Density functional study of the H_3N-Cl_2 system - the importance of Hartree-Fock exchange in density functional methods.

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Streszczenie

Studies on the abilities of different density functional methods applied to charge transfer complexes have been carried out on the ammonia-chlorine, $H_3N\cdots Cl_2$, complex. Various non-local exchange-correlation and hybrid functionals have been used in the investigation of the structure and energetic properties of the 1:1 complex. A triple-zeta basis set, added with diffuse functions and multiple sets of polarization functions (e.g. 6-311++G(2df,2p)), has been used throughout the study. Comparison with experimental data from pulsed-nozzle Fourier-transform microwave spectroscopy and also with results from the second-order Møller-Plesset perturbation theory shows that most variants of the density functional theory (DFT) yield the intermolecular distance too short. The agreement is best for the hybrid methods mixing the Hartree-Fock exchange with Slater exchange.

Słowa kluczowe

Charge transfer complex, Density functional method, Hybrid functional

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