Helder M Marques

List of Publications by Year in Descending Order

154 papers	4,164 citations	34 h-index	57 g-index
155 ext. papers	4,525 ext. citations	4.6 avg, IF	5.61 L-index

#	Paper	IF	Citations
154	Chalcogen Bonding in the Molecular Dimers of WCh (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,	6.3	5
153	Chalcogen□□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	2.9	4
152	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,	4.8	3
151	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		3
150	The Pnictogen Bond: The Covalently Bound Arsenic Atom in Molecular Entities in Crystals as a Pnictogen Bond Donor. *Molecules*, **2022**, 27, 3421	4.8	2
149	The CsAgRhCl Halide Double Perovskite: A Dynamically Stable Lead-Free Transition-Metal Driven Semiconducting Material for Optoelectronics. *Frontiers in Chemistry*, **2020**, 8, 796	5	3
148	Does Chlorine in CH3Cl Behave as a Genuine Halogen Bond Donor?. *Crystals*, **2020**, 10, 146	2.3	10
147	Physical and optoelectronic features of lead-free A2AgRhBr6 (A = Cs, Rb, K, Na, Li) with halide double perovskite composition. *Journal of Materials Chemistry C*, **2020**, 8, 12968-12983	7.1	9
146	Is the Fluorine in Molecules Dispersive? Is Molecular Electrostatic Potential a Valid Property to Explore Fluorine-Centered Non-Covalent Interactions?. *Molecules*, **2019**, 24,	4.8	45
145	Nature of halogen-centered intermolecular interactions in crystal growth and design: Fluorine-centered interactions in dimers in crystalline hexafluoropropylene as a prototype. *Journal of Computational Chemistry*, **2019**, 40, 1836-1860	3.5	9
144	Halogen Bonding: A Halogen-Centered Noncovalent Interaction Yet to Be Understood. *Inorganics*, **2019**, 7, 40	2.9	77
143	The chalcogen bond: can it be formed by oxygen?. *Physical Chemistry Chemical Physics*, **2019**, 21, 19969-19986	3.6	22
142	C Fullerene Cage as a Novel Catalyst for Efficient Proton Transfer Reactions between Small Molecules: A Theoretical study. *Scientific Reports*, **2019**, 9, 10650	4.9	3
141	Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the CHNHPbI hybrid organic-inorganic halide perovskite solar cell semiconductor. *Scientific Reports*, **2019**, 9, 50	4.9	57
140	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	2.7	0
139	Revealing Factors Influencing the Fluorine-Centered Non-Covalent Interactions in Some Fluorine-Substituted Molecular Complexes: Insights from First-Principles Studies. *ChemPhysChem*, **2018**, 19, 1486-1499	3.2	16
138	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	6.2	23

137	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	2.1	1
136	Do surfaces of positive electrostatic potential on different halogen derivatives in molecules attract? like attracting like!. *Journal of Computational Chemistry*, **2018**, 39, 343-350	3.5	24
135	Revealing the Chemistry between Band Gap and Binding Energy for Lead-/Tin-Based Trihalide Perovskite Solar Cell Semiconductors. *ChemSusChem*, **2018**, 11, 449-463	8.3	22
134	Halogen in materials design: Chloroammonium lead triiodide perovskite (ClNH PbI) a dynamical bandgap semiconductor in 3D for photovoltaics. *Journal of Computational Chemistry*, **2018**, 39, 1902-1912	3.5	2
133	Can Combined Electrostatic and Polarization Effects Alone Explain the F⋯F Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective. *Computation*, **2018**, 6, 51	2.2	21
132	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	3.6	18
131	Revealing the Cooperative Chemistry of the Organic Cation in the Methylammonium Lead Triiodide Perovskite Semiconductor System. *ChemistrySelect*, **2018**, 3, 7269-7282	1.8	6
130	Hybrid organic-inorganic CH NH PbI perovskite building blocks: Revealing ultra-strong hydrogen bonding and mulliken inner complexes and their implications in materials design. *Journal of Computational Chemistry*, **2017**, 38, 2802-2818	3.5	23
129	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	6.8	42
128	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	2.7	6
127	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	3.7	35
126	The kinetics of the substitution of coordinated H2O on Co(III) by cyanide in aquacobalamin (vitamin B12a) and in a corrole analogue. *Inorganic Chemistry Communication*, **2015**, 57, 15-17	3.1	3
125	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	2.7	4
124	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, 31624-45	3.6	28
123	Ligand(s)-to-metal charge transfer as a factor controlling the equilibrium constants of late first-row transition metal complexes: revealing the Irving-Williams thermodynamical series. *Physical Chemistry Chemical Physics*, **2015**, 17, 805-11	3.6	13
122	Hexahalogenated and their mixed benzene derivatives as prototypes for the understanding of halogen⋯halogen intramolecular interactions: New insights from combined DFT, QTAIM-, and RDG-based NCI analyses. *Journal of Computational Chemistry*, **2015**, 36, 2328-43	3.5	17
121	Fluorines in tetrafluoromethane as halogen bond donors: Revisiting address the nature of the fluorine‐fluorine hole. *International Journal of Quantum Chemistry*, **2015**, 115, 453-470	2.1	36
120	The synthesis of a corrole analogue of aquacobalamin (vitamin B12a) and its ligand substitution reactions. *Inorganic Chemistry*, **2014**, 53, 4418-29	5.1	7

