1. Record Nr. UNISA996396343703316

Autore	Leybourn William <1626-1716.>
Titolo	The art of measuring, or, The carpenters new rule described and explained [[electronic resource]] : furnished with variety of scales, fitted for the more speedy mensuration of divers superficies and solids, with all necessary requisits appertaining thereunto, as a plain and easie introduction to the principals of geometry, which is the ground and foundation of all kind of mensuration : together with the description and use of the logarithmical tables of proportions in arithmetick and geometry, also their particular application in the measuring of superficies and solids ... / / composed and published by W. Leybourne ... ; unto which is annexed a supplement, containing the description of the line of numbers, with its use explained and illustrated in divers practical examples of mensuration, by John Wiblin .
Pubbl/distr/stampa	London, : Printed for Richard Jones ..., 1669
Descrizione fisica	2 pts. : ill
Altri autori (Persone)	WiblinJohn
Soggetti	Carpentry - Mathematics Carpentry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	"A supplement, wherein is contained and plainly demonstrated the use of the scale of logarithms" has special t.p. Reproduction of original in British Library.
Sommario/riassunto	eebo-0018

2. Record Nr. UNINA9910254055303321

Titolo	9th Congress on Electronic Structure: Principles and Applications (ESPA 2014) : A Conference Selection from Theoretical Chemistry Accounts / / edited by Manuel F. Ruiz-Lopez, Francisco J. Olivares del Valle
Pubbl/distr/stampa	Berlin, Heidelberg : , : Springer Berlin Heidelberg : , : Imprint : Springer, , 2016
ISBN	3-662-49221-0
Edizione	[1st ed. 2016.]
Descrizione fisica	1 online resource (229 p.)
Collana	Highlights in theoretical chemistry ; ; volume 11
Disciplina	540
Soggetti	Chemistry, Physical and theoretical Atomic structure Molecular structure Theoretical and Computational Chemistry Atomic/Molecular Structure and Spectra Physical Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di contenuto	Contents; Preface to the ESPA-2014 special issue; AMOEBA force field parameterization of the azabenzenes; 1 Introduction; 2 Computational details; 2.1 Quantum calculations; 2.2 Force field; 2.2.1 The AMOEBA formalism; 2.2.2 Details of AMOEBA calculations; 2.3 Parameterization; 2.4 Atomic multipoles; 3 Force field validation and refinement of vdW parameters; 3.1 Bonded interactions, force constants, and vibrational frequencies; 3.2 Molecular multipoles and electrostatic potential; 3.3 Intermolecular interactions; 4 Conclusions; 5 Supporting information; References Triplet-singlet gap in structurally flexible organic diradicals1 Introduction; 2 Model systems; 2.1 Computational approach; 3 Results and discussion; 3.1 Local minima, isomers and enantiomers; 3.2 Triplet-singlet gaps; 4 Conclusions; References; Separating nuclear spin isomers using a pump-dump laser scheme; 1 Introduction; 2 Methods; 3 Results and discussion; 3.1 Pump process; 3.2 Dump process; 4 Conclusion; References; Spin delocalization in hydrogen

chains described with the spin-partitioned total position-spread tensor; 1 Introduction; 2 General formalism: spin partition of TPS tensor
3 Computational details4 Results and discussions; 4.1 Equally spaced hydrogen chains; 4.2 Dimerized chains; 4.2.1 Fixed-bond dimerized hydrogen chains; 4.2.2 Homothetic dimerized hydrogen chains; 4.3 Asymptotic behavior of the longitudinal position-spread tensors; 5 Conclusions; References; Invariant time-dependent exchange perturbation theory and its application to the particles collision problem; 1 Introduction; 2 Exchange perturbation theory (EPT), time-dependent perturbation; 3 Perturbation theory to the first order; 4 Perturbation theory to the second and higher orders
5 S-scattering and T-matrix elements6 Collisions with exchange of electrons; 7 Scattering of proton by lithium atom with electron exchange; 8 Conclusions; Appendix 1; Appendix 2; Appendix 3; References; On the definition of molecular dynamic magnetizability; 1 Introduction; 2 Electromagnetic multipole moment operators and the interaction Hamiltonian; 3 Induced electric dipole moment; 4 Induced magnetic dipole moment; 5 Change of response properties and equivalence conditions in a translation of coordinates; 5.1 Magnitude of origin-shift vectors
5.2 Translation of frequency-dependent response tensors6 Variation of frequency-dependent moments in acoordinate translation; 7 Orders of magnitude; 8 Concluding remarks; References; Toward (car)borane-based molecular magnets; 1 Introduction; 1.1 The theoretical models; 1.1.1 Two magnetic sites system; 1.1.2 Three magnetic sites systems; 1.1.3 Four magnetic sites system; 2 Results and discussion; 3 Concluding remarks; References; Theoretical analysis of vibrational modes in uranyl aquo chloro complexes; 1 Introduction; 2 Computational aspects; 3 Results and discussion; 4 Conclusions References

Sommario/riassunto

This volume collects research findings presented at the 9th Edition of the Electronic Structure: Principles and Applications (ESPA-2014) International Conference, held in Badajoz, Spain, on July 2–4, 2014. The contributions cover research work on theory, methods and foundations, materials science, structure and chemical reactivity as well as environmental effects and modelling. Originally published in the journal Theoretical Chemistry Accounts, these outstanding papers are now available in a hardcover print format, as well as a special electronic edition. This volume provides valuable content for all researchers in theoretical chemistry, and will especially benefit those research groups and libraries with limited access to the journal.