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Edward I. Solomon • Robert A. Scott • R. Bruce King

Computational

Inorganic and Bioinorganic Chemistry

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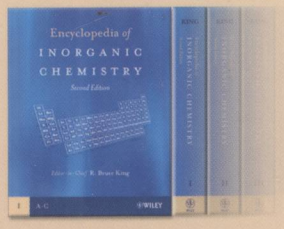

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EIC Books

COMPUTATIONAL Inorganic and Bioinorganic Chemistry

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Periodic Table of the Elements

Group →	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period → 1	1 H 1.0079																	2 He 4.0026
2	3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.0107	7 N 14.0067	8 O 15.9994	9 F 18.9984	10 Ne 20.179
3	11 Na 22.9898	12 Mg 24.305											13 Al 26.9815	14 Si 28.0855	15 P 30.9738	16 S 32.066	17 Cl 35.453	18 Ar 39.948
4	19 K 39.0983	20 Ca 40.078	21 Sc 44.9559	22 Ti 47.867	23 V 50.9415	24 Cr 51.996	25 Mn 54.9380	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.409	31 Ga 69.723	32 Ge 72.64	33 As 74.9216	34 Se 78.96	35 Br 79.904	36 Kr 83.798
5	37 Rb 85.4678	38 Sr 87.62	39 Y 88.9059	40 Zr 91.224	41 Nb 92.9064	42 Mo 95.94	43 Tc 98.9062	44 Ru 101.07	45 Rh 102.9055	46 Pd 106.42	47 Ag 107.8682	48 Cd 112.41	49 In 114.818	50 Sn 118.710	51 Sb 121.760	52 Te 127.60	53 I 126.9045	54 Xe 131.29
6	55 Cs 132.9054	56 Ba 137.327	57 * La 138.9055	72 Hf 178.49	73 Ta 180.9479	74 W 183.84	75 Re 186.207	76 Os 190.2	77 Ir 192.22	78 Pt 195.08	79 Au 196.9665	80 Hg 200.59	81 Tl 204.3833	82 Pb 207.2	83 Bi 208.9804	84 Po (209)	85 At (210)	86 Rn (222)
7	87 Fr (223)	88 Ra (226.0254)	89 ** Ac (227.0277)	104 Rf (261.1088)	105 Db (262.1141)	106 Sg (266.1219)	107 Bh (264.12)	108 Hs (277)	109 Mt (268.1388)	110 Ds (271)	111 Rg (272)							

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* LANTHANIDES	58 Ce 140.12	59 Pr 140.9077	60 Nd 144.24	61 Pm (147)	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.9254	66 Dy 162.50	67 Ho 164.9304	68 Er 167.26	69 Tm 168.9342	70 Yb 173.04	71 Lu 174.967
** ACTINIDES	90 Th 232.0381	91 Pa 231.0359	92 U 238.0289	93 Np 237.0482	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (260)	102 No (259)	103 Lr (262)

Based on information from IUPAC, the International Union of Pure and Applied Chemistry (version dated 1st November 2004).
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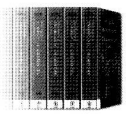

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Encyclopedia of Inorganic Chemistry

In 1994 John Wiley & Sons published the *Encyclopedia of Inorganic Chemistry* (EIC). This 8-volume work was well received by the community, and has become a standard publication in all libraries serving the inorganic, coordination chemistry, organometallic and bioinorganic communities. The 10-volume Second Edition of the *Encyclopedia* was published in print in 2005, and online in 2006, on the major reference platform Wiley InterScience:

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Series Preface

The success of the *Encyclopedia of Inorganic Chemistry* (EIC) has been very gratifying to the Editors. We felt, however, that not everyone would necessarily need access to the full ten volumes of EIC. Some readers might prefer to have more concise thematic volumes targeted to their specific area of interest. This idea encouraged us to produce a series of EIC Books, focusing on topics of current interest. These books will continue to appear on a regular basis and will feature leading scholars in their fields. Like the Encyclopedia, we hope that EIC Books will give both the starting research student and the confirmed research worker a critical distillation of the leading concepts and provide a structured entry into the fields covered.

