

1. Record Nr.	UNINA9910154920803321
Autore	Jensen Frank
Titolo	Introduction to computational chemistry // Frank Jensen
Pubbl/distr/stampa	Chichester, UK ; ; Hoboken, NJ : , : John Wiley & Sons, , [2017] ©2017
Edizione	[Third edition.]
Descrizione fisica	1 online resource (663 pages) : illustrations
Disciplina	541.0285
Soggetti	Chemistry, Physical and theoretical - Data processing Chemistry, Physical and theoretical - Mathematics Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Introduction -- Force field methods -- Hartree-Fock theory -- Electron correlation methods -- Basis sets -- Density functional methods -- Semi-empirical methods -- Valence bond methods -- Relativistic methods -- Wave function analysis -- Molecular properties -- Illustrating the concepts -- Optimization techniques -- Statistical mechanics and transition state theory -- Simulation techniques -- Qualitative theories -- Mathematical methods -- Statistics and QSAR -- Concluding remarks
Sommario/riassunto	"Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields; Tight-binding DFT; More extensive DFT functionals, excited states and time dependent molecular properties; Accelerated Molecular Dynamics methods; Tensor decomposition methods; Cluster analysis; Reduced scaling and reduced prefactor methods" -- From the publisher.

2. Record Nr.	UNISA996280485803316
Titolo	IEEE Std 1858-2016 (Incorporating IEEE Std 1858-2016/Cor 1-2017) : IEEE Standard for Camera Phone Image Quality // Institute of Electrical and Electronics Engineers
Pubbl/distr/stampa	New York, NY, USA : , : IEEE, , 2017
ISBN	1-5044-2388-7
Descrizione fisica	1 online resource (xi, 131 pages) : illustrations
Collana	IEEE Standard
Disciplina	621.380414
Soggetti	Image transmission Imaging systems - Image quality
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di contenuto	Overview -- Normative references -- Definitions, acronyms, and abbreviations -- Test conditions and apparatus -- Spatial frequency response (SFR) -- Lateral chromatic displacement -- Chroma level -- Color uniformity -- Local geometric distortion -- Visual noise -- Texture blur -- Annex A (normative) Subjective evaluation methodology -- Annex B (normative) Viewing conditions and conversion to angular spatial frequency -- Annex C (normative) Slanted edge SFR algorithm -- Annex D (normative) Visual noise processing -- Annex E (normative) Steps to calculate texture acutance -- Annex F (informative) SFR data processing -- Annex G (informative) Linearization by inversion of gamma curve -- Annex H (informative) Example acutance calculation -- Annex I (informative) Color uniformity illustrative example -- Annex J (informative) Lateral chromatic displacement -- illustrative example -- Annex K (informative) Extracting the dots from the target -- Annex L (informative) Dot center validation -- Annex M (informative) Local geometric distortion -- illustrative example and validation -- Annex N (informative) Grid sort -- Annex O (informative) Derivation of objective metric to JND mapping -- Annex P (informative) Fitting the texture MTF -- Annex Q (informative) Example texture analysis -- Annex R (informative) Example texture blur results -- Annex S (informative) Texture blur chart design -- Annex T (informative) Subjective data and models -- Annex U (informative) Bibliography.