119	Halogen bonding interaction of chloromethane with several nitrogen donating molecules: addressing the nature of the chlorine surface hole. *Physical Chemistry Chemical Physics*, **2014**, 16, 19573-89	3.6	34
118	Outer-sphere anion recognition by a cyclen-based octadentate europium(III) complex: pH dependent recognition of ortho-phthalic acid. *Chemical Communications*, **2014**, 50, 1582-4	5.8	4
117	Modulating Cavity Size in an Acyclic Amino Alcohol Assembly. *Journal of Chemical Crystallography*, **2014**, 44, 229-235	0.5	
116	Significant evidence of C···O and C···C long-range contacts in several heterodimeric complexes of CO with CH3-X, should one refer to them as carbon and dicarbon bonds!. *Physical Chemistry Chemical Physics*, **2014**, 16, 17238-52	3.6	51
115	Polymorphic Diversity: N-Phenylbenzamide as a Possible Polymorphophore. *Crystal Growth and Design*, **2013**, 13, 3463-3474	3.5	12
114	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, 1077-83	5.1	4
113	DFT studies of trans and cis influences in the homolysis of the Co-C bond in models of the alkylcobalamins. *Journal of Physical Chemistry A*, **2013**, 117, 3057-68	2.8	17
112	Phenylvinylcobalamin: an alkenylcobalamin featuring a ligand with a large trans influence. *Dalton Transactions*, **2013**, 42, 7555-61	4.3	4
111	The preparation of N-acetyl-Co(III)-microperoxidase-8 (NAcCoMP8) and its ligand substitution reactions: a comparison with aquacobalamin (vitamin B(12a)). *Journal of Inorganic Biochemistry*, **2013**, 123, 66-79	4.2	10
110	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, o383-6		3
109	Can a single molecule of water be completely isolated within the subnano-space inside the fullerene C60 cage? A quantum chemical prospective. *Chemistry - A European Journal*, **2012**, 18, 15345-60	4.8	39
108	cis influence in models of cobalt corrins by DFT and TD-DFT studies. *Journal of Physical Chemistry B*, **2012**, 116, 8836-45	3.4	15
107	5,10,15,20-Tetra-p-phenylsulfonyporphinatocobalt(III), a water-soluble Co(III) porphyrin. *Inorganica Chimica Acta*, **2012**, 392, 108-111	2.7	4
106	The cis influence of the corrin in vitamin B12 models. *Chemical Physics Letters*, **2012**, 550, 150-155	2.5	7
105	An electronic structure theory investigation of the physical chemistry of the intermolecular complexes of cyclopropenylidene with hydrogen halides. *Journal of Computational Chemistry*, **2012**, 33, 2073-82	3.5	11
104	Bis-(2-hy-droxy-eth-yl)ammonium 2-bromo-phenolate. *Acta Crystallographica Section E: Structure Reports Online*, **2012**, 68, o2610		2
103	(2-Amino-phen-yl)methanol. *Acta Crystallographica Section E: Structure Reports Online*, **2012**, 68, o174		2
102	4-(Dimeth-oxy-meth-yl)phenyl 2,3,4,6-tetra-O-acetyl-d-glucopyran-oside. *Acta Crystallographica Section E: Structure Reports Online*, **2012**, 68, o1202		