Computer literature searches have become so easy that one could be led into thinking that the problem of efficient access to chemical knowledge is now solved. In fact, these searches often produce such a vast mass of material that the reader is overwhelmed. As Henry Kissinger has remarked, the end result is often a shrinking of one's perspective. From studying the volumes that comprise the EIC Books series, we hope that readers will find an expanding perspective to furnish ideas for research, and a solid, up-to-date digest of current knowledge to provide a basis for instructors and lecturers.

I take this opportunity of thanking Bruce King, who pioneered the *Encyclopedia of Inorganic Chemistry*, my fellow editors, as well as the Wiley personnel, and, most particularly, the authors of the articles for the tremendous effort required to produce such a series on time. I hope that EIC Books will allow readers to benefit in a more timely way from the insight of the authors and thus contribute to the advance of the field as a whole.

Robert H. Crabtree
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January 2009

Volume Preface

Over the past several decades there have been major advances in our ability to evaluate computationally the electronic structure of inorganic molecules, particularly transition metal systems. This is due to the Moore's Law increase in computing power as well as the impact of density functional theory (DFT) and its implementation in commercial and freeware programs for quantum chemical calculations. Improved pure and hybrid density functionals are now allowing DFT calculations with accuracy comparable to high level Hartree–Fock (HF) treatments, and the results of these calculations can now be evaluated based on experiment. The latter is made possible through the development of modules for the calculation of spin-Hamiltonian parameters and other ground state properties (vibrational frequencies, g and A matrices, D tensor, etc.) and ΔSCF and time-dependent density functional theory (TDDFT) methods for correlation to electronic excited states. Developments in wave function methods have also extended their use to a wide range of transition metal systems.

The availability and ease in utility of electronic structure codes have led to their becoming a significant component of the experimental chemist's toolbox. Indeed many papers on inorganic systems in the major chemical literature now contain electronic structure calculations as a complement to experimental results. Despite the significant advances in theory, the accuracy of computational methods is still limited when applied to transition metal systems, and different DFT functionals, levels of implementation of HF based methods (Moeller-Plesset perturbation theory (MP), complete active space (CAS), coupled cluster (CC), configurational interaction (CI)), and model designs can give different results. It is therefore of critical importance to calibrate calculations with experiments. However, when calculations are correlated to and supported by experimental data they can provide fundamental insight into electronic structure and its contributions to physical properties and chemical reactivity. This interplay will continue to expand and contribute to both improved value of experimental results and improved accuracy of computational predictions.

The purpose of this volume is to provide state-of-the-art presentations of quantum mechanical and related methods and their applications by many of the leaders in the field. Part 1 of this volume focuses on methods, their background and implementation, and their use in describing bonding properties, energies, transition states and spectroscopic features. Then we focus on applications in bioinorganic chemistry (Part 2) and inorganic chemistry (Part 3) where electronic structure calculations have already had a major impact. We believe this volume will be of significant value to both experimentalists and theoreticians, and anticipate that it will stimulate both further development of the methodology and its applications in the many interdisciplinary fields that comprise modern inorganic chemistry.

