Helder M Marques

List of Publications by Year
in descending order

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155 papers	4,947 citations	125106 35 h-index	134545 62 g-index
155 all docs	155 docs citations	155 times ranked	4469 citing authors

#	Article	IF	Citations
1	Chalcogen Bonding in the Molecular Dimers of WCh2 (Ch = S, Se, Te): On the Basic Understanding of the Local Interfacial and Interlayer Bonding Environment in 2D Layered Tungsten Dichalcogenides. International Journal of Molecular Sciences, 2022, 23, 1263.	1.8	12
2	ChalcogenÂ·Â·Â·Chalcogen Bonding in Molybdenum Disulfide, Molybdenum Diselenide and Molybdenum Ditelluride Dimers as Prototypes for a Basic Understanding of the Local Interfacial Chemical Bonding Environment in 2D Layered Transition Metal Dichalcogenides. Inorganics, 2022, 10, 11.	1.2	8
3	The Phosphorus Bond, or the Phosphorus-Centered Pnictogen Bond: The Covalently Bound Phosphorus Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. Molecules, 2022, 27, 1487.	1.7	17
4	The Nitrogen Bond, or the Nitrogen-Centered Pnictogen Bond: The Covalently Bound Nitrogen Atom in Molecular Entities and Crystals as a Pnictogen Bond Donor. Compounds, 2022, 2, 80-110.	1.0	20
5	The Stibium Bond or the Antimony-Centered Pnictogen Bond: The Covalently Bound Antimony Atom in Molecular Entities in Crystal Lattices as a Pnictogen Bond Donor. International Journal of Molecular Sciences, 2022, 23, 4674.	1.8	10
6	The Pnictogen Bond: The Covalently Bound Arsenic Atom in Molecular Entities in Crystals as a Pnictogen Bond Donor. Molecules, 2022, 27, 3421.	1.7	13
7	Physical and optoelectronic features of lead-free A₂AgRhBr₆ (A = Cs, Rb, K,) Tj ETQq1 1 0.784314 rgBT /Ov 12968-12983.	2.7	19
8	The Cs2AgRhCl6 Halide Double Perovskite: A Dynamically Stable Lead-Free Transition-Metal Driven Semiconducting Material for Optoelectronics. Frontiers in Chemistry, 2020, 8, 796.	1.8	24
9	Does Chlorine in CH3Cl Behave as a Genuine Halogen Bond Donor?. Crystals, 2020, 10, 146.	1.0	18
10	The chalcogen bond: can it be formed by oxygen?. Physical Chemistry Chemical Physics, 2019, 21, 19969-19986.	1.3	32
11	C70 Fullerene Cage as a Novel Catalyst for Efficient Proton Transfer Reactions between Small Molecules: A Theoretical study. Scientific Reports, 2019, 9, 10650.	1.6	8
12	Is the Fluorine in Molecules Dispersive? Is Molecular Electrostatic Potential a Valid Property to Explore Fluorine-Centered Non-Covalent Interactions?. Molecules, 2019, 24, 379.	1.7	69
13	Nature of halogenâ€centered intermolecular interactions in crystal growth and design: Fluorineâ€centered interactions in dimers in crystalline hexafluoropropylene as a prototype. Journal of Computational Chemistry, 2019, 40, 1836-1860.	1.5	17
14	Halogen Bonding: A Halogen-Centered Noncovalent Interaction Yet to Be Understood. Inorganics, 2019, 7, 40.	1.2	115
15	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CH3NH3PbI3 hybrid organic-inorganic halide perovskite solar cell semiconductor. Scientific Reports, 2019, 9, 50.	1.6	95
16	Probing the nature of the Co(III) ion in corrins: The reactions of aquacyano-5-seco-cobyrinic acid heptamethyl ester with anionic ligands. Inorganica Chimica Acta, 2019, 484, 402-413.	1.2	2
17	Revealing Factors Influencing the Fluorineâ€Centered Nonâ€Covalent Interactions in Some Fluorineâ€Substituted Molecular Complexes: Insights from Firstâ€Principles Studies. ChemPhysChem, 2018, 19, 1486-1499.	1.0	21
18	Halogen in materials design: Revealing the nature of hydrogen bonding and other non-covalent interactions in the polymorphic transformations of methylammonium lead tribromide perovskite. Materials Today Chemistry, 2018, 9, 1-16.	1.7	33

