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Dr. Richard S. Miller

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COMPUTED HEATS OF FORMATION

by

Peter Politzer, M. Edward Grice and Pat Lane

Department of Chemistry
University of New Orleans
New Orleans, LA 70148

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Peter Politzer, M. Edward Grice and Pat Lane

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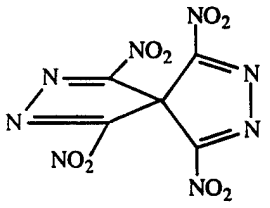
Computed heats of formation for **1 - 4.**



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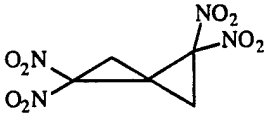

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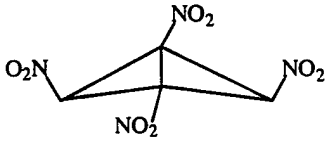

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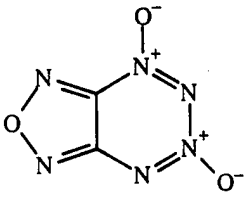

4

1: ΔH_f^{298K} (solid) = 157 kcal/mole = 524 cal/g

2: ΔH_f^{298K} (solid) = 46 kcal/mole = 183 cal/g

3: ΔH_f^{298K} (solid) = 59 kcal/mole = 250 cal/g

4: ΔH_f^{298K} (solid) = 143 kcal/mole = 918 cal/g

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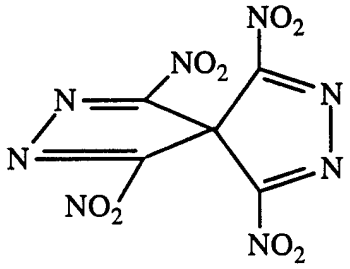
We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **4**, in response to a request from R. Naylor (Allegany Ballistics Laboratory). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the liquid and solid state values by subtracting, respectively, the heat of vaporization and the heat of sublimation. These are obtained by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [3,4].

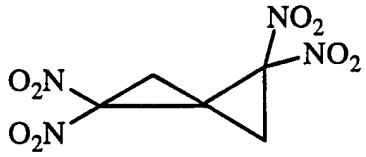
Results:

1



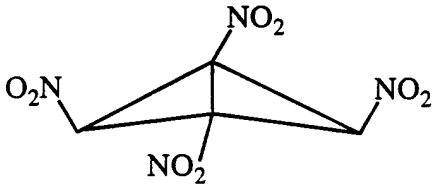
ΔH_f^{298K} (gas) = 189 kcal/mole = 630 cal/g
ΔH_f^{298K} liquid = 174 kcal/mole = 579 cal/g
ΔH_f^{298K} (solid) = 157 kcal/mole = 524 cal/g

2



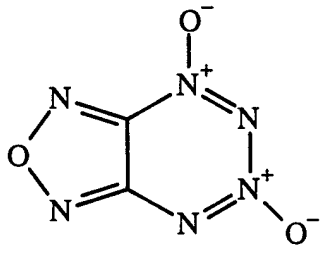
ΔH_f^{298K} (gas) = 76 kcal/mole = 304 cal/g
ΔH_f^{298K} liquid = 60 kcal/mole = 243 cal/g
ΔH_f^{298K} (solid) = 46 kcal/mole = 183 cal/g

3



ΔH_f^{298K} (gas) = 85 kcal/mole = 364 cal/g
ΔH_f^{298K} liquid = 71 kcal/mole = 303 cal/g
ΔH_f^{298K} (solid) = 59 kcal/mole = 250 cal/g

4



ΔH_f^{298K} (gas) = 165 kcal/mole = 1058 cal/g
ΔH_f^{298K} liquid = 152 kcal/mole = 974 cal/g
ΔH_f^{298K} (solid) = 143 kcal/mole = 918 cal/g

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [5,6].

References:

1. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem. **16**, 654 (1995).
2. M. E. Grice and P. Politzer, Chem. Phys. Lett. **244**, 295 (1995).
3. J. S. Murray and P. Politzer, *Quantitative Treatments of Solute/Solvent Interactions*, J.S . Murray and P. Politzer, Eds., Elsevier, Amsterdam, 1994, ch. 8.
4. P. Politzer, J. S. Murray, M. E. Grice, M. DeSalvo and E. Miller, Mol. Phys. **91**, 235 (1997).
5. D. R. Stull, E. F. Westrum and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds*, Wiley, New York, 1969.
6. J. M. Rosen and C. Dickinson, J. Chem. Eng. Data **14**, 120 (1969).