Catharine Esterhuysen

List of Publications by Year
in descending order

77 papers	1,736 citations	257101 24 h-index	301761 39 g-index
81 all docs	81 docs citations	81 times ranked	2111 citing authors

#	Article	IF	Citations
1	Conferences in the time of COVID: Perspectives on organising ISXB-4 Virtual. CrystEngComm, 2021, 23, 4889-4895.	1.3	0
2	Nature of halogen bond adducts of carbones with XCF3 (XÂ=ÂCl, Br, I) species. Polyhedron, 2021, 200, 115107.	1.0	3
3	Halogen Bonding: From Fundamentals to Applications. ChemPlusChem, 2021, 86, 1229-1230.	1.3	5
4	Direct Determination of Enthalpies of Sorption Using Pressureâ€Gradient Differential Scanning Calorimetry: CO 2 â€‰Sorption by Cuâ€HKUST. ChemSusChem, 2020, 13, 102-105.	3.6	10
5	Pressureâ€Gradient Sorption Calorimetry of Flexible Porous Materials: Implications for Intrinsic Thermal Management. ChemSusChem, 2020, 13, 5220-5223.	3.6	5
6	CO₂-induced single-crystal to single-crystal transformations of an interpenetrated flexible MOF explained by in situ crystallographic analysis and molecular modeling. Chemical Science, 2019, 10, 10018-10024.	3.7	39
7	Steric and Electronic Effects in Gold Nâ€Heterocyclic Carbene Complexes Revealed by Computational Analysis. ChemistryOpen, 2019, 8, 539-550.	0.9	1
8	Computational investigation of AuÂ·H hydrogen bonds involving neutral AuI N-heterocyclic carbene complexes and amphiprotic binary hydrides. Journal of Molecular Modeling, 2019, 25, 135.	0.8	4
9	A thermo-responsive structural switch and colossal anisotropic thermal expansion in a chiral organic solid. Chemical Communications, 2018, 54, 3727-3730.	2.2	16
10	Prevalent polymorphism in benzophenones. Acta Crystallographica Section C, Structural Chemistry, 2018, 74, 465-471.	0.2	4
11	Ligand-driven formation of halogen bonds involving Au(<scp>i</scp>) complexes. New Journal of Chemistry, 2018, 42, 10529-10538.	1.4	12
12	Trifluoromethyl: An Amphiphilic Noncovalent Bonding Partner. ChemPhysChem, 2017, 18, 772-784.	1.0	47
13	Solvatochromism as a probe to observe the solvent exchange process in a 1-D porous coordination polymer with 1-D solvent accessible channels. Chemical Communications, 2017, 53, 5618-5621.	2.2	12
14	Solvent- and Pressure-Induced Phase Changes in Two 3D Copper Glutarate-Based Metalâ€“Organic Frameworks via Glutarate (+gauche â‡„ â^'gauche) Conformational Isomerism. Journal of the American Chemical Society, 2017, 139, 5923-5929.	6.6	38
15	Gold setting the â€œgold standardâ€•among transition metals as a hydrogen bond acceptor â€“ a theoretical investigation. Dalton Transactions, 2017, 46, 4960-4967.	1.6	29
16	The halogen bond in solution: general discussion. Faraday Discussions, 2017, 203, 347-370.	1.6	5
17	Computational approaches and sigma-hole interactions: general discussion. Faraday Discussions, 2017, 203, 131-163.	1.6	17
18	Beyond the halogen bond: general discussion. Faraday Discussions, 2017, 203, 227-244.	1.6	2

