylor and S. P. Kirby, *Thermochemical Data of Organic Compounds*, 2nd ed. (Chapman and Hall, London, 1986).