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19	Halogen in materials design: Fluoroammonium lead triiodide (FNH₃PbI₃) perovskite as a newly discovered dynamical bandgap semiconductor in 3D. International Journal of Quantum Chemistry, 2018, 118, e25621.	1.0	2
20	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. Journal of Computational Chemistry, 2018, 39, 343-350.	1.5	33
21	Revealing the Chemistry between Band Gap and Binding Energy for Leadâ€/Tinâ€Based Trihalide Perovskite Solar Cell Semiconductors. ChemSusChem, 2018, 11, 449-463.	3.6	27
22	Halogen in materials design: Chloroammonium lead triiodide perovskite (ClNH 3 PbI 3) a dynamical bandgap semiconductor in 3D for photovoltaics. Journal of Computational Chemistry, 2018, 39, 1902-1912.	1.5	2
23	Can Combined Electrostatic and Polarization Effects Alone Explain the FÂ·Â·Â·F Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. Computation, 2018, 6, 51.	1.0	32
24	A DFT assessment of some physical properties of iodine-centered halogen bonding and other non-covalent interactions in some experimentally reported crystal geometries. Physical Chemistry Chemical Physics, 2018, 20, 15316-15329.	1.3	23
25	Revealing the Cooperative Chemistry of the Organic Cation in the Methylammonium Lead Triiodide Perovskite Semiconductor System. ChemistrySelect, 2018, 3, 7269-7282.	0.7	12
26	Hybrid organicâ€“inorganic CH₃NH₃PbI₃ perovskite building blocks: Revealing ultraâ€strong hydrogen bonding and mulliken inner complexes and their implications in materials design. Journal of Computational Chemistry, 2017, 38, 2802-2818.	1.5	32
27	Synthesis of copper and zinc 2-(pyridin-2-yl)imidazo[1,2-a]pyridine complexes and their potential anticancer activity. European Journal of Medicinal Chemistry, 2017, 126, 353-368.	2.6	61
28	Probing the nature of the Co(III) ion in cobalamins: The ligand substitution reactions of aquacyanocobester, aquacyano(10-nitro)cobester and aquacyano(10-amino)cobester. Inorganica Chimica Acta, 2016, 450, 269-278.	1.2	7
29	Can an entirely negative fluorine in a molecule, viz. perfluorobenzene, interact attractively with the entirely negative site(s) on another molecule(s)? Like liking like!. RSC Advances, 2016, 6, 19098-19110.	1.7	42
30	Hexahalogenated and their mixed benzene derivatives as prototypes for the understanding of halogenÂ·Â·Â·halogen intramolecular interactions: New insights from combined DFT, QTAIMâ€, and RDGâ€based NCI analyses. Journal of Computational Chemistry, 2015, 36, 2328-2343.	1.5	20
31	Fluorines in tetrafluoromethane as halogen bond donors: Revisiting address the nature of the fluorine'sÏƒ_{hole}. International Journal of Quantum Chemistry, 2015, 115, 453-470.	1.0	44
32	The kinetics of the substitution of coordinated H2O on Co(III) by cyanide in aquacobalamin (vitamin) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.8	4
33	Probing the nature of the Co(III) ion in cobalamins: The reactions of aquacobalamin (vitamin B12a), aqua-10-chlorocobalamin and aqua-10-bromocobalamin with anionic and neutral ligands. Inorganica Chimica Acta, 2015, 436, 29-38.	1.2	6
34	Unusual bonding modes of perfluorobenzene in its polymeric (dimeric, trimeric and tetrameric) forms: entirely negative fluorine interacting cooperatively with entirely negative fluorine. Physical Chemistry Chemical Physics, 2015, 17, 31624-31645.	1.3	34
35	Ligand(s)-to-metal charge transfer as a factor controlling the equilibrium constants of late first-row transition metal complexes: revealing the Irvingâ€“Williams thermodynamical series. Physical Chemistry Chemical Physics, 2015, 17, 805-811.	1.3	19
36	Significant evidence of Câ‹¯O and Câ‹¯C long-range contacts in several heterodimeric complexes of CO with CH₃â€“X, should one refer to them as carbon and dicarbon bonds!. Physical Chemistry Chemical Physics, 2014, 16, 17238-17252.	1.3	56

