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COMPUTED HEATS OF FORMATION

by

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Computed heats of formation for 1 - 8.

1: $\Delta H_f^{298K}$ (solid) = 231 cal/g
2: $\Delta H_f^{298K}$ (solid) = 491 cal/g
3: $\Delta H_f^{298K}$ (solid) = 150 cal/g
4: $\Delta H_f^{298K}$ (solid) = 157 cal/g
5: $\Delta H_f^{298K}$ (solid) = 132 cal/g
6: $\Delta H_f^{298K}$ (solid) = 235 cal/g
7: $\Delta H_f^{298K}$ (solid) = -1.5 cal/g
8: $\Delta H_f^{298K}$ (solid) = -584 cal/g

Subject Terms:
Energetic compounds; heats of formation
We have computed heats of formation for compounds 1 - 8 (Table 1). The first five are target compounds proposed by M. Trudell (University of New Orleans); 6 - 8 have recently been prepared by R. Schmitt and J. Bottaro (SRI). For the molecular systems 1 - 7, we used our density functional procedure to obtain gas phase heats of formation, which were converted to liquid and solid state values by subtracting, respectively, the heats of vaporization and sublimation. The latter are determined by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [2,3]. (Vibrational energies were obtained from the molecular stoichiometries [4].) For the ionic solid 8, the heat of formation was calculated using the lattice enthalpy and the gas phase heats of formation of the positive and negative ions; the lattice enthalpy was computed from our recently-developed relationship involving anionic surface electrostatic potentials [5]. For comparison, the experimental solid phase heats of formation of HMX and RDX are, respectively, 60.4 cal/g and 76.1 cal/g [6].

References:

Table 1. Computed heats of formation.

| 1 | ![Image 1] | $\Delta H_f^{298K}$ (gas) = 73.6 kcal/mole = 341 cal/g  
$\Delta H_f^{298K}$ (liquid) = 60.0 kcal/mole = 278 cal/g  
$\Delta H_f^{298K}$ (solid) = 49.8 kcal/mole = 231 cal/g |
| 2 | ![Image 2] | $\Delta H_f^{298K}$ (gas) = 155 kcal/mole = 604 cal/g  
$\Delta H_f^{298K}$ (liquid) = 139 kcal/mole = 544 cal/g  
$\Delta H_f^{298K}$ (solid) = 126 kcal/mole = 491 cal/g |
| 3 | ![Image 3] | $\Delta H_f^{298K}$ (gas) = 80.6 kcal/mole = 263 cal/g  
$\Delta H_f^{298K}$ (liquid) = 64.3 kcal/mole = 210 cal/g  
$\Delta H_f^{298K}$ (solid) = 45.8 kcal/mole = 150 cal/g |
| 4 | ![Image 4] | $\Delta H_f^{298K}$ (gas) = 104 kcal/mole = 264 cal/g  
$\Delta H_f^{298K}$ (liquid) = 87.5 kcal/mole = 221 cal/g  
$\Delta H_f^{298K}$ (solid) = 62.2 kcal/mole = 157 cal/g |
| 5 | ![Image 5] | $\Delta H_f^{298K}$ (gas) = 96.5 kcal/mole = 236 cal/g  
$\Delta H_f^{298K}$ (liquid) = 79.1 kcal/mole = 194 cal/g  
$\Delta H_f^{298K}$ (solid) = 54.0 kcal/mole = 132 cal/g |
| 6 | ![Image 6] | $\Delta H_f^{298K}$ (gas) = 108 kcal/mole = 370 cal/g  
$\Delta H_f^{298K}$ (liquid) = 91.1 kcal/mole = 312 cal/g  
$\Delta H_f^{298K}$ (solid) = 68.7 kcal/mole = 235 cal/g |

(continued)
Table 1. Computed heats of formation (continued).

| 7 | \[ \text{O}_2\text{N} \text{N} \text{F} \text{N} \text{O}_2\text{N} \] | \( \Delta H_f^{298K} \) (gas) = 20.5 kcal/mole = 124 cal/g  
\( \Delta H_f^{298K} \) (liquid) = 8.23 kcal/mole = 49.8 cal/g  
\( \Delta H_f^{298K} \) (solid) = 0.24 kcal/mole = 1.5 cal/g |
| 8 | \( \text{K}^+ \left[ \text{N} \text{F} \text{NO}_2^- \right] \) | \( \Delta H_f^{298K} \) (solid) = \(-69.0\) kcal/mole = \(-584\) cal/g |