1. Record Nr. UNISA996395648503316

Autore	Holloway James <d. 1684.>
Titolo	The free and voluntary confession and narrative of James Holloway [[electronic resource]] : (addressed to His Majesty) written with his own hand, and delivered by himself to Mr. Secretary Jenkins ; as also the proceedings against the said James Holloway, in His Majesties Kings Bench Court, Westminster. And his petition to His Majesty
Pubbl/distr/stampa	[Dublin], : Printed by the appointment of Peter Daniel and Samuel Dashwood sheriffs, and re-printed at Dublin by Mary Crook at Ormonde-Key, 1684
Descrizione fisica	28 p
Soggetti	Trials (Treason) - England - London Great Britain History Charles II, 1660-1685 Sources Early works to 1800
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Caption title. Signed at end: James Holloway. Place and date of publication suggested by Wing (2nd ed.). Reproduction of original in: Beinecke Rare Book and Manuscript Library.
Sommario/riassunto	eebo-0009

2. Record Nr. UNINA9910437819603321

Autore	Brandan Silvia A
Titolo	A structural and vibrational study of the chromyl chlorosulfate, fluorosulfate, and nitrate compounds / / Silvia A. Brandan
Pubbl/distr/stampa	Dordrecht ; ; New York, : Springer, c2013
ISBN	1-283-90909-X 94-007-5763-8
Edizione	[1st ed. 2013.]
Descrizione fisica	1 online resource (89 p.)
Collana	SpringerBriefs in molecular science
Disciplina	530.12
Soggetti	Chemical structure Vibration
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 Analysis of Chromyl Chlorosulfate -- Structural and Vibrational Study of Chromyl Fluorosulfate -- Structural and Vibrational Study of Chromyl Nitrate.
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.