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37	The Synthesis of a Corrole Analogue of Aquacobalamin (Vitamin B_{12a}) and Its Ligand Substitution Reactions. Inorganic Chemistry, 2014, 53, 4418-4429.	1.9	9
38	Halogen bonding interaction of chloromethane with several nitrogen donating molecules: addressing the nature of the chlorine surface Ïƒ-hole. Physical Chemistry Chemical Physics, 2014, 16, 19573-19589.	1.3	38
39	Outer-sphere anion recognition by a cyclen-based octadentate europium(<scp>iii</scp>) complex: pH dependent recognition of ortho-phthalic acid. Chemical Communications, 2014, 50, 1582-1584.	2.2	4
40	Modulating Cavity Size in an Acyclic Amino Alcohol Assembly. Journal of Chemical Crystallography, 2014, 44, 229-235.	0.5	0
41	Polymorphic Diversity: N-Phenylbenzamide as a Possible Polymorphophore. Crystal Growth and Design, 2013, 13, 3463-3474.	1.4	15
42	Probing the Nature of the Co(III) Ion in Corrins: Comparison of Reactions of Aquacyanocobyrinic Acid Heptamethyl Ester and Aquacyano-Stable Yellow Cobyrinic Acid Hexamethyl Ester with Neutral N-Donor Ligands. Inorganic Chemistry, 2013, 52, 1077-1083.	1.9	6
43	DFT Studies of Trans and Cis Influences in the Homolysis of the Coâ€“C Bond in Models of the Alkylcobalamins. Journal of Physical Chemistry A, 2013, 117, 3057-3068.	1.1	19
44	Phenylvinylcobalamin: an alkenylcobalamin featuring a ligand with a large trans influence. Dalton Transactions, 2013, 42, 7555.	1.6	5
45	The preparation of N-acetyl-Co(III)-microperoxidase-8 (NAcCoMP8) and its ligand substitution reactions: A comparison with aquacobalamin (vitamin B12a). Journal of Inorganic Biochemistry, 2013, 123, 66-79.	1.5	13
46	Bis(2-hydroxyethyl)ammonium 2-bromophenolate. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2610-o2610.	0.2	2
47	(2-Aminophenyl)methanol. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o174-o174.	0.2	2
48	4-(Dimethoxymethyl)phenyl 2,3,4,6-tetra-O-acetyl-Î²-D-glucopyranoside. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o1202-o1202.	0.2	0
49	Bis(2-bromoethyl)ammonium bromide. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2570-o2571.	0.2	0
50	Helical self-assembly of 2-(1,4,7,10-tetraazacyclododecan-1-yl)cyclohexan-1-ol (cycyclen). Acta Crystallographica Section C: Crystal Structure Communications, 2012, 68, o383-o386.	0.4	3
51	Can a Single Molecule of Water be Completely Isolated Within the Subnanoâ€Space Inside the Fullerene C₆₀ Cage? A Quantum Chemical Prospective. Chemistry - A European Journal, 2012, 18, 15345-15360.	1.7	44
52	cis Influence in Models of Cobalt Corrins by DFT and TD-DFT Studies. Journal of Physical Chemistry B, 2012, 116, 8836-8845.	1.2	18
53	5,10,15,20-Tetra-p-phenylsulfonyporphinatocobalt(III), a water-soluble Co(III) porphyrin. Inorganica Chimica Acta, 2012, 392, 108-111.	1.2	5
54	The cis influence of the corrin in vitamin B12 models. Chemical Physics Letters, 2012, 550, 150-155.	1.2	8

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55	An electronic structure theory investigation of the physical chemistry of the intermolecular complexes of cyclopropenylidene with hydrogen halides. Journal of Computational Chemistry, 2012, 33, 2073-2082.	1.5	11
56	A Density Functional Theory and Quantum Theory of Atoms-in-Molecules Analysis of the Stability of Ni(II) Complexes of Some Amino Alcohol Ligands. Journal of Physical Chemistry A, 2011, 115, 6629-6640.	1.1	8
57	Hydrogen-bond interactions in morpholinium bromide. Acta Crystallographica Section E: Structure Reports Online, 2011, 67, o2594-o2594.	0.2	5
