1. Record Nr. UNINA9910166053703321

Autore	Traviglia Arianna
Titolo	Across space and time : papers from the 41st Conference on Computer Applications and Quantitative Methods in Archaeology, Perth, 25-28 March 2013 / / edited by Arianna Traviglia
Pubbl/distr/stampa	Amsterdam University Press, 2017 Amsterdam, Netherlands : , : Amsterdam University Press, , 2017 ©2015
ISBN	9789048524433 9789089647153
Descrizione fisica	1 online resource (515 pages) : illustrations, maps; digital, PDF file(s)
Disciplina	930.1028
Soggetti	Archaeology - Methodology Archaeology - Data processing
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Sommario/riassunto	This volume presents a selection of the best papers presented at the forty-first annual Conference on Computer Applications and Quantitative Methods in Archaeology. The theme for the conference was "Across Space and Time", and the papers explore a multitude of topics related to that concept, including databases, the semantic Web, geographical information systems, data collection and management, and more.

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.