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COMPUTED HEATS OF FORMATION OF THREE DIAZAPENTALENES, AND TWO GEM-DINITRO/GEM-DIFLUORAMINO ANALOGUES OF RDX

by

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Computed Heats of Formation of Three Diazapentalenes and Two Gem-Dinitro/Gem-Difluoramino Analogues of RDX

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Computed heats of formation for 1 - 5.

1: $\Delta H_f^{298K}$ (solid) = 61 kcal/mole = 402 cal/g
2: $\Delta H_f^{298K}$ (solid) = 67 kcal/mole = 276 cal/g
3: $\Delta H_f^{298K}$ (solid) = 78 kcal/mole = 273 cal/g
4: $\Delta H_f^{298K}$ (solid) = -51 kcal/mole = -160 cal/g
5: $\Delta H_f^{298K}$ (solid) = -77 kcal/mole = -230 cal/g

heats of formation; diazapentalenes; gem-dinitro/gem-difluoramino analogues of RDX

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We have used our density functional procedure [1] to compute the heats of formation of the compounds 1 - 5. 1 and 2 have been prepared by R. Schmitt and J. Bottaro at SRI and 3 is under consideration. The syntheses of 4 and 5 are being pursued by T. Axenrod (CUNY). 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 solid state value by subtracting the heat of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:

1
\[ \Delta H_f^{298K} \text{(gas)} = 84 \text{ kcal/mole} = 553 \text{ cal/g} \]
\[ \Delta H_f^{298K} \text{(solid)} = 61 \text{ kcal/mole} = 402 \text{ cal/g} \]

2
\[ \Delta H_f^{298K} \text{(gas)} = 97 \text{ kcal/mole} = 401 \text{ cal/g} \]
\[ \Delta H_f^{298K} \text{(solid)} = 67 \text{ kcal/mole} = 276 \text{ cal/g} \]

3
\[ \Delta H_f^{298K} \text{(gas)} = 113 \text{ kcal/mole} = 394 \text{ cal/g} \]
\[ \Delta H_f^{298K} \text{(solid)} = 78 \text{ kcal/mole} = 273 \text{ cal/g} \]

4
\[ \Delta H_f^{298K} \text{(gas)} = -13 \text{ kcal/mole} = -42 \text{ cal/g} \]
\[ \Delta H_f^{298K} \text{(solid)} = -51 \text{ kcal/mole} = -160 \text{ cal/g} \]

5
\[ \Delta H_f^{298K} \text{(gas)} = -40 \text{ kcal/mole} = -120 \text{ cal/g} \]
\[ \Delta H_f^{298K} \text{(solid)} = -77 \text{ kcal/mole} = -230 \text{ cal/g} \]

For comparison, the experimental gas phase \( \Delta H_f^{298K} \) value for RDX is 206 cal/g [4,5].
References: