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Study of the Lewis complexes of electronic structure on the basis of DFT method

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Abstract

We have analyzed by means of DFT calculations of a range of halogenide metal complexes of I, IV and V groups, halogen and interhalogen molecules and SO_3 complexes with ligands of different donor ability. Density functional theory included in the GAUSSIAN and ADF program packages were used. The geometrical parameters, rotational constants and vibrational frequencies calculated from GAUSSIAN and ADF are in agreement with the data of microwave spectroscopy in the gas phase. All-electron basis DGDZVP and ZORA approximation have shown good results in calculating constants of quarupole interaction on halogen, nitrogen and metal atoms. For the first time the correlations between charge transfer and bond energies in SO_3 and halogen complexes were obtained. It has been shown that there exists difference between halogen and SO_3 complexes on the one hand and metal halogenides on other hand. From electron partitioning analyses and Klopman's approximation it follows that for the metal and interhalogen complexes the electrostatic bonding is predominant and for SO_3 complexes there is a large contribution of covalent bonding.