101	Bis-(2-bromo-eth-yl)ammonium bromide. *Acta Crystallographica Section E: Structure Reports Online*, **2012**, 68, o2570-1		
100	Hydrogen-bond inter-actions in morpholinium bromide. *Acta Crystallographica Section E: Structure Reports Online*, **2011**, 67, o2594		3
99	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, 8700-18	5.1	18
98	Probing the nature of the Co(III) ion 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, 8719-27	5.1	27
97	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, 5592-601	2.8	37
96	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, 13180-90	2.8	28
95	Polymorphs of N-[2-(Hydroxymethyl)phenyl]benzamide: Structural Characterization and Analysis of Molecule□Molecule Interactions by Means of Atom□Atom Potentials and DFT. *Crystal Growth and Design*, **2011**, 11, 1431-1436	3.5	6
94	A gold(III) complex and a tetrachloroaurate salt of the neuroepileptic drug gabapentin. *Inorganic Chemistry Communication*, **2011**, 14, 534-538	3.1	4
93	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, 6629-40	2.8	6
92	Amino-alcohol ligands: synthesis and structure of N,NPbis(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, 8003-11	5.1	5
91	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, 2126-38	3.6	57
90	The physical chemistry of [M(H2O)4(NO3)2] (M = Mn2+, 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	1.9	29
89	Crystallographic and computational investigation of nitrate salts of nickel(II) ethylenediamine complexes. *Inorganic Chemistry Communication*, **2010**, 13, 584-588	3.1	6
88	Hydrogen-bonding controls the solid-state and enantiomeric conformations of the amino alcohol ligand 2-[(2-hydroxyethyl)amino]cyclohexanol. *Acta Crystallographica Section C: Crystal Structure Communications*, **2010**, 66, o229-32		3
87	N,NPbis(2-hydroxycyclohexyl)-N,NPbis(2-hydroxyethyl)ethane-1,2-diaminium dichloride. *Acta Crystallographica Section C: Crystal Structure Communications*, **2010**, 66, o553-6		3
86	Structure and Function: Insights into Bioinorganic Systems from Molecular Mechanics Calculations **2010**, 87-109		
85	Low-spin complexes of Ni2+ with six NH3 and H2O ligands: A DFT□RX3LYP study. *Computational and Theoretical Chemistry*, **2009**, 902, 21-32		8
84	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		9

83	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**, 424-33	4.3	19
82	The structure of N,NPbis(2-hydroxyethyl)ethane-1,2-diamine and its complexes with Zn(II) and Cd(II). *Dalton Transactions*, **2009**, 10208-18	4.3	9
81	DFT-UX3LYP studies on the coordination chemistry of Ni2+. Part 1: Six coordinate [Ni(NH3)n(H2O)(6-n)]2+ complexes. *Journal of Physical Chemistry A*, **2008**, 112, 10657-66	2.8	50
80	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	3.4	6
79	The crystal structure of halofantrine-ferriprotoporphyrin IX and the mechanism of action of arylmethanol antimalarials. *Journal of Inorganic Biochemistry*, **2008**, 102, 1660-7	4.2	85
78	Insights into porphyrin chemistry provided by the microperoxidases, the haempeptides derived from cytochrome c. *Dalton Transactions*, **2007**, 4371-85	4.3	86
77	Influence of electronic and steric effects on stability constants and electrochemical reversibility of divalent ion complexes with glycine and sarcosine. A glass electrode potentiometric, sampled direct current polarographic, virtual potentiometric, and molecular modelling study. *Analytica Chimica Acta*, **2007**, 590, 203-16	6.6	4
76	2-Chloro-N-methylacetamide revisited: a low-temperature study. *Acta Crystallographica Section E: Structure Reports Online*, **2007**, 63, o1642-o1644		
75	Speciation and structure of ferriprotoporphyrin IX in aqueous solution: spectroscopic and diffusion measurements demonstrate dimerization, but not mu-oxo dimer formation. *Journal of Biological Inorganic Chemistry*, **2007**, 12, 101-17	3.7	113
74	Modelling the interaction of several bisphosphonates with hydroxyapatite using the generalised AMBER force field. *Journal of Molecular Structure*, **2006**, 825, 134-142	3.4	28
73	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	3.4	7
72	Peroxidase activity of the hemeoctapeptide N-acetylmicroperoxidase-8. *Inorganic Chemistry*, **2005**, 44, 6146-8	5.1	6
71	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**, 889-95	4.3	33
70	The solution structure of some cobalamins determined by NMR-restrained molecular modelling. *Journal of Molecular Structure*, **2005**, 737, 245-258	3.4	7
69	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	3.4	13
68	Product stabilization in the enzymatic activation of coenzyme B12: a molecular modeling study. *Computational and Theoretical Chemistry*, **2005**, 714, 209-215		9
67	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	4.2	7
66	Diisopropylphosphitocobalamin-acetone-water (1/3.48/7.56). *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, m88-90		1