58	Probing the Nature of the Co^{III}Ion in Corrins: The Structural and Electronic Properties of Dicyano- and Aquacyanocobyrinic Acid Heptamethyl Ester and a Stable Yellow Dicyano- and Aquacyanocobyrinic Acid Heptamethyl Ester. Inorganic Chemistry, 2011, 50, 8700-8718.	1.9	21
59	Probing the Nature of the CoIIIIon in Corrins: A Comparison of the Thermodynamics and Kinetics of the Ligand Substitution Reactions of Aquacyanocobyrinic Acid Heptamethyl Ester and Stable Yellow Aquacyanocobyrinic Acid Heptamethyl Ester. Inorganic Chemistry, 2011, 50, 8719-8727.	1.9	29
60	DFT-B3LYP, NPA-, and QTAIM-Based Study of the Physical Properties of [M(II)(H₂O)₂(15-crown-5)] (M = Mn, Fe, Co, Ni, Cu, Zn) Complexes. Journal of Physical Chemistry A, 2011, 115, 5592-5601.	1.1	46
61	Conformational Analysis of 18-Azacrown-6 and Its Bonding with Late First Transition Series Divalent Metals: Insight from DFT Combined with NPA and QTAIM Analyses. Journal of Physical Chemistry A, 2011, 115, 13180-13190.	1.1	33
62	Polymorphs of N-[2-(Hydroxymethyl)phenyl]benzamide: Structural Characterization and Analysis of MoleculeÂ·Â·Â·Molecule Interactions by Means of Atomâ^'Atom Potentials and DFT. Crystal Growth and Design, 2011, 11, 1431-1436.	1.4	7
63	A gold(III) complex and a tetrachloroaurate salt of the neuroepileptic drug gabapentin. Inorganic Chemistry Communication, 2011, 14, 534-538.	1.8	7
64	The physical chemistry of [M(H2O)4(NO3)2] (MÂ=ÂMn2+, Co2+, Ni2+, Cu2+, Zn2+) complexes: computational studies of their structure, energetics and the topological properties of the electron density. Theoretical Chemistry Accounts, 2010, 127, 711-725.	0.5	33
65	Crystallographic and computational investigation of nitrate salts of nickel(II) ethylenediamine complexes. Inorganic Chemistry Communication, 2010, 13, 584-588.	1.8	6
66	Hydrogen-bonding controls the solid-state and enantiomeric comformations of the amino alcohol ligand 2-[(2-hydroxyethyl)amino]cyclohexanol. Acta Crystallographica Section C: Crystal Structure Communications, 2010, 66, o229-o232.	0.4	3
67	N,Nâ€²-Bis(2-hydroxycyclohexyl)-N,Nâ€²-bis(2-hydroxyethyl)ethane-1,2-diaminium dichloride. Acta Crystallographica Section C: Crystal Structure Communications, 2010, 66, o553-o556.	0.4	3
68	Amino-Alcohol Ligands: Synthesis and Structure of N,Nâ€²-bis(2-hydroxycyclopentyl)ethane-1,2-diamine and Its Salts, and an Assessment of Its Fitness and That of Related Ligands for Complexing Metal Ions. Inorganic Chemistry, 2010, 49, 8003-8011.	1.9	6
69	The physical chemistry of coordinated aqua-, ammine-, and mixed-ligand Co2+ complexes: DFT studies on the structure, energetics, and topological properties of the electron density. Physical Chemistry Chemical Physics, 2010, 12, 2126.	1.3	69
70	Structure and Function: Insights into Bioinorganic Systems from Molecular Mechanics Calculations. , 2010, , 87-109.		0
71	Low-spin complexes of Ni2+ with six NH3 and H2O ligands: A DFTâ€“RX3LYP study. Computational and Theoretical Chemistry, 2009, 902, 21-32.	1.5	9
72	DFT RX3LYP and RPBEPBE studies on the structural, electronic, and vibrational properties of some amino-alcohol ligands. Computational and Theoretical Chemistry, 2009, 915, 20-32.	1.5	12

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73	NMR spectroscopy and molecular modelling studies of nitrosylcobalamin: further evidence that the deprotonated, base-off form is important for nitrosylcobalamin in solution. Dalton Transactions, 2009, , 424-433.	1.6	23
74	The structure of N,Nâ€²-bis(2-hydroxyethyl)ethane-1,2-diamine and its complexes with Zn(ii) and Cd(ii). Dalton Transactions, 2009, , 10208.	1.6	9
75	Sc(III) porphyrins. The molecular structure of two Sc(III) porphyrins and a re-evaluation of the parameters for the molecular mechanics modelling of Sc(III) porphyrins. Journal of Molecular Structure, 2008, 872, 47-55.	1.8	7
