Carole A Morrison

List of Publications by Year
in descending order

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144 papers	4,396 citations	126708 33 h-index	133063 59 g-index
148 all docs	148 docs citations	148 times ranked	5316 citing authors

#	Article	IF	Citations
1	Structure Analysis Restrained by ab Initio Calculations:â€‰ The Molecular Structure of 2,5-Dichloropyrimidine in Gaseous and Crystalline Phases. The Journal of Physical Chemistry, 1996, 100, 12280-12287.	2.9	178
2	Elucidating the Breathing of the Metalâ€“Organic Framework MIL-53(Sc) with ab Initio Molecular Dynamics Simulations and in Situ X-ray Powder Diffraction Experiments. Journal of the American Chemical Society, 2013, 135, 15763-15773.	6.6	173
3	Challenges and opportunities in the recovery of gold from electronic waste. RSC Advances, 2020, 10, 4300-4309.	1.7	159
4	Understanding the adsorption process in ZIF-8 using high pressure crystallography and computational modelling. Nature Communications, 2018, 9, 1429.	5.8	146
5	Amino acids as highly efficient modulators for single crystals of zirconium and hafnium metalâ€“organic frameworks. Journal of Materials Chemistry A, 2016, 4, 6955-6963.	5.2	137
6	Three-dimensional protonic conductivity in porous organic cage solids. Nature Communications, 2016, 7, 12750.	5.8	133
7	The Effect of High Pressure on MOFâ€5: Guestâ€Induced Modification of Pore Size and Content at High Pressure. Angewandte Chemie - International Edition, 2011, 50, 11138-11141.	7.2	128
8	Spontaneous Generation of Stable Pnictinyl Radicals from â€œJack-in-the-Boxâ€•Dipnictines:Â A Solid-State, Gas-Phase, and Theoretical Investigation of the Origins of Steric Stabilization1. Journal of the American Chemical Society, 2001, 123, 9045-9053.	6.6	124
9	A Simple Primary Amide for the Selective Recovery of Gold from Secondary Resources. Angewandte Chemie - International Edition, 2016, 55, 12436-12439.	7.2	116
10	Persistent phosphinyl radicals from a bulky diphosphine: an example of a molecular jack-in-the-box. Chemical Communications, 2000, , 2045-2046.	2.2	106
11	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie - International Edition, 2016, 55, 2401-2405.	7.2	103
12	Improving Predictions of Gas Adsorption in Metalâ€“Organic Frameworks with Coordinatively Unsaturated Metal Sites: Model Potentials, ab initio Parameterization, and GCMC Simulations. Journal of Physical Chemistry C, 2012, 116, 18899-18909.	1.5	102
13	Effect of pressure on the crystal structure of L-serine-I and the crystal structure of L-serine-II at 5.4â€…GPa. Acta Crystallographica Section B: Structural Science, 2005, 61, 58-68.	1.8	97
14	Tetraborane(10), B4H10: structures in gaseous and crystalline phases. Journal of the Chemical Society Dalton Transactions, 1996, , 4589.	1.1	96
15	Femtosecond Dynamics of the Ring Closing Process of Diarylethene: A Case Study of Electrocyclic Reactions in Photochromic Single Crystals. Journal of Physical Chemistry A, 2011, 115, 13158-13168.	1.1	96
16	Lead-free pseudo-three-dimensional organicâ€“inorganic iodobismuthates for photovoltaic applications. Sustainable Energy and Fuels, 2017, 1, 308-316.	2.5	90
17	Dihydrogen Bonds in Solid BH3NH3. Angewandte Chemie - International Edition, 2004, 43, 4780-4782.	7.2	85
18	Temperature- and Pressure-Induced Proton Transfer in the 1:1 Adduct Formed between Squaric Acid and 4,4â€²-Bipyridine. Journal of the American Chemical Society, 2009, 131, 3884-3893.	6.6	82