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September 2009

Abbreviations and Acronyms used in this Volume

ABL	Alternating ''short-and-long'' Bond Length
ABS	Absorption Spectroscopy
ACS	Acetyl-Coenzyme A Synthase
ADF	Amsterdam Density Functional
AdNDP	Adaptive Natural Density Partitioning
Ado	Adenosyl
$AdoCbi^+$	Adenosylcobinamide
AdoCbl	Adenosylcobalamin
AE	All-Electron
AF	Antiferromagnetic
AIM	Atoms-In-Molecules
AIMP	Ab Initio Model Potential
AM1	Austin Method 1
ANL	Argonne National Laboratory
ANO	Atomic Natural Orbital
AO	Atomic Orbital
APS	Advanced Photon Source
ARCS	Aromatic Ring-Current Shielding
ASM	Adiabatic Simulation Method
ATP	Adenosine Triphosphate
ATR	Adenosyltransferase
B3	Becke Hybrid
B3LYP	Becke's Three-parameter Hybrid Functional for Exchange Combined with the Lee-Yang-Par Correlation Functional
BCPs	Bond Critical Points
BDE	Bond Dissociation Energy
BKB-HB	Backbone Hydrogen Bond
BLYP	Becke–Lee–Yang–Parr
BNCT	Boron Neutron Capture Therapy
BO	Born–Oppenheimer
BP86	Nonhybrid Functional by Becke and Perdew
BS	Broken Symmetry
BSSE	Basis Set Superposition Errors
CA	Carbonic Anhydrase
CAS	Complete Active Space
CASPT2	Complete Active Space Perturbation Theory Second Order
CASSCF	Complete Active Space Self-Consistent Field
Cbi^+	Cobinamide
Cbl	Cobalamin
CBS	Complete Basis Set
CC	Computational Chemistry
cc-pVDZ	Correlation-consistent polarized Valence Double-Zeta
cc-pVnZ	Correlation-consistent polarized Valence n-Zeta
cc-pVQZ	Correlation-consistent polarized Valence Quadruple-Zeta
cc-pVTZ	Correlation-consistent polarized Valence Triple-Zeta
cc-pwCVnZ	Correlation-consistent Weighted Core-Valence n-Zeta
CC	Coupled Cluster
CCO	Cytochrome *c* Oxidase
CCSD(T)	Coupled Cluster with Single, Double, and Perturbative Triple Excitation
CD	Cholesky Decomposition
CD	Circular Dichroism
CDA	Charge Decomposition Analysis
CF	Configuration Function
CFeSP	Corrinoid/Iron–Sulfur Protein
CG	Cowan–Griffin
CH3-THF	Methyl-Tetrahydrofolate
CI	Configuration Interaction
CIS	CI with Single Excitation
