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Dr. Richard S. Miller

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6. AUTHOR(S)

Peter Politzer, Jane S. Murray and M. Edward Grice

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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

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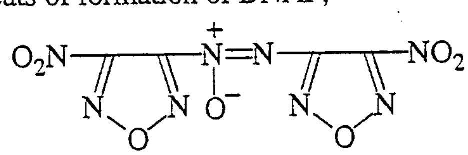

based on computational analyses, are: ΔH_f(gaseous) = 169 kcal/mole = 621 cal/g; ΔH_f(liquid) = 155 kcal/mole = 570 cal/g; ΔH_f(solid) = 137 kcal/mole = 504 cal/g.

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Dr. Richard S. Miller

Technical Report No. 85

PREDICTED HEATS OF FORMATION OF DNAF IN GASEOUS, LIQUID AND SOLID PHASES

by

Peter Politzer, Jane S. Murray and M. Edward Grice

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

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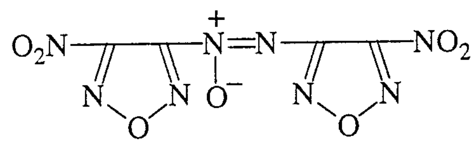
One of the compounds for which we have recently computed the gas phase heats of formation, ΔH_f(gaseous), is DNAF, **1** [1]. This was done using our density functional procedure [2].



DNAF, **1**

In response to interest expressed by the Air Force Armament Laboratory (Eglin AFB), we have now estimated the liquid and solid phase heats of formation of **1**. For this purpose, we needed the heats of vaporization, ΔH_{vap}, and sublimation, ΔH_{sub}, which we obtained using general correlations between these properties and computed quantities related to electrostatic potentials on molecular surfaces [3].

$$\Delta H_f(\text{liquid}) = \Delta H_f(\text{gaseous}) - \Delta H_{vap} \qquad (1)$$

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{sub} \qquad (2)$$

We found ΔH_{vap} = 14 kcal/mole and ΔH_{sub} = 32 kcal/mole. Then,

$$\Delta H_f(\text{gaseous}) = 169 \text{ kcal/mole} = 621 \text{ cal/g}$$

$$\Delta H_f(\text{liquid}) = 155 \text{ kcal/mole} = 570 \text{ cal/g}$$

$$\Delta H_f(\text{solid}) = 137 \text{ kcal/mole} = 504 \text{ cal/g}$$

References

1. P. Politzer and M. E. Grice, Technical Report No. 78, Office of Naval Research, Contract No. N00014-95-1-0028, March 16, 1995.
2. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, J. Comp. Chem., **16**, 654 (1995).
3. M. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.