ADDITIONS AND CORRECTIONS

2008, Volume 112A

Vitaly G. Kiselev and Nina P. Gritsan*: Theoretical Study of the Nitroalkane Thermolysis. 1. Computation of the Formation Enthalpy of the Nitroalkanes, Their Isomers and Radical Products

Pages 4458−4464. Using the G3 technique and the atomization energy approach, the gas-phase formation enthalpy of $C(NO_2)_4$ (**10**) was calculated to be $\Delta_f H^0_{gas} = 19.6$ kcal/mol, in perfect agreement with the experimental value (19.7 ± 0.5 kcal/mol) [Lebedev, V. P.; Miroshnichenko, E. A.; Matyushin, Yu. N.; Larionov, V. P.; Romanov, V. S.; Bukolov, Yu. E.; Denisov, G. M.; Balepin, A. A.; Lebedev, Yu. A. *Russ. J. Phys. Chem. (Engl. Transl.)* **1975**, *49*, 1133 (p 1927 in original publication)]. Thus, the G3 procedure gives accurate results (within 1 kcal/mol) for formation enthalpies not only of nitrosubstituted methane and ethane but of polynitrosubstituted methanes as well.

The enthalpies of the isodesmic reactions (1) and (2) (from the original paper) were also calculated using the G3 technique and were found to be 21.9 and 17.8 kcal/mol, respectively. Using these reaction enthalpies and the experimental $\Delta_f H^0_{gas}$ of CH_4, **1** and **10**, the gas-phase formation enthalpies of **4** and **7** were estimated to be −10.1 and 1.8 kcal/mol, respectively. These values are in very good agreement with the ones calculated at the G3 level using the atomization energy approach (Table 1).

10.1021/jp804942q
Published on Web 06/21/2008