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19	Ring-Closing Reaction in Diarylethene Captured by Femtosecond Electron Crystallography. Journal of Physical Chemistry B, 2013, 117, 15894-15902.	1.2	79
20	Recycling copper and gold from e-waste by a two-stage leaching and solvent extraction process. Separation and Purification Technology, 2021, 263, 118400.	3.9	78
21	High-Pressure Experimental and DFT-D Structural Studies of the Energetic Material FOX-7. Journal of Physical Chemistry C, 2015, 119, 2322-2334.	1.5	69
22	Experimental and DFT-D Studies of the Molecular Organic Energetic Material RDX. Journal of Physical Chemistry C, 2013, 117, 8062-8071.	1.5	56
23	Tuning the Swing Effect by Chemical Functionalization of Zeolitic Imidazolate Frameworks. Journal of the American Chemical Society, 2018, 140, 382-387.	6.6	55
24	Predicting the reactivity of energetic materials: an ab initio multi-phonon approach. Journal of Materials Chemistry A, 2019, 7, 19539-19553.	5.2	52
25	Liquid Methanol from DFT and DFT/MM Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 106-118.	2.3	51
26	The First Alkaline Earth Metal Complex Containing a Î¼-Î·1:Î·1 Allyl Ligand: Structure of [{HC[C(tBu)NC6H3(CHMe2)2]2Mg(C3H5)}6] The financial support of the UK EPSRC (S.T.L., S.P.) and The Royal Society (C.A.M.) is gratefully acknowledged.. Angewandte Chemie - International Edition, 2001, 40, 4463.	7.2	46
27	Cold ablation driven by localized forces in alkali halides. Nature Communications, 2014, 5, 3863.	5.8	41
28	Determining the Strengths of Hydrogen Bonds in Solid-State Ammonia and Urea: Insight from Periodic DFT Calculations. Chemistry - A European Journal, 2003, 9, 628-634.	1.7	40
29	Toward Understanding Mobile Proton Behavior from First Principles Calculation:Â The Short Hydrogen Bond in Crystalline Ureaâ^'Phosphoric Acid. Journal of the American Chemical Society, 2005, 127, 4042-4048.	6.6	39
30	A symmetric hydrogen bond revisited: potassium hydrogen maleate by variable temperature, variable pressure neutron diffraction and plane-wave DFT methods. Chemical Physics Letters, 2003, 381, 102-108.	1.2	36
31	Tuneable separation of gold by selective precipitation using a simple and recyclable diamide. Nature Communications, 2021, 12, 6258.	5.8	36
32	Outer-Sphere Coordination Chemistry: Amido-Ammonium Ligands as Highly Selective Tetrachloridozinc(II)ate Extractants. Inorganic Chemistry, 2012, 51, 12805-12819.	1.9	35
33	Metal-binding motifs of alkyl and aryl phosphinates; versatile mono and polynucleating ligands. Coordination Chemistry Reviews, 2017, 335, 150-171.	9.5	35
34	Extending lead-free hybrid photovoltaic materials to new structures: thiazolium, aminothiazolium and imidazolium iodobismuthates. Dalton Transactions, 2018, 47, 7050-7058.	1.6	34
35	Polymorphism in the Crystal Structures of the Group 13 Trimethyls. Organometallics, 2003, 22, 2450-2457.	1.1	33
36	Predicting the impact sensitivities of energetic materials through zone-center phonon up-pumping. Journal of Chemical Physics, 2021, 154, 064105.	1.2	33