76	The crystal structure of halofantrineâ€“ferriprotoporphyrin IX and the mechanism of action of arylmethanol antimalarials. Journal of Inorganic Biochemistry, 2008, 102, 1660-1667.	1.5	91
77	DFT-UX3LYP Studies on the Coordination Chemistry of Ni²⁺. Part 1: Six Coordinate [Ni(NH₃)_n(H₂O)_{6â^'n}]²⁺Complexes. Journal of Physical Chemistry A, 2008, 112, 10657-10666.	1.1	61
78	Insights into porphyrin chemistry provided by the microperoxidases, the haempeptides derived from cytochrome c. Dalton Transactions, 2007, , 4371.	1.6	93
79	Influence of electronic and steric effects on stability constants and electrochemical reversibility of divalent ion complexes with glycine and sarcosine. Analytica Chimica Acta, 2007, 590, 203-216.	2.6	5
80	2-Chloro-N-methylacetamide revisited: a low-temperature study. Acta Crystallographica Section E: Structure Reports Online, 2007, 63, o1642-o1644.	0.2	0
81	Speciation and structure of ferriprotoporphyrin IX in aqueous solution: spectroscopic and diffusion measurements demonstrate dimerization, but not Î¼-oxo dimer formation. Journal of Biological Inorganic Chemistry, 2007, 12, 101-117.	1.1	129
82	Modelling the interaction of several bisphosphonates with hydroxyapatite using the generalised AMBER force field. Journal of Molecular Structure, 2006, 825, 134-142.	1.8	29
83	Using artificial neural networks to develop molecular mechanics parameters for the modelling of metalloporphyrins: Part IV. Five-, six-coordinate metalloporphyrins of Mn, Co, Ni and Cu. Journal of Molecular Structure, 2006, 783, 21-33.	1.8	9
84	The solution structure of some cobalamins determined by NMR-restrained molecular modelling. Journal of Molecular Structure, 2005, 737, 245-258.	1.8	9
85	Using artificial neural networks to develop molecular mechanics parameters for the modelling of metalloporphyrins. III. Five coordinate Zn(II) porphyrins and the metalloprophyrins of the early 3d metals. Journal of Molecular Structure, 2005, 738, 67-78.	1.8	16
86	Product stabilization in the enzymatic activation of coenzyme B12: a molecular modeling study. Computational and Theoretical Chemistry, 2005, 714, 209-215.	1.5	9
87	Peroxidase Activity of the HemeoctapeptideN-Acetylmicroperoxidase-8. Inorganic Chemistry, 2005, 44, 6146-6148.	1.9	6
88	Probing the nature of the Co(iii) ion in cobalamins: a comparison of the reaction of aquacobalamin (vitamin B12a) and aqua-10-chlorocobalamin with some anionic and N-donor ligands. Dalton Transactions, 2005, , 889.	1.6	35
89	Solution structure, enzymatic, and non-enzymatic reactivity of 3-isoadenosylcobalamin, a structural isomer of coenzyme B12 with surprising coenzymic activity. Journal of Inorganic Biochemistry, 2004, 98, 287-300.	1.5	7
90	Diisopropylphosphitocobalaminâ€“acetoneâ€“water (1/3.48/7.56). Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, m88-m90.	0.4	1

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91	Isoamylcobalaminâ€“acetoneâ€“water (1/0.385/12.650). Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, m165-m167.	0.4	5
92	Synergistic anion-directed coordination of ferric and cupric ions to bovine serum transferrin â€“ an inorganic perspective. Journal of Inorganic Biochemistry, 2004, 98, 199-208.	1.5	13
93	The coordination of imidazole and substituted pyridines by the hemeoctapeptide N-acetyl-ferromicroperoxidase-8 (FeIINAcMP8). Journal of Inorganic Biochemistry, 2004, 98, 1471-1482.	1.5	26
94	Solution Structure and Thermolysis ofCoÎ²-5â€˜-Deoxyadenosylimidazolylcobamide, a Coenzyme B12Analogue with an Imidazole Axial Nucleoside. Inorganic Chemistry, 2004, 43, 8130-8142.	1.9	23
