DFT and G2MP2 Calculations of the N-N Bond Dissociation Enthalpies and Enthalpies of Formation of Hydrazine, Monomethylhydrazine and Symmetrical and Unsymmetrical Dimethylhydrazine

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In a combined DFT (B3LYP) and G2MP2 theoretical study the following enthalpies of formation ($\Delta H^{\circ}{}_{f}$) and bond dissociation enthalpies (*BDE*) for hydrazine, methylhydrazine (MMH), 1,1-dimethylhydrazine (UDMH) and 1,2-dimethylhydrazine (SDMH) were determined: *BDE*/kJ mol^{-1}: N_2H_4, 278 ± 4; MMH, 272 ± 4; UDMH, 259 ± 12; SDMH, 272 ± 12. $\Delta H^{\circ}{}_{f}$/kJ mol^{-1}: N_2H_4, 95 ± 6; MMH, 94 ± 4; UDMH, 80 ± 4; SDMH, 91 ± 4. The bond enthalpy for the N-N bond in hydrazine amounts to *BE* (N-N, H_2N-NH_2) = 159 ± 4 kJ mol^{-1}.

Key words: Dimethylhydrazine, Hydrazine, MMH, Monomethylhydrazine, N-N Bond Dissociation Energies, UDMH