Ian Gordon Dance

List of Publications by Year
in descending order

76 papers	3,303 citations	117625 34 h-index	161849 54 g-index
78 all docs	78 docs citations	78 times ranked	2562 citing authors

#	Article	IF	Citations
1	Structures and reaction dynamics of N₂ and H₂ binding at FeMo-co, the active site of nitrogenase. Dalton Transactions, 2021, 50, 18212-18237.	3.3	10
2	Computational Investigations of the Chemical Mechanism of the Enzyme Nitrogenase. ChemBioChem, 2020, 21, 1671-1709.	2.6	36
3	How feasible is the reversible S-dissociation mechanism for the activation of FeMo-co, the catalytic site of nitrogenase?. Dalton Transactions, 2019, 48, 1251-1262.	3.3	32
4	Survey of the Geometric and Electronic Structures of the Key Hydrogenated Forms of FeMo-co, the Active Site of the Enzyme Nitrogenase: Principles of the Mechanistically Significant Coordination Chemistry. Inorganics, 2019, 7, 8.	2.7	25
5	Evaluations of the accuracies of DMol3 density functionals for calculations of experimental binding enthalpies of N₂, CO, H₂, C₂H₂ at catalytic metal sites. Molecular Simulation, 2018, 44, 568-581.	2.0	38
6	What is the role of the isolated small water pool near FeMoâ€¢co, the active site of nitrogenase?. FEBS Journal, 2018, 285, 2972-2986.	4.7	5
7	New insights into the reaction capabilities of His195 adjacent to the active site of nitrogenase. Journal of Inorganic Biochemistry, 2017, 169, 32-43.	3.5	17
8	Mechanisms of the S/CO/Se interchange reactions at FeMo-co, the active site cluster of nitrogenase. Dalton Transactions, 2016, 45, 14285-14300.	3.3	19
9	Activation of N₂, the Enzymatic Way. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2015, 641, 91-99.	1.2	25
10	Protonation of bridging sulfur in cubanoid Fe₄S₄clusters causes large geometric changes: the theory of geometric and electronic structure.. Dalton Transactions, 2015, 44, 4707-4717.	3.3	10
11	Misconception of reductive elimination of H₂, in the context of the mechanism of nitrogenase. Dalton Transactions, 2015, 44, 9027-9037.	3.3	14
12	The pathway for serial proton supply to the active site of nitrogenase: enhanced density functional modeling of the Grotthuss mechanism. Dalton Transactions, 2015, 44, 18167-18186.	3.3	47
13	What is the trigger mechanism for the reversal of electron flow in oxygen-tolerant [NiFe] hydrogenases?. Chemical Science, 2015, 6, 1433-1443.	7.4	20
14	Large structural changes upon protonation of Fe4S4 clusters: the consequences for reactivity. Dalton Transactions, 2014, 43, 16213-16226.	3.3	14
15	Nitrogenase: a general hydrogenator of small molecules. Chemical Communications, 2013, 49, 10893.	4.1	68
16	A molecular pathway for the egress of ammonia produced by nitrogenase. Scientific Reports, 2013, 3, 3237.	3.3	25
17	The Stereochemistry and Dynamics of the Introduction of Hydrogen Atoms onto FeMo-co, the Active Site of Nitrogenase. Inorganic Chemistry, 2013, 52, 13068-13077.	4.0	27
18	Ramifications of C-centering rather than N-centering of the active site FeMo-co of the enzyme nitrogenase. Dalton Transactions, 2012, 41, 4859.	3.3	39

