STRUCTURE AND SPECTRA OF THE MOLECULES OF MANGANESE, IRON, AND COBALT TRIFLUORIDES: A CCSD(T) STUDY IN THE COMPLETE BASIS SET*

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The coupled-cluster singles and doubles with perturbative triples (CCSD(T)) method in triple-, quadruple-, and quintuple-zeta basis sets with extrapolation to the complete basis set limit is used to analyze the properties of MnF_3, FeF_3, and CoF_3 molecules. The relative energies of low-lying electronic states are determined. The Jahn–Teller effect is investigated in the ground electronic state $^5E'$ of the MnF_3 molecule and the first excited electronic state $^5E''$ of the CoF_3 molecule. Geometric parameters, atomization enthalpies, vibrational frequencies, intensities in the infrared and Raman spectra are found with high accuracy. The assignment of the bands observed in the low-frequency region of the IR and Raman spectra of MnF_3 and CoF_3 molecules are revised.

Keywords: manganese trifluoride, iron trifluoride, cobalt trifluoride, structure of molecules, Jahn–Teller effect, vibrational frequencies, atomization enthalpy, coupled cluster method, extrapolation to the complete basis set limit.