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19	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	1.6	2
20	Highlights from the Faraday Discussion: Halogen Bonding in Supramolecular and Solid State Chemistry, July 10â€“12th 2017, Ottawa, Canada. Chemical Communications, 2017, 53, 11615-11621.	2.2	9
21	Electrostatic surface potential analysis of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>I</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow> ion in the gas phase, the condensed phase and a novel extrapolation to the solid state. Computational and Theoretical Chemistry, 2016, 1090, 225-232.	1.1	11
22	Preparing Gold(I) for Interactions with Proton Donors: The Elusive [Au]â‹…â‹…â‹…HO Hydrogen Bond. Angewandte Chemie, 2016, 128, 1726-1730.	1.6	12
23	Ab initio studies of the structures and vibrational spectra of the hydrogen halide and lithium halide homo- and heterodimers and some mixed hydrogen halide/lithium halide heterodimers. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	0
24	Preparing Gold(I) for Interactions with Proton Donors: The Elusive [Au]â‹…â‹…â‹…HO Hydrogen Bond. Angewandte Chemie - International Edition, 2016, 55, 1694-1698.	7.2	33
25	Elucidating the mechanism responsible for anomalous thermal expansion in a metalâ€“organic framework. Dalton Transactions, 2016, 45, 4141-4149.	1.6	5
26	Concomitant polymorphs of p-iso-propylcalix[4]arene. CrystEngComm, 2015, 17, 5129-5133.	1.3	10
27	Extreme Carbon Dioxide Sorption Hysteresis in Openâ€Channel Rigid Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2015, 54, 2079-2083.	7.2	48
28	Hydrogen-Bond Analysis: Statistical and Computational versus Experimental Position Refinement. Crystal Growth and Design, 2014, 14, 3480-3484.	1.4	2
29	Polymorphic Co-crystals from Polymorphic Co-crystal Formers: Competition between Carboxylic AcidÂ·Â·Â·Pyridine and PhenolÂ·Â·Â·Pyridine Hydrogen Bonds. Crystal Growth and Design, 2013, 13, 3935-3952.	1.4	80
30	Complexation behavior of two-coordinated carbon compounds containing fluorenyl ligands. Dalton Transactions, 2013, 42, 13349.	1.6	15
31	Extensive theoretical investigation: influence of the electrostatic environment on the I3 â¯Â·Â·Â·I3 â¯ anionâ€“anion interaction. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	29
32	In Situ Xâ€ray Structural Studies of a Flexible Host Responding to Incremental Gas Loading. Angewandte Chemie - International Edition, 2012, 51, 4913-4916.	7.2	62
33	A Tale of Two Polymorphic Pharmaceuticals: Pyrithyldione and Propyphenazone and their 1937 Coâ€crystal Patent. Chemistry - A European Journal, 2011, 17, 13445-13460.	1.7	21
34	Distinguishing Carbones from Allenes by Complexation to AuCl. Chemistry - A European Journal, 2011, 17, 9944-9956.	1.7	84
35	OHphenolâ‹¯OHalcohol hydrogen-bonding as the preferred hydrogen-bonded interaction in the crystal structures of three isomers of methylolphenol: analysis of hydrogen-bonding interactions in phenol and alcohol containing molecules. CrystEngComm, 2011, 13, 5773.	1.3	11
36	Synthesis Characterization Molecular Modeling of a Pharmaceutical Co-Crystal: (2-Chloro-4-Nitrobenzoic Acid):(Nicotinamide). Journal of Pharmaceutical Sciences, 2010, 99, 4054-4071.	1.6	47

