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Sommario/riassunto	A Structural and Vibrational Study of the Chromyl Chlorosulfate, Fluorosulfate and Nitrate Compounds presents important studies related to the structural and vibrational properties on the chromyl compounds based on Ab-initio calculations. The synthesis and the study of such properties are of chemical importance because the stereo-chemistries and reactivities of these compounds are strongly dependent on the coordination modes that adopt the different ligands linked to the chromyl group. In this book, the geometries of all stable structures in gas phase for chromyl chlorosulfate, fluorosulfate, and nitrate are optimized by using Density functional Theory (DFT). Then, the complete assignments of all observed bands in the infrared and Raman spectra are performed combining DFT calculations with Pulay´s Scaled Quantum Mechanics Force Field (SQMFF) methodology and taking into account the type of coordination adopted by the chlorosulfate, fluorosulfate and nitrate ligands as monodentate and bidentate. Moreover, the force constants for each compound at the same levels of theory are calculated. As a result, the bond orders calculated and the topological properties of electronic charge density

reveal the characteristics and nature of the different bonds in each structure.