65	Isoamylcobalamin-acetone-water (1/0.385/12.650). *Acta Crystallographica Section C: Crystal Structure Communications*, **2004**, 60, m165-7		4
64	Synergistic anion-directed coordination of ferric and cupric ions to bovine serum transferrin--an inorganic perspective. *Journal of Inorganic Biochemistry*, **2004**, 98, 199-208	4.2	12
63	The coordination of imidazole and substituted pyridines by the hemeoctapeptide N-acetyl-ferromicroperoxidase-8 (FeIINAcMP8). *Journal of Inorganic Biochemistry*, **2004**, 98, 1471-82	4.2	25
62	Solution structure and thermolysis of Cobeta-5Pdeoxyadenosylimidazolylcobamide, a coenzyme B12 analogue with an imidazole axial nucleoside. *Inorganic Chemistry*, **2004**, 43, 8130-42	5.1	22
61	Molecular mechanics parameters for the modelling of four-coordinate Zn(II) porphyrins. *Physical Chemistry Chemical Physics*, **2003**, 5, 5499-5506	3.6	16
60	Molecular mechanics and molecular dynamics simulations of porphyrins, metalloporphyrins, heme proteins and cobalt corrinoids. *Coordination Chemistry Reviews*, **2002**, 225, 123-158	23.2	82
59	Fate of haem iron in the malaria parasite Plasmodium falciparum. *Biochemical Journal*, **2002**, 365, 343-7	3.8	222
58	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		23
57	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		17
56	Complexes of cobalt(III) with phenolate-containing polydentate ligands and bovine serum apo-transferrin: towards creating spectroscopic models for cobalt(III)Tyrosinate interactions. *Dalton Transactions RSC*, **2002**, 4064-4069		12
55	Molecular mechanics modelling of porphyrins. Using artificial neural networks to develop metal parameters for four-coordinate metalloporphyrins. *Physical Chemistry Chemical Physics*, **2002**, 4, 5878-5887	3.6	17
54	Molecular modeling of the mechanochemical triggering mechanism for catalysis of carbon-cobalt bond homolysis in coenzyme B12. *Journal of Inorganic Biochemistry*, **2001**, 83, 121-32	4.2	36
53	Manganese(III) in a pseudo-compressed mixed-donor octahedral environment: synthesis, X-ray crystal structure and physicochemical properties. *Polyhedron*, **2001**, 20, 2195-2201	2.7	5
52	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 NAcMP8. *Dalton Transactions RSC*, **2000**, 1335-1342		17
51	Structure-function relationships in aminoquinolines: effect of amino and chloro groups on quinoline-hematin complex formation, inhibition of beta-hematin formation, and antiplasmodial activity. *Journal of Medicinal Chemistry*, **2000**, 43, 283-91	8.3	271
50	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	23.2	18
49	The role of haem in the activity of chloroquine and related antimalarial drugs. *Coordination Chemistry Reviews*, **1999**, 190-192, 493-517	23.2	70
48	Coordination of N-Donor Ligands by the Monomeric Ferric PorphyrinN-Acetylmicroperoxidase-8. *Inorganic Chemistry*, **1999**, 38, 2312-2319	5.1	30

