A theoretical study of NO_2 complexes with aluminium and gallium based on topological analysis of electron density and electron localization function.

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Streszczenie

Results of DFT and MP4 calculations on $AlNO_2$ and $GaNO_2$ molecules are presented. One C_s and two C_{2v} structures (two minima and one TS) are found and their energies and vibrational frequencies are reported and discussed. The minima are close in energy and lie ca. 70 kcal mol^{-1} below reactants (M + NO_2). More insight is obtained via topological analysis of electron density and electron localization function (ELF). It is shown that the molecules are bound mainly via electrostatic interactions, and there is a significant charge transfer from metal atom to the NO_2 moiety. Detailed analysis of the ELF shows that the loss of stability of gallium complexes with respect to aluminium structures is best explained by (antibonding) influence of gallium semi-core d electrons.

Adres publiczny

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