Theoretical study of aluminum and gallium atom complexes with CO_2, CS_2 and COS.

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Streszczenie

Various possible structures for neutral ML complexes (M = Al, Ga; L = $C0_2$, CS_2, and COS) are investigated using density functional methods and the Moller-Plesset perturbation approach. Formation of C_{2v} and C_s species is observed. Obtained vibrational frequencies are compared with experimental data. Differences between CO_2 and CS_2 adducts are discussed. Absence of C_{2v} species for MCS_2 complexes, as seen in experiments, is consistent with calculated relative energies. Erratic behavior of the MP2 method when excluding core electrons from correlation suggests that for gallium 3d semi-core electrons of $GaCO_22$ complex play an important role in complex formation. Very small (ca. -3 kcal/mol) binding energies explain major difficulties in experimental observation of $GaCO_2$ complexes. To investigate this matter further, calculations for experimentally unknown MCOS complexes have been performed.

Adres publiczny

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https://www.acs.org/content/acs/en.html