

Study of chemical bonding in the complexes of interhalogen based on density functional theory

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Abstract

The density functional theory analysis was used for a number XYL complexes, formed between molecules I₂, ICl, IBr and pyridine. The calculated geometrical parameters, IR spectra and nuclear quadrupole interaction constants of iodine are consistent with the data of microwave spectroscopy and nuclear quadrupole resonance. The good correlation between the experimental and calculated binding energies of the inner electrons of iodine, chlorine and nitrogen atoms were found with the calculation of Gaussian and Slater functions. The comparison of experimental and calculated changes in the electron density on the atoms upon complex formation allowed choosing the scheme of calculating the effective charge on the atoms, which allow us to interpret the experimental spectra. It is shown that the use of both calculated schemes allows calculating the enthalpy of complex formation, close to the experimental values. The energy analysis shows that in the complexes the electrostatic binding is of dominates to that of covalent binding.