CISD	CI with Single and Double Excitation
CNCbl	Cyanocobalamin
CNDO	Complete Neglect of Differential Overlap
$Co^{1+}Cbl$	Cob(I)alamin
$Co^{2+}Cbl$	Cob (II)alamin
$Co^{2+}Cbi^+$	Cob(II)inamide
$Co^{3+}Cbi^+$	Cob(III)inamide
$Co^{3+}Cbl$	Cob(III)alamin
COSMO	Conductor-like Screening Model
CP-SCF	Coupled-Perturbed Self-Consistent Field
CPA	Carboxypeptidase A
CPCM	Conductor-Like Polarizable Continuum Model
CPMD	Car–Parrinello Molecular Dynamics
CSF	Configuration State Function
CT	Charge Transfer
CV	Core–Valence
CVE	Cluster Valence Electron
DCD	Dewar–Chatt–Duncanson
DF	Density Functional
DFG	Deutsche Forschungsgemeinschaft
DFT	Density Functional Theory
DK	Douglas–Kroll
DKH	Douglas–Kroll–Hess
DMB	5,6-Dimethylbenzimidazole
DNIC	Dinitrosyl Iron Complex
DOC	Differential Orbital Covalency
DOS	Density of States
DSD	Diamond–Square–Diamond
DTMA	Di(thiomethyl) Amine
DZ	Double-Zeta
EA	Electron Affinity
EAN	Effective Atomic Number
EBO	Effective Bond Order
ECDA	Extended Charge Decomposition Analysis
ECP	Effective Core Potential
EDA	Energy Decomposition Analysis
EE	Electrostatic Embedding
EFG	Electric Field Gradient
EFP	Effective Fragment Potential
EHT	Extended Hückel Theory
ELF	Electron Localization Function
EM	Electromagnetic
ENDOR	Electron Nuclear Double Resonance
EOM-CCSD	Equation-of-Motion CCSD
EPR	Electron Paramagnetic Resonance
ERI	Electron Repulsion Integral
ESEEM	Electron Spin-Echo Envelope Modulation
ESP	Electrostatic Potential
ESR	Electron Spin Resonance
ET	Electron Transfer
EVB	Empirical Valence Bond
EXAFS	Extended X-ray Absorption Fine Structure
FCI	Fond der Chemischen Industrie
FE	Free Energy
FEP	Free-Energy Perturbation
FF	Force Field
FMM	Fast Multipole Methods
FMO	Frontier Molecular Orbital
FPP	Farnesyl Diphosphate
FTase	Farnesyltransferase
FTICR-MS	Fourier Transform Ion Cyclotron Resonance Mass Spectrometry
GAFF	General AMBER Force Field
GB	Gas Phase Basicity
GC	Guanylyl Cyclase
GFP	Green Fluorescent Protein
GGA	Generalized Gradient Approximation
GIAO	Gauge-Including Atomic Orbital
GIPAW	Gauge-Including Projector-Augmented Wave