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37	Extraction and transport of gold(III) using some acyl(aroyl)thiourea ligands and a crystal structure of one of the complexes. Inorganic Chemistry Communication, 2010, 13, 468-470.	1.8	33
38	Concomitant Polymorphs of the Antihyperlipoproteinemic Bezafibrate. Crystal Growth and Design, 2009, 9, 2646-2655.	1.4	27
39	Pentacarbonyl-2Î¹5C-chlorido-1Î¹Cl-bis[1(Î·5)-cyclopentadienyl](Î¼-1-oxidoethylene-1:2Î¹2O:C)chromium(0)zirconium(IV). Acta Crystallographica Section E: Structure Reports Online, 2009, 65, m125-m125.	0.2	2
40	Preparation of tris(azolyl)phosphine gold(<scp>i</scp>) complexes: digold(<scp>i</scp>) coordination and variation in solid state intermolecular interactions. New Journal of Chemistry, 2008, 32, 138-150.	1.4	13
41	Pentacarbonyl-2Î¹⁵ C-chlorido-1Î¹Cl-bis[1(Î·⁵)-cyclopentadienyl][Î¼-oxido(phenyl)methylene-1:2Î¹² O:C]hafnium(IV)tungsten(0). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, m1150-m1150.	0.2	4
42	Pentacarbonyl-2Î¹5C-chlorido-1Î¹Cl-bis[1(Î·5)-cyclopentadienyl][Î¼2-oxido(methyl)methylene-1:2Î¹2O:C]tungsten(0)zirconium(IV). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, m1252-m1252.	0.2	4
43	Pentacarbonyl-2Î¹5C-chlorido-1Î¹Cl-bis[1(Î·5)-cyclopentadienyl](Î¼-Î±-oxidobenzylidene-1:2Î¹2O:C)titanium(IV)tungsten(0). Acta Crystallographica Section E: Structure Reports Online, 2008, 64, m1534-m1534.	0.2	1
44	Reaction and subsequent transformation of anionic acetylideâ€“carbene complexes using the Ph3PAu+ fragment. Dalton Transactions, 2007, , 5684.	1.6	9
45	Aurolysis of Î±-C-deprotonated group 6 aminocarbene and thiocarbene complexes with Ph3PAu+. Dalton Transactions, 2006, , 4580-4589.	1.6	14
46	Aqua[3,6-bis(methoxycarbonylmethyl)-3,6-diazaoctanedioato]copper(II) dihydrate. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m355-m357.	0.2	0
47	Tetrakis(Î¼2-2,2-dimethylpropanoato-Î¹2O,Oâ€²)bis[(pyridine-Î¹N)copper(II)]. Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m420-m422.	0.2	2
48	Pentacarbonyl[methyl(n-propylsulfanyl)carbene]chromium(0). Acta Crystallographica Section E: Structure Reports Online, 2006, 62, m1625-m1626.	0.2	1
49	High and selective Ag(I) bulk liquid membrane transport with N,N-diethyl-Nâ€²-camphanyl thiourea and structure of the complex. Inorganic Chemistry Communication, 2006, 9, 99-102.	1.8	19
50	4-Membered metallodithiophosphinate rings â€“ flat or puckered? A comparison of two crystal structures with computational and literature data. Inorganica Chimica Acta, 2006, 359, 609-616.	1.2	8
51	Reply to â€œComment on the Comparative Use of the Electron Density and Its Laplacianâ€• Chemistry - A European Journal, 2006, 12, 7773-7774.	1.7	22
52	Solid-State Self-Inclusion: The Missing Link. Angewandte Chemie - International Edition, 2006, 45, 5354-5358.	7.2	39
53	Guest-Induced Conformational Switching in a Single Crystal. Angewandte Chemie - International Edition, 2006, 45, 5856-5859.	7.2	86
54	New reactions and new products derived from Î±-deprotonated Fischer-type carbene complexes. Inorganica Chimica Acta, 2005, 358, 1581-1594.	1.2	6

