

1. Record Nr.	UNINA9910437819103321
Autore	Brandan Silvia A
Titolo	A structural and vibrational investigation into chromylazide, acetate, perchlorate, and thiocyanate compounds // Silvia A. Brandan
Pubbl/distr/stampa	New York, : Springer Verlag, c2013
ISBN	1-283-90908-1 94-007-5754-9
Edizione	[1st ed. 2013.]
Descrizione fisica	1 online resource (90 p.)
Collana	SpringerBriefs in molecular science
Disciplina	541.2
Soggetti	Azides Acetates
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	Structural and Vibrational Properties of Chromyl Azide -- Structural and Vibrational Study on Chromyl Acetate in Different Media -- Theoretical Study on the Structural and Vibrational Properties of Chromyl Perchlorate -- Theoretical Structural and Vibrational DFT Calculations of Chromyl Thiocyanate.
Sommario/riassunto	A Structural and Vibrational Investigation into Chromyl Azide, Acetate, Perchlorate and Thiocyanate Compounds reviews the structural and vibrational properties of chromyl azide, acetate, perchlorate, and thiocyanate from a theoretical point of view by using Density Functional Theory (DFT) methods. These compounds are extensively used in organic syntheses and the study of their structure and spectroscopy has become fundamental. This book evaluates the best theoretical level and basis set to reproduce the experimental data existing for those compounds. To this end, the optimized geometries and wavenumbers for the normal modes of vibration are calculated and the obtained results are compared and analyzed. Also, the nature of the different types of bonds and their corresponding topological properties of electronic charge density are systematically and quantitatively investigated by using the NBO analysis and the atoms in molecules theory (AIM).