#	Article	IF	Citations
19	The controlled relay of multiple protons required at the active site of nitrogenase. Dalton Transactions, 2012, 41, 7647.	3.3	50
20	Calculated vibrational frequencies for FeMo-co, the active site of nitrogenase, bearing hydrogen atoms and carbon monoxide. Dalton Transactions, 2011, 40, 6480.	3.3	21
21	Electronic Dimensions of FeMo-co, the Active Site of Nitrogenase, and Its Catalytic Intermediates. Inorganic Chemistry, 2011, 50, 178-192.	4.0	41
22	How does vanadium nitrogenase reduce CO to hydrocarbons?. Dalton Transactions, 2011, 40, 5516.	3.3	34
23	Alternative metal grid structures formed by [M(terpy)2]2+ and [M(terpyOH)2]2+ complexes with small and large tetrahedral dianions, and by [Ru(terpy)2]0. CrystEngComm, 2010, 12, 2700.	2.6	26
24	Mimicking nitrogenase. Dalton Transactions, 2010, 39, 2972.	3.3	53
25	Alternative two-dimensional embrace nets formed by metal complexes of 4â€²-phenylterpyridine crystallised with hydrophilic anions. CrystEngComm, 2010, 12, 3207.	2.6	27
26	Crystal packing in metal complexes of 4â€²-phenylterpyridine and related ligands: occurrence of the 2D and 1D terpy embrace arrays. CrystEngComm, 2009, 11, 1141.	2.6	55
27	Molecules embracing in crystals. CrystEngComm, 2009, 11, 2233.	2.6	119
28	The chemical mechanism of nitrogenase: hydrogen tunneling and further aspects of the intramolecular mechanism for hydrogenation of Î·2-N2 on FeMo-co to NH3. Dalton Transactions, 2008, , 5992.	3.3	47
29	The chemical mechanism of nitrogenase: calculated details of the intramolecular mechanism for hydrogenation of Î·2-N2 on FeMo-co to NH3. Dalton Transactions, 2008, , 5977.	3.3	77
30	A pragmatic method for location of transition states and calculation of reaction paths. Molecular Simulation, 2008, 34, 923-929.	2.0	17
31	The Mechanistically Significant Coordination Chemistry of Dinitrogen at FeMo-co, the Catalytic Site of Nitrogenase. Journal of the American Chemical Society, 2007, 129, 1076-1088.	13.7	68
32	Elucidating the Coordination Chemistry and Mechanism of Biological Nitrogen Fixation. Chemistry - an Asian Journal, 2007, 2, 936-946.	3.3	59
33	Crystals of isomeric tritolylamines: embrace motifs in crystals, and their thermochemical properties. CrystEngComm, 2006, 8, 59.	2.6	6
34	The Correlation of Redox Potential, HOMO Energy, and Oxidation State in Metal Sulfide Clusters and Its Application to Determine the Redox Level of the FeMo-co Active-Site Cluster of Nitrogenase. Inorganic Chemistry, 2006, 45, 5084-5091.	4.0	77
35	Mechanistic Significance of the Preparatory Migration of Hydrogen Atoms around the FeMo-co Active Site of Nitrogenase. Biochemistry, 2006, 45, 6328-6340.	2.5	52
36	Intermolecular Embraces and Intermolecular Energies. Molecular Crystals and Liquid Crystals, 2005, 440, 265-293.	0.9	26

