PRECISE THEORETICAL STUDY OF SPECTROSCOPIC CONSTANTS IN DIATOMICS

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During the last decade a significant progress in methods of molecular spectroscopy was achieved. One of the most important applications of these methods is a measurement of an electron electric dipole moment in diatomic molecules and cations containing heavy elements. In order to speed up such experiments, which usually prepared for many years, one can apply accurate *ab initio* quantum-chemical methods to predict different spectroscopic constants of a molecule or cation under consideration: scheme of electronic terms, vibrational and rotation constants, hyperfine structure constants, g-factors, lifetimes etc. In such calculations both correlation and relativistic effects should be taken into account. This is not a trivial problem for systems containing transition elements and especially lanthanides and actinides. We report results of our recent investigations of a number of diatomics including theoretical investigation of HfF^{+} [b]. Details of used methods are discussed.

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