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55	Gold acyls and imidoyls prepared from anionic Fischer-type carbene complexes. Inorganica Chimica Acta, 2005, 358, 4217-4228.	1.2	19
56	The Nature of the Chemical Bond Revisited: An Energy-Partitioning Analysis of Nonpolar Bonds. Chemistry - A European Journal, 2005, 11, 1813-1825.	1.7	137
57	Resolution of (S,S)-4-(2,2,4-trimethylchroman-4-yl)phenyl camphanate and its 4-chromanyl epimer by crystallization. Acta Crystallographica Section C: Crystal Structure Communications, 2005, 61, o32-o34.	0.4	5
58	1,1-Dibenzoyl-3,3-dimethylurea. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o4042-o4044.	0.2	0
59	Thione complexes of Rh(i): a first comparison with the bonding and catalytic activity of related carbene and imine compounds. Dalton Transactions, 2005, , 181.	1.6	56
60	Reactions of halogens with Pt(ii) complexes of N-alkyl- and N,N-dialkyl-Nâ€²-benzoylthioureas: oxidative addition and formation of an I2 inclusion compound. Dalton Transactions, 2005, , 2162.	1.6	31
61	The nature of the chemical bond revisited. An energy partitioning analysis of diatomic molecules E2 (E=Nâ€“Bi, Fâ€“I), CO and BF. Theoretical Chemistry Accounts, 2004, 111, 381-389.	0.5	134
62	Intramolecular hydrogen-bond-directed coordination:trans-bis(N-benzoyl-Nâ€²-propylthiourea-ÎºS)diiodoplatinum(II) andtrans-bis(N-benzoyl-Nâ€²-propylthiourea-ÎºS)dibromoplatinum(II). Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, m395-m398.	0.4	11
63	The first bipodal thiocarbamic acid ester,O,Oâ€²-diethylN,Nâ€²-(p-phenylenedicarbonyl)bis(thiocarbamate). Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o862-o864.	0.4	6
64	Anionic Fischer-type carbene complexes as bidentate (N,O) ligandsElectronic supplementary information (ESI) available: molecular structures of 4b, 5, 7 and 8. See http://www.rsc.org/suppdata/dt/b3/b316998g/. Dalton Transactions, 2004, , 1173.	1.6	22
65	Comparison of Side-On and End-On Coordination of E2 Ligands in Complexes [W(CO)5E2] (E=N, P, As, Sb,) Tj ETQq1 1 0.784314 rgB	1.7	36
66	Synthesis and characterisation of N-coordinated pentafluorophenyl gold(i) thiazole-derived complexes and an unusual self-assembly to form a tetrameric gold(i) complexElectronic supplementary information (ESI) available: Characterisation data for 1. See http://www.rsc.org/suppdata/dt/b3/b303625a/. Dalton Transactions, 2003, , 2859.	1.6	24
67	Biphasic hydroformylation in new molten saltsâ€”analogies and differences to organic solvents. Dalton Transactions RSC, 2002, , 1132.	2.3	35
68	Mono- and bi-dentate Group 6-coordinated and titanium-containing isocyanide ligands prepared from benzoxazole. Dalton Transactions RSC, 2002, , 2386.	2.3	6
69	New Rhodium Complexes Coordinated by Bidentate Imine Ligands with Benzothiazolyl Functionalities. Helvetica Chimica Acta, 2002, 85, 3737-3747.	1.0	6
70	Synthesis, X-ray characterization and single molecule magnetic behaviour of [Mn12O12(O2CCH2X)16(H2O)4]Â·mCH2Cl2Â·nH2O (1: X = Cl, mÂ= 2, nÂ= 6; 2: X = Br, mÂ= 4, nÂ= 0). Dalton Transactions RSC, 2001, , 3352.	2.3	22
71	Tricarbonylbis(4-methyl-1,3-thiazole-2(3H)-thionato-N,S2)tungsten(II). Acta Crystallographica Section E: Structure Reports Online, 2001, 57, m72-m74.	0.2	1
72	Thioether- and selenoether-carboxylates in palladium chemistry: conclusive proof of hemilabile properties of Oâ€“Se ligands. Journal of Organometallic Chemistry, 2001, 619, 164-178.	0.8	13

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73	Synthesis and crystallographic characterization of thiazole-2-dithiocarboxylate methyl ester complexes of chromium, tungsten and iron carbonylsâ€Šâ€. Dalton Transactions RSC, 2000, , 3016-3021.	2.3	10
74	trans-(2-Methylthiobenzoato-O)phenylbis(triphenylphosphine)palladium(II), two conformational isomers. Acta Crystallographica Section C: Crystal Structure Communications, 2000, 56, 329-331.	0.4	0
75	Group 6 carbene complexes derived from lithiated azoles and the crystal structure of a molybdenum thiazolinylidene complex. Journal of Organometallic Chemistry, 1999, 590, 158-168.	0.8	49
76	Thioethercarboxylates in palladium chemistry: First proof of hemilabile properties of Sâ€“O ligands. Journal of Organometallic Chemistry, 1998, 553, 83-90.	0.8	16
77	Palladiumâ€Catalyzed Activation of Carbonâ€“Halogen Bonds: Electrostaticsâ€Controlled Reactivity. European Journal of Organic Chemistry, 0, , .	1.2	4