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37	Structural and theoretical investigations of short hydrogen bonds: neutron diffraction and plane-wave DFT calculations of ureaâ€“phosphoric acid. Chemical Physics Letters, 2002, 362, 85-89.	1.2	32
38	Evaluation of Simple Amides in the Selective Recovery of Gold from Secondary Sources by Solvent Extraction. ACS Sustainable Chemistry and Engineering, 2019, 7, 15019-15029.	3.2	32
39	Pore Shape Modification of a Microporous Metalâ€“Organic Framework Using High Pressure: Accessing a New Phase with Oversized Guest Molecules. Chemistry of Materials, 2016, 28, 466-473.	3.2	31
40	Anisotropic lattice softening near the structural phase transition in the thermosalient crystal 1,2,4,5-tetrabromobenzene. Physical Chemistry Chemical Physics, 2018, 20, 8523-8532.	1.3	31
41	Cooperative Heterometallic Catalysts for Lactide Ring-Opening Polymerization: Combining Aluminum with Divalent Metals. Inorganic Chemistry, 2021, 60, 2294-2303.	1.9	30
42	Preparation and Properties of Gallaborane, GaBH6:Â Structure of the Gaseous Molecule H2Ga(Î¼-H)2BH2As Determined by Vibrational, Electron Diffraction, and ab Initio Studies, and Structure of the Crystalline Solid at 110 K As Determined by X-ray Diffractionâ€. Inorganic Chemistry, 2001, 40, 3484-3497.	1.9	29
43	Combined Experimental and Computational Hydrostatic Compression Study of Crystalline Ammonium Perchlorate. Journal of Physical Chemistry C, 2011, 115, 18782-18788.	1.5	29
44	Early Events in the Nonadiabatic Relaxation Dynamics of 4-(N,N-Dimethylamino)benzonitrile. Journal of Chemical Theory and Computation, 2015, 11, 1118-1128.	2.3	29
45	Perfluorocyclopropene:Â Experimental and Theoretical Studies of Its Structure in Gaseous, Solution, and Crystalline Phases. Journal of the American Chemical Society, 1996, 118, 209-216.	6.6	28
46	Assessing the performance of density functional theory in optimizing molecular crystal structure parameters. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 259-267.	0.5	28
47	Anion Receptor Design: Exploiting Outer-Sphere Coordination Chemistry To Obtain High Selectivity for Chloridometalates over Chloride. Inorganic Chemistry, 2015, 54, 8685-8692.	1.9	28
48	Conformational Properties of Substituted Ferrocenes:Â Experimental and Theoretical Studies of the Molecular Structures of 1,1â€˜-Di-tert-butylferrocene and Isopropylferrocene. Organometallics, 2001, 20, 2309-2320.	1.1	26
49	A Pathway to the Athermal Impact Initiation of Energetic Azides. Journal of Physical Chemistry C, 2018, 122, 19395-19408.	1.5	26
50	The Influence of the Hofmeister Bias and the Stability and Speciation of Chloridolanthanates on Their Extraction from Chloride Media. Solvent Extraction and Ion Exchange, 2016, 34, 579-593.	0.8	25
51	A Computational and Experimental Approach Linking Disorder, Highâ€Pressure Behavior, and Mechanical Properties in UiO Frameworks. Angewandte Chemie, 2016, 128, 2447-2451.	1.6	24
52	Dimethylalane, [Me2AlH]n, in the Vapor Phase and in Hydrocarbon Solution:Â Gas-Phase Electron Diffraction, Spectroscopic, Colligative, and ab Initio Studies. Organometallics, 2000, 19, 527-538.	1.1	23
53	Car-Parrinello and path integral molecular dynamics study of the hydrogen bond in the chloroacetic acid dimer system. Journal of Chemical Physics, 2007, 127, 064304.	1.2	22
54	Spin crossover in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msup><mml:mrow><mml:mtext>CsFe</mml:mtext></mml:mrow><mml:mrow><mml:mtext>II</mml:mr Physical Review B, 2010, 81, .	1.1	22

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55	A Simple Primary Amide for the Selective Recovery of Gold from Secondary Resources. Angewandte Chemie, 2016, 128, 12624-12627.	1.6	22
56	Vibrationally induced metallisation of the energetic azide Î±-NaN‹sub›3‹/sub›. Physical Chemistry Chemical Physics, 2018, 20, 29061-29069.	1.3	21
57	C‹sub›70‹/sub› Oxides and Ozonides and the Mechanism of Ozonolysis on the Fullerene Surface. A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 9891-9898.	1.1	19
58	Molecular Structure of 1,3,5-Triazine in Gas, Solution, and Crystal Phases and by ab Initio Calculationsâ€. Journal of Physical Chemistry A, 1997, 101, 10029-10038.	1.1	18
59	Proton Chelating Ligands Drive Improved Chemical Separations for Rhodium. Inorganic Chemistry, 2019, 58, 8720-8734.	1.9	18
60	Interpreting Molecular Crystal Disorder in Plumbocene, Pb(C5H5)2:Â Insight from Theory. Journal of the American Chemical Society, 2002, 124, 6775-6780.	6.6	17
61	Small energy differences in molecular crystals: A first principles study of tautomerism and dynamics in benzoic acid derivatives. CrystEngComm, 2007, 9, 777.	1.3	17
62	Aluminiumâ€Catalyzed C(sp)â^'H Borylation of Alkynes. Angewandte Chemie - International Edition, 2021, 60, 20672-20677.	7.2	17
63	Modifying the Fullerene Surface Using Endohedral Noble Gas Atoms: Density Functional Theory Based Molecular Dynamics Study of C‹sub›70‹/sub›O‹sub›3‹/sub›. Journal of Physical Chemistry A, 2012, 116, 3413-3419.	1.1	16
64	Hybrid QM/QM simulations of photochemical reactions in the molecular crystal N-salicylidene-2-chloroaniline. Physical Chemistry Chemical Physics, 2013, 15, 10803.	1.3	16
65	A Computational and Experimental Study on the Binding of Dithio Ligands to Sperrylite, Pentlandite, and Platinum. Journal of Physical Chemistry C, 2016, 120, 22476-22488.	1.5	16
66	Coherent ultrafast lattice-directed reaction dynamics of triiodide anion photodissociation. Nature Chemistry, 2017, 9, 516-522.	6.6	16
67	High-Pressure Study of Two Polymorphs of 2,4,6-Trinitrotoluene Using Neutron Powder Diffraction and Density Functional Theory Methods. Journal of Physical Chemistry C, 2019, 123, 26095-26105.	1.5	16
68	1,1,2-Tri-tert-butyldisilane, But2HSiSiH2But: vibrational spectra and molecular structure in the gas phase by electron diffraction and ab initio calculations. Journal of the Chemical Society Dalton Transactions, 1999, , 2303-2310.	1.1	15
69	Heavier alkali metal complexes of 2-phenylamidopyridine: An X-ray crystallographic and theoretical study of a structurally diverse series of crown ether adducts. Dalton Transactions, 2004, , 2514.	1.6	15
70	Experimental equilibrium crystal structures: Molecular dynamics as a probe for atomic probability density functions. Chemical Physics Letters, 2007, 448, 61-64.	1.2	15
71	Simulating thermal motion in crystalline phase-I ammonia. Journal of Chemical Physics, 2010, 132, 134511.	1.2	15
72	Pressure induced phase transitions in the tripeptide glutathione to 5.24 GPa: the crystal structure of glutathione-II at 2.94 GPa and glutathione-III at 3.70 GPa. CrystEngComm, 2010, 12, 2587.	1.3	15

