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Theoretical Investigations on Fundamental Performances of All-nitrogen Materials: Ⅱ. Prediction of Enthalpies of Formation

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Abstract: To accurately predict the enthalpies of formation of all-nitrogen materials, nine density functionals including B3PW91, B3P86, B3LYP, X3LYP, O3LYP, M052X, M062X, M06HF, B2PLYP52 were employed to calculate the enthalpies of formation of nitrogen-rich compounds via atomization reaction. The calculation results show that double hybrid functional B2PLYP has the smallest mean absolute deviation of 30.1 kJ·mol^{-1}, which is more accurate than G4 method. Hence, the enthalpies of formation of five all-nitrogen molecules with cage structure, namely, $N_4(T_d)$, $N_6(D_{3h})$, $N_8(O_h)$, $N_{10}(D_{5h})$, and $N_{12}(D_{6h})$, were predicted by B2PLYP functional, and the corresponding results were 756.4, 1338.2, 1878.5, 2144.3, 2787.0 kJ·mol^{-1}, respectively.

Key words: density functionals; cage structures; atomization reactions; all-nitrogen materials
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