47	NMR-restrained molecular modeling of cobalt corrinoids: cyanocobalamin (vitamin B12) and methylcobalt corrinoids. *Computational and Theoretical Chemistry*, **1998**, 453, 209-224		27
46	Conformational studies of 5?-deoxyadenosyl-13-epicobalamin, a coenzymatically active structural analog of coenzyme B12. *Polyhedron*, **1998**, 17, 2213-2224	2.7	20
45	Haempeptide models for haemoproteins. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 1743-1752		19
44	Structural and enzymatic studies of a new analogue of coenzyme B12 with an alpha-adenosyl upper axial ligand. *Biochemistry*, **1998**, 37, 9704-15	3.2	38
43	Molecular Mechanics Modeling of the Cobaloximes and Reevaluation of the Parameters for Modeling of the Cobalt Corrins. *Inorganic Chemistry*, **1998**, 37, 2578-2581	5.1	37
42	Factors affecting the rate of ligand substitution reactions of aquacobalamin (vitamin B12a)□ *Journal of the Chemical Society Dalton Transactions*, **1997**, 3827-3834		28
41	Cis Effects in the Cobalt Corrins. 1. Crystal Structures of 10-Chloroaquacobalamin Perchlorate, 10-Chlorocyanocobalamin, and 10-Chloromethylcobalamin. *Inorganic Chemistry*, **1997**, 36, 3666-3675	5.1	56
40	An Analysis of Porphyrin Molecular FlexibilityUse of Porphyrin Diacids. *Journal of the American Chemical Society*, **1997**, 119, 10732-10742	16.4	145
39	Thermodynamic factors controlling the interaction of quinoline antimalarial drugs with ferriprotoporphyrin IX. *Journal of Inorganic Biochemistry*, **1997**, 68, 137-45	4.2	139
38	Heme-Peptide Models for Hemoproteins. 1. Solution Chemistry of N-Acetylmicroperoxidase-8. *Inorganic Chemistry*, **1996**, 35, 3752-3767	5.1	80
37	Heme-Peptide Models for Hemoproteins. 2. N-Acetylmicroperoxidase-8: Study of the pi-pi Dimers Formed at High Ionic Strength Using a Modified Version of Molecular Exciton Theory. *Inorganic Chemistry*, **1996**, 35, 3768-3779	5.1	31
36	Solution structure of cyanocobalamin (vitamin B12) by NMR-restrained molecular dynamics and simulated annealing calculations. *Chemical Communications*, **1996**, 1427	5.8	21
35	Reactions of ferric porphyrins and thiols. The reaction of the haem octapeptide, N-acetylmicroperoxidase-8, with cysteine. *Inorganica Chimica Acta*, **1996**, 248, 115-119	2.7	12
34	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	4.2	29
33	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	4.2	27
32	A molecular mechanics force field for the cobalt corrinoids. *Computational and Theoretical Chemistry*, **1995**, 340, 97-124		40
31	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	5.1	31
30	Molecular Mechanics of Cobalt Corrinoids. 2. Structure of Alkylcobalamins and Thermolysis of the Cobalt-Carbon Bond. *Inorganic Chemistry*, **1995**, 34, 3733-3740	5.1	34

29	Structural and Molecular Mechanics Studies on Highly Ruffled Low-Spin (Porphinato)iron(III) Complexes. *Journal of the American Chemical Society*, **1995**, 117, 935-954	16.4	112
28	A force field for molecular mechanics studies of iron porphyrins. *Journal of the Chemical Society, Faraday Transactions*, **1995**, 91, 1741		33
27	Analysis of malaria pigment from Plasmodium falciparum. *Journal of Pharmacological and Toxicological Methods*, **1994**, 32, 25-30	1.7	14
26	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		15
25	Hemes and hemoproteins. Part 7. Co-ordination of ammonia, aniline and pyridine by the iron(III) porphyrin microperoxidase-8. *Journal of the Chemical Society Dalton Transactions*, **1993**, 1633		12
24	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	2.7	15
23	A Mössbauer study on an iron porphyrin model of ferric hemoproteins. *Nuclear Instruments & Methods in Physics Research B*, **1993**, 76, 315-317	1.2	3
22	The ligand-substitution reactions of aquahydroxocobinamide proceed through a dissociative interchange mechanism. *Journal of the Chemical Society Dalton Transactions*, **1993**, 3475		24
21	Molecular mechanics study of the ruffling of metalloporphyrins. *Journal of the American Chemical Society*, **1992**, 114, 7218-7230	16.4	94
20	Ligand substitution reactions of aquacobalamin: evidence for a dissociative interchange mechanism. *Journal of the Chemical Society Dalton Transactions*, **1992**, 2019		35
19	Coordination of N-donor ligands by hematohemin. *Inorganica Chimica Acta*, **1992**, 196, 221-229	2.7	27
18	A spectrophotometric determination of the binding constants of cyanide by hemin in aqueous ethanol solutions. *Inorganica Chimica Acta*, **1991**, 190, 291-295	2.7	7
17	Kinetics of reaction of aquacobalamin with azide ion and hydrazoic acid: pH profile and activation parameters. *Journal of the Chemical Society Dalton Transactions*, **1991**, 2941		11
16	Notes. Activation parameters for the reaction of aquocobalamin (vitamin B12a) with small anionic and neutral ligands. *Journal of the Chemical Society Dalton Transactions*, **1991**, 339		18
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14	The effects of anions on the kinetics of reductive elimination of iron from monoferrictransferrins by thiols. *BBA - Proteins and Proteomics*, **1990**, 1038, 1-9		11
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