GM	Glutamate Mutase
GPx	Glutathione Peroxidase
GTO	Gaussian-Type Orbital
GUGA	Graphical Unitary Group Approach
GVB	Generalized Valence Bond
GVB-CI	Generalized Valence Bond Plus Configuration Interaction
H_2OCbl^+	Aquacobalamin
hATR	Human Adenosyltransferase
Hcy	Homocysteine
HF	Hartree–Fock
HF-SCF	Hartree–Fock Self-Consistent Field
HFC	Hyperfine Coupling
His	Histidine
HK	Hohenberg and Kohn
HMG	High Mobility Group
HMPT	H2 to N5, N10-Methylene-Tetrahydromethanopterin
HOMO	Highest Occupied Molecular Orbital
HPA	Heteropolyoxoanion
HS	High-Spin
HSE	Heyd, Scuseria and Ernzerhof
HYSCORE	Hyperfine Sublevel Correlation Spectroscopy
H-L	HOMO–LUMO
ICR	Ion Cyclotron Resonance
IEF-PCM	Integral Equation Formalism Polarizable Continuum Model
IGLOs	Individual Gauge for Localized Orbitals
IL	Intraligand
IMOMM	Integrated Molecular Orbital Molecular Mechanics
INDO	Intermediate Neglect of Differential Overlap
IP	Ionization Potential
IPA	Isopolyoxoanion
IPN	Isopenicillin N
IPNS	Isopenicillin N Synthase
IR	Infrared
IRC	Internal Reaction Coordinate
ISC	Intersystem Crossing
ISTLS	Inhomogeneous Singwi–Tosi–Land-Sjölander
JST	Japan Science and Technology
KS	Kohn–Sham
LA	Long Axis
LDA	Local Density Approximation
LED	Light Emitting Diode
LF	Ligand Field
LFER	Linear Free Energy Relationship
LFMM	Ligand Field Molecular Mechanics
LFSE	Ligand Field Stabilization Energy
LHF	Localized Hartree–Fock
LLCT	Ligand–Ligand-Charge-Transfer
LM	Large Model
LMCT	Ligand to Metal Charge Transfer
LMO	Localized Molecular Orbital
LOC	Localized Orbital Correction
lp	Lone-Pair
ls	Low-spin
LUMO	Lowest Unoccupied Molecular Orbital
LYP	Lee–Yang–Parr
MAE	Mean Absolute Error
MAs	Minor Actinide
MAS	Magic-Angle Spinning
MB	Mössbauer
MBPT	Many-Body Perturbation Theory
MC	Multiconfiguration
MCA	Methyl Cation Affinity
MCD	Magnetic Circular Dichroism
MCO	Multicopper Oxidase
MCPF	Modified Coupled Pair Functional
MCSCF	Multiconfiguration Self-Consistent Field
MD	Molecular Dynamics
ME	Mechanical Embedding
Me	Methyl
$MeCbi^+$	Methylcobinamide
MeCbl	Methylcobalamin
MeIm	Methylimidazole
MEP	Molecular Electrostatic Potential
Met	Methionine
meta-GGA	Meta-generalized Gradient Approximation
MetAP	Methionine Aminopeptidase
MetH	Methionine Synthase
MLCT	Metal-to-Ligand Charge Transfer
MM	Molecular Mechanics
MMCM	Methylmalonyl-CoA Mutase
MMCoA	Methylmalonyl-CoA
MMFF	Merck Molecular Force Field
MMO	Methane Monooxygenase
MNDO	Modified Neglect of Differential Overlap
MO	Molecular Orbital
MP	Møller–Plesset
MP2	Møller–Plesset Second-order Perturbation Theory
MPn	Møllet–Plesset nth order Perturbation Theory
MPU	Modeled Peptide Unit
MRCI	Multireference Configuration Interaction
MSBCT	Metal-to-Sigma-Bond-Charge-Transfer
MVD	Mass–Velocity and One-Electron Darwin
mve	Metallic Valence Electron
NBO	Natural Bond Orbital
NCA	Normal Coordinate Analysis
NDDO	Neglect of Diatomic Differential Overlap
NICS	Nuclear-Independent Chemical Shift
NIR	Near-Infrared
NLO	Nonlinear Optical
NMR	Nuclear Magnetic Resonance
NO	Nitric Oxide
NQC	Nuclear Quadrupole Coupling
NRVS	Nuclear Resonance Vibrational Spectroscopy
OEC	Oxygen-Evolving Complex
OEP	Optimized Effective Potential
ONIOM	Our own N-layered Integrated Molecular Orbital + Molecular Mechanics
op-sym	out-of-plane Symmetry
OPDOS	Overlap-Population Density of States
OR	Optical Rotation
ORD	Optical Rotatory Dispersion
PA	Proton Affinity
PAW	Projector-Augmented Wave
PBE	Poisson Equation or Poisson–Boltzmann Equation
PBSA	Poisson–Boltzmann Solvation, Combined with a Surface-Area Method
Pc	Plastocyanin
pc-n	Polarization-Consistent n-zeta
PCET	Proton Coupled Electron Transfer
PCM	Polarizable Continuum Model
PDB	Protein Data Bank
pdt	Propanedithiolate
MPT^+	N5, N10-Methenyl-Tetrahydromethanopterin
PES	Photoelectron Spectroscopy
PES	Potential Energy Surface
Phe	Phenylalanine
PHVA	Partial Hessian Vibrational Analysis
PI	Photoionization
PJT	Pseudo-Jahn–Teller
PMF	Potential of Mean Force