#	Article	IF	Citations
37	Engineering grids of metal complexes: development of the 2D M(terpy)2 embrace motif in crystals. CrystEngComm, 2005, 7, 216.	2.6	97
38	The crystallisation of polyoxo-molybdate and -tungstate anions with phenylated phosphonium and arsonium cations, in relation to the crystal packing and species in solution. CrystEngComm, 2005, 7, 491.	2.6	20
39	The Hydrogen Chemistry of the FeMo-co Active Site of Nitrogenase. Journal of the American Chemical Society, 2005, 127, 10925-10942.	13.7	73
40	Engineering the metal-terpy grid with complexes containing 4â€²-hydroxy terpyridine. CrystEngComm, 2005, 7, 230-236.	2.6	44
41	The Mechanism of Nitrogenase. Computed Details of the Site and Geometry of Binding of Alkyne and Alkene Substrates and Intermediates. Journal of the American Chemical Society, 2004, 126, 11852-11863.	13.7	51
42	Questions for crystal engineering of halocuprate complexes: concepts for a difficult system. CrystEngComm, 2004, 6, 257.	2.6	134
43	Inorganic intermolecular motifs, and their energiesThis article is based (partly) on a presentation which will be made at the European Research Conference (EURESCO) on "Molecular Crystal Engineering - EuroConference on Design and Preparation of Molecular Materials" (Acquafredda di) Tj ETQq1 1 0.784314 rgBT /Overlock European Commission, Research DG, Human Potential Programme, High-Level Scientific Conferences, Contract HPCF-CT-2002-00270. T. CrystEngComm, 2003, 5, 208.	2.6	86
44	The consequences of an interstitial N atom in the FeMo cofactor of nitrogenase. Chemical Communications, 2003, , 324-325.	4.1	101
45	Dimorphs of (Ph4P)2[Cd2(SPh)6]:â€‰ Crystal Packing Analyses and the Interplay of Intermolecular and Intramolecular Energies. Crystal Growth and Design, 2002, 2, 601-607.	3.0	9
46	Supramolecular motifs in four pseudo-polymorphic crystals of [Fe(phen)3](I3)2Â·(solvent): solvent = acetone, CH2Cl2, CH3CN, toluene or H2O. CrystEngComm, 2002, 4, 7-12.	2.6	20
47	Three-Coordinate [CuIIX3]â^' (X=Cl, Br), Trapped in a Molecular Crystal. Chemistry - A European Journal, 2002, 8, 1269-1278.	3.3	40
48	Towards Rational Syntheses of the Elusive Metallocarbohedrenes: Density Functional Prescriptions for Electronic and Geometric Structures. Chemistry - A European Journal, 2002, 8, 3497.	3.3	6
49	Dimorphic Intra- and Intermolecular Aryl Motifs in Symmetrical Hexafaceted Molecules (ArnX)3Y-Z-Y(XArn)3. Chemistry - A European Journal, 2002, 8, 5456-5468.	3.3	31
50	The Geometric and Electronic Structures of Niobium Carbon Clusters. Journal of Physical Chemistry A, 2001, 105, 3340-3358.	2.5	36
51	The crystal supramolecularity of metal phenanthroline complexes. Dalton Transactions RSC, 2001, , 789-799.	2.3	149
52	Crystal packing motifs for mixed oxalate/phenanthroline metal complexes. CrystEngComm, 2001, 3, 96.	2.6	20
53	Contrasting crystal supramolecularity for [Fe(phen)3]I8 and [Mn(phen)3]I8: complementary orthogonality and complementary helicity. CrystEngComm, 2001, 3, 1.	2.6	63
54	Principles of crystal packing and intermolecular motifs for Ph3XSnXPh3, XâŠ•âŠ•C, Si, Ge, Sn. CrystEngComm, 2001, 3, 120-127.	2.6	3