95	Molecular mechanics parameters for the modelling of four-coordinate Zn(ii) porphyrins. Physical Chemistry Chemical Physics, 2003, 5, 5499-5506.	1.3	17
96	Fate of haem iron in the malaria parasite Plasmodium falciparum. Biochemical Journal, 2002, 365, 343-347.	1.7	253
97	Probing the nature of the Co(iii) ion in cobalamins: deactivation of the metal towards ligand substitution in 10-nitrosoaquacobalamin, and the kinetics of the ligand substitution reactions of iodocobalamin. Dalton Transactions RSC, 2002, , 3195.	2.3	24
98	The co-ordination of ligands by iron porphyrins: a comparison of ligand binding by myoglobin from sperm whale and the haem undecapeptide from cytochrome c. Dalton Transactions RSC, 2002, , 449-457.	2.3	18
99	Complexes of cobalt(iii) with phenolate-containing polydentate ligands and bovine serum apo-transferrin: towards creating spectroscopic models for cobalt(iii)â€“tyrosinate interactions. Dalton Transactions RSC, 2002, , 4064-4069.	2.3	13
100	Molecular mechanics modelling of porphyrins. Using artificial neural networks to develop metal parameters for four-coordinate metalloporphyrinsElectronic supplementary information (ESI) available: Molecular mechanics parameters, comparisons between crystallographic and molecular mechanics geometries, error response surfaces, and crystal structures. See http://www.rsc.org/suppdata/cp/b2/b203360g/. Physical Chemistry Chemical Physics, 2002, 4, 5878-5887.	1.3	19
101	Molecular mechanics and molecular dynamics simulations of porphyrins, metalloporphyrins, heme proteins and cobalt corrinoids. Coordination Chemistry Reviews, 2002, 225, 123-158.	9.5	90
102	Molecular modeling of the mechanochemical triggering mechanism for catalysis of carbonâ€“cobalt bond homolysis in coenzyme B12. Journal of Inorganic Biochemistry, 2001, 83, 121-132.	1.5	37
103	Manganese(III) in a pseudo-compressed mixed-donor octahedral environment: synthesis, X-ray crystal structure and physicochemical properties. Polyhedron, 2001, 20, 2195-2201.	1.0	7
104	Co-ordination of weak field ligands by N-acetylmicroperoxidase-8 (NAcMP8), a ferric haempeptide from cytochrome c, and the influence of the axial ligand on the reduction potential of complexes of NAcMP8â€Šâ€. Dalton Transactions RSC, 2000, , 1335-1342.	2.3	20
105	Structureâˆ’Function Relationships in Aminoquinolines:Â Effect of Amino and Chloro Groups on Quinolineâˆ’Hematin Complex Formation, Inhibition of Î²-Hematin Formation, and Antiplasmodial Activity. Journal of Medicinal Chemistry, 2000, 43, 283-291.	2.9	301
106	The structure of cobalt corrinoids based on molecular mechanics and NOE-restrained molecular mechanics and dynamics simulations. Coordination Chemistry Reviews, 1999, 190-192, 127-153.	9.5	22
107	The role of haem in the activity of chloroquine and related antimalarial drugs. Coordination Chemistry Reviews, 1999, 190-192, 493-517.	9.5	78
108	Coordination of N-Donor Ligands by the Monomeric Ferric PorphyrinN-Acetylmicroperoxidase-8. Inorganic Chemistry, 1999, 38, 2312-2319.	1.9	34

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109	NMR-restrained molecular modeling of cobalt corrinoids: cyanocobalamin (vitamin B12) and methylcobalt corrinoids. Computational and Theoretical Chemistry, 1998, 453, 209-224.	1.5	30
110	Conformational studies of 5â€²-deoxyadenosyl-13-epicobalamin, a coenzymatically active structural analog of coenzyme B12. Polyhedron, 1998, 17, 2213-2224.	1.0	21
111	Haempeptide models for haemoproteins Part 3 N-Acetylmicroperoxidase-8: EPR, MÃ¶ssbauer and magnetic susceptibility studies on an iron(III) porphyrin in thermal equilibrium between S=3/2, 5/2 and S=1/2 states. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 1743-1752.	1.7	22