PMn	nth Parameterization Method For Neglect of Diatomic Differential Overlap
pNMR	Paramagnetic NMR
POM	Polyoxometalate
POS	Points on a Sphere
PP	Pseudopotential
PRDDO	Partial Retention of Diatomic Differential Overlap
PSBR	Protonated Schiff Base of Retinal
PSEP	Polyhedral Skeletal Electron Pair
PSI	Photosystem I
PSII	Photosystem II
QC	Quantum Chemical
QCA-NCA	Quantum Chemistry Assisted Normal Coordinate Analysis
QCPE	Quantum Chemistry Program Exchange
QIT-MS	Quadrupole Ion-Trap Mass Spectrometer
QM	Quantum Mechanical
QM/MM	Quantum Mechanics/Molecular Mechanics
QM/MM/PCM	Quantum Mechanics/Molecular Mechanics/ Polarizable Continuum Model
QTCP	QM/MM Thermodynamic Cycle Perturbation
RAMO	Redox-Active Molecular Orbital
RASSCF	Restricted Active Space Self-Consistent Field
RC	Reaction Coordinate
Rd	Rubredoxin
RE	Resonance Energy
RECP	Relativistic Effective Core Potential
RFO	Rational Function Optimization
RG	Runge and Gross
RM1	Recife Model 1
RMS	Root Mean Square
RMSD	Root Mean Square Deviation
RPA	Random-Phase Approximation
rR	Resonance Raman
RRS	Roussin's Red Salt
RTK	Receptor Tyrosine Kinase
SA	Short Axis
SAC	Symmetry-Adapted Cluster
SAM	S-Adenosylmethionine
SBB	N-(4-sulfamylbenzoyl) Benzylamine
SBSBCT	Sigma-Bond-to-Sigma-Bond-Charge-Transfer
SC	Side Chain
SCC	Self-Consistent Charge
SCF	Self-Consistent Field
STR-HB	Strong Low-Barrier Hydrogen Bond
SCoA	Succinyl-CoA
SCRF	Self-Consistent Reaction Field
SCS-MP2	Spin-Component-Scaled MP2
SDC-HB	Side Chain Hydrogen Bond
SDD	Stuttgart–Dresden
SEN	Schrödinger Equation for Nuclear Motion
SERS	Surface-Enhanced Raman Spectroscopy
sGC	Soluble Guanylate Cyclase
SHE	Standard Hydrogen Electrode
SHFC	Super Hyperfine Coupling Constant
SIC	Self-Interaction Corrected
SLBO	Strictly Localized Bond Orbital
SM	Small Model
SO	Sulfite Oxidase
SO-RASSI	Spin-Orbit Restricted Active Space State Interaction
SOC	Spin-Orbit Coupling
SOC-CI	Spin-Orbit Coupling Configuration Interaction
SOMO	Singly Occupied Molecular Orbital
SORCI	Spectroscopy-Oriented Configuration Interaction
SQM	Scaled Quantum Mechanical
SR	Sarcoplasmic Reticulum
SRP	Specific Reaction Parameters
STO	Slater-Type Orbital
SVD	Singular Value Decomposition
TAE	Total Atomization Energy
TD-DFT	Time-Dependent Density Functional Theory
TERI	Two-Electron Repulsion Integral
THF	Tetrahydrofolate
TLN	Thermolysine
TM	Transition Metal
TS	Transition State
TSH	Tensor Spherical Harmonic
TSH	Tensor Surface Harmonic
TSR	Two-State Reactivity
TS	Transition State
TST	Transition State Theory
TZP or TZ2P	Polarized Triple-Zeta
UAHF	United Atomic Hartree–Fock
UKS-DFT	Unrestricted Kohn–Sham DFT
UV	Ultraviolet
VB	Valence Bond
VBCI	Valence Bond Configuration Interaction
VCPO	Vanadium-Containing Chloroperoxidase
VDE	Vertical Detachment Energy
VDOS	Vibrational Density of States
vdW	van der Waals
VO	Valence-Only
VRI	Valley-Ridge Inflection Point
VS	Very Small
VSEPR	Valence Shell Electron-Pair Repulsion
VT	Variable-Temperature
VTVH	Variable-Temperature, Variable-Field
WB	Wood–Boring
WF	Wave Function
WFT	Wave Function Theory
XAFS	X-ray Absorption Fine Structure
XANES	X-ray Absorption Near-Edge Structure
XAS	X-ray Absorption Spectroscopy
XC	Exchange Correlation
XDH	Xanthine Dehydrogenase
XLCT	Halide-to-Ligand Charge-Transfer
XO	Xanthine Oxidase
yCD	Yeast Cytosine Deaminase
ZDO	Zero Differential Overlap
ZFS	Zero-Field Splitting
ZORA	Zero-Order Regular Approximation
ZPC	Zero-Point Correction
ZPVE	Zero-Point Vibrational Energy