#	Article	IF	Citations
55	The first endoannular metal halideâ€“cucurbituril: cis-SnCl4(OH2)2@cucurbit[7]uril. CrystEngComm, 2001, 3, 230-236.	2.6	17
56	Analyses of the crystal packing of (Ph3P)2Ag(O2C2O2)Ag(PPh3)2 and related heavily phenylated molecules: substitutional trimorphism. CrystEngComm, 2001, 3, 84.	2.6	5
57	High symmetry crystal supramolecularity: â€“XPh3 molecules in cubic latticesElectronic supplementary information (ESI) available: additional figures (Fig. S1â€“3) described in the text. See http://www.rsc.org/suppdata/nj/b1/b104324m/. New Journal of Chemistry, 2001, 25, 1500-1509.	2.8	19
58	A diamondoid supramolecular crystal lattice maintained entirely by sixfold phenyl embraces. CrystEngComm, 2001, 3, 46.	2.6	9
59	Crystal structures, crystal packing and supramolecular motifs in [Fe(phen)3]I14 and [M(phen)3]I18 (MâŠ•=âŠ•Fe, Ni): complementary orthogonality of [M(phen)3]2+ cations and polyiodide anions. CrystEngComm, 2001, 3, 9-14.	2.6	21
60	Coordination and Dehydrogenation of PH3by 23 Transition Metal Ions in the Gas Phase:Â FTICR Experiments and Density Functional Interpretations. Inorganic Chemistry, 2001, 40, 6972-6982.	4.0	3
61	Supramolecular Assemblies of Quaternary Ammonium Cations and Halide Anions in the Gas Phase: ESMS-FTICR Data and Computer Modelling. Chemistry - A European Journal, 2000, 6, 3671-3678.	3.3	9
62	Crystal supramolecularity: multiple phenyl embraces formed by [AsPh4]+ cations. Inorganica Chimica Acta, 2000, 306, 160-167.	2.4	17
63	Sixfold phenyl embraces with substituted phenyl in PPh3â€Šâ€. Dalton Transactions RSC, 2000, , 2909-2915.	2.3	35
64	Crystal supramolecularity. Multiple phenyl embraces by [PPN]+ cationsâ€Šâ€. Dalton Transactions RSC, 2000, , 299-306.	2.3	33
65	Crystal supramolecularity: sixfold phenyl embraces between PPh3 ligands, forming extended nets in one-, two-, and three-dimensions. Dalton Transactions RSC, 2000, , 1587-1594.	2.3	36
66	Supramolecular potentials and embraces for fluorous aromatic molecules. New Journal of Chemistry, 2000, 24, 295-304.	2.8	98
67	Intramolecular and supramolecular geometry of coordinated PPh3. Dalton Transactions RSC, 2000, , 1579-1585.	2.3	61
68	Crystal supramolecular motifs for [Ph4P]+ salts of [M(mnt)2]2â^', [M(mnt)2]â^', [{M(mnt)2}2]2â^', [M(mnt)3]3â^' and [M(mnt)3]2â^' (mnt2â^'â€...=â€...maleonitriledithiolate)â€Šâ€. Dalton Transactions RSC, 2000, , 3176-3185.	2.3	49
69	Crystal Supramolecular Motifs:â€‰ Columns of Embracing Ph3PMe+ or Ph3PCl+ Cations Controlling Formation of [Cu3X82- (X = Cl, Br). Inorganic Chemistry, 2000, 39, 401-405.	4.0	19
70	Understanding structure and reactivity of new fundamental inorganic molecules: metal sulfides, metallocarbohedrenes, and nitrogenase. Chemical Communications, 1998, , 523-530.	4.1	61
71	Ti8C12:Â Barrierless Transformation of theThIsomer to theTdIsomer. Journal of the American Chemical Society, 1996, 118, 6309-6310.	13.7	56
72	Computational Methods for Metal Sulfide Clusters. ACS Symposium Series, 1996, , 135-152.	0.5	7

#	Article	IF	Citations
73	Supramolecular Motifs: Concerted Multiple Phenyl Embraces between Ph₄P⁺ Cations Are Attractive and Ubiquitous. Chemistry - A European Journal, 1996, 2, 481-486.	3.3	255
74	Bildung und Struktur neuer Metalloâ€•und Metallapolysulfane [MS_y]⁺ (y = 2â€“16). Angewandte Chemie, 1995, 107, 215-218.	2.0	10
75	Selbstorganisation von Zinkâ€•und Cadmiumâ€cyaniden [M_x(CN)_{2x + 1}]^{â^'}, x â©½ 27, zu Helicaten. Angewandte Chemie, 1995, 107, 366-368.	2.0	0
76	Metal Chalcogenide Cluster Chemistry. Progress in Inorganic Chemistry, 0, , 637-803.	3.0	156