112	Structural and Enzymatic Studies of a New Analogue of Coenzyme B12with an Î±-Adenosyl Upper Axial Ligandâ€. Biochemistry, 1998, 37, 9704-9715.	1.2	42
113	Molecular Mechanics Modeling of the Cobaloximes and Reevaluation of the Parameters for Modeling of the Cobalt Corrins. Inorganic Chemistry, 1998, 37, 2578-2581.	1.9	41
114	Factors affecting the rate of ligand substitution reactions of aquacobalamin (vitamin B12a)â€Šâ€¡. Journal of the Chemical Society Dalton Transactions, 1997, , 3827-3834.	1.1	29
115	CisEffects in the Cobalt Corrins. 1. Crystal Structures of 10-Chloroaquacobalamin Perchlorate, 10-Chlorocyanocobalamin, and 10-Chloromethylcobalamin. Inorganic Chemistry, 1997, 36, 3666-3675.	1.9	61
116	An Analysis of Porphyrin Molecular FlexibilityUse of Porphyrin Diacids. Journal of the American Chemical Society, 1997, 119, 10732-10742.	6.6	160
117	Thermodynamic factors controlling the interaction of quinoline antimalarial drugs with ferriprotoporphyrin IX. Journal of Inorganic Biochemistry, 1997, 68, 137-145.	1.5	152
118	Hemeâ^'Peptide Models for Hemoproteins. 1. Solution Chemistry ofN-Acetylmicroperoxidase-8. Inorganic Chemistry, 1996, 35, 3752-3767.	1.9	85
119	Hemeâ^'Peptide Models for Hemoproteins. 2.N-Acetylmicroperoxidase-8:Â Study of the Ï€â^'Ï€ Dimers Formed at High Ionic Strength Using a Modified Version of Molecular Exciton Theory. Inorganic Chemistry, 1996, 35, 3768-3779.	1.9	33
120	Solution structure of cyanocobalamin (vitamin B12) by NMR-restrained molecular dynamics and simulated annealing calculations. Chemical Communications, 1996, , 1427.	2.2	22
121	Reactions of ferric porphyrins and thiols. The reaction of the haem octapeptide, N-acetylmicroperoxidase-8, with cysteine. Inorganica Chimica Acta, 1996, 248, 115-119.	1.2	14
122	The interaction of the heme-octapeptide, N-acetylmicroperoxidase-8 with antimalarial drugs: Solution studies and modeling by molecular mechanics methods. Journal of Inorganic Biochemistry, 1996, 64, 7-23.	1.5	30
123	Release of iron from C-terminal monoferric transferrin to phosphate and pyrophosphate at pH 5.5 proceeds through two pathways. Journal of Inorganic Biochemistry, 1995, 57, 11-21.	1.5	29
124	A molecular mechanics force field for the cobalt corrinoids. Computational and Theoretical Chemistry, 1995, 340, 97-124.	1.5	43
125	Side Chain Entropy and the Activation of Organocobalamins for Carbon-Cobalt Bond Homolysis: Thermolysis of Neopentylcobalamin-c-monocarboxylate, -c-N-methylamide, -c-N,N-dimethylamide, and -c-N-isopropylamide. Inorganic Chemistry, 1995, 34, 3038-3049.	1.9	36
126	Molecular Mechanics of Cobalt Corrinoids. 2. Structure of Alkylcobalamins and Thermolysis of the Cobalt-Carbon Bond. Inorganic Chemistry, 1995, 34, 3733-3740.	1.9	40

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127	Structural and Molecular Mechanics Studies on Highly Ruffled Low-Spin (Porphinato)iron(III) Complexes. Journal of the American Chemical Society, 1995, 117, 935-954.	6.6	120
128	A force field for molecular mechanics studies of iron porphyrins. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1741.	1.7	36
129	Analysis of malaria pigment from Plasmodium falciparum. Journal of Pharmacological and Toxicological Methods, 1994, 32, 25-30.	0.3	19
130	Ligand substitution reactions of aquacobalamin: further evidence for a dissociative interchange mechanism, and factors controlling reaction rates. Journal of the Chemical Society Dalton Transactions, 1994, , 297.	1.1	16
131	Placing hydroxide in the thermodynamic trans influence order of the cobalt corrinoids: equilibrium constants for the reaction of some ligands with aquahydroxocobinamide. Inorganica Chimica Acta, 1993, 209, 161-169.	1.2	18
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