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73	Predicting anisotropic displacement parameters using molecular dynamics: density functional theory plus dispersion modelling of thermal motion in benzophenone. Journal of Applied Crystallography, 2013, 46, 656-662.	1.9	15
74	Understanding the Recovery of Rare-Earth Elements by Ammonium Salts. Metals, 2018, 8, 465.	1.0	15
75	Synthesis and structures of anionic rhenium polyhydride complexes of boronâ€“hydride ligands and their application in catalysis. Chemical Science, 2020, 11, 9994-9999.	3.7	15
76	A theoretical and experimental study of weak silaneâ€“electron donor interactions. Journal of Molecular Structure, 2000, 554, 163-172.	1.8	14
77	Using molecular-dynamics simulations to understand and improve the treatment of anharmonic vibrations. I. Study of positional parameters. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, 336-345.	0.3	14
78	Contributions of inner and outer coordination sphere bonding in determining the strength of substituted phenolic pyrazoles as copper extractants. Dalton Transactions, 2016, 45, 3055-3062.	1.6	14
79	On the Extraction of HCl and H₂PtCl₆ by Tributyl Phosphate: A Mode of Action Study. Solvent Extraction and Ion Exchange, 2017, 35, 531-548.	0.8	14
80	A Review of the Catalytic Effects of Leadâ€Based Ballistic Modifiers on the Combustion Chemistry of Double Base Propellants. Propellants, Explosives, Pyrotechnics, 2021, 46, 13-25.	1.0	14
81	Predicting the impact sensitivity of a polymorphic high explosive: the curious case of FOX-7. Chemical Communications, 2021, 57, 11213-11216.	2.2	14
82	The molecular structure of thiazole, determined by the combined analysis of gas-phase electron diffraction (GED) data and rotational constants and by ab initio calculations. Physical Chemistry Chemical Physics, 1999, 1, 2421-2426.	1.3	13
83	Nitric acid dihydrate at ambient and high pressure: An experimental and computational study. Physical Review B, 2006, 73, .	1.1	13
84	Hybrid QM/QM Simulations of Excited-State Intramolecular Proton Transfer in the Molecular Crystal 7-(2-Pyridyl)-indole. Journal of Chemical Theory and Computation, 2013, 9, 1182-1192.	2.3	13
85	First-Principles Study on Ligand Binding and Positional Disorder in Pentlandite. Journal of Physical Chemistry C, 2015, 119, 25457-25468.	1.5	13
86	Direct evidence for distinct colour origins in ROY polymorphs. Chemical Science, 2021, 12, 12711-12718.	3.7	13
87	Optimization of process parameters for the selective leaching of copper, nickel and isolation of gold from obsolete mobile phone PCBs. Cleaner Engineering and Technology, 2021, 4, 100180.	2.1	13
88	Gaseous and crystalline phase molecular structures of 4,6-dichloropyrimidine, 2,6-dichloropyrazine and 3,6-dichloropyridazine. Journal of the Chemical Society Perkin Transactions II, 1997, , 857-868.	0.9	12
89	Simulating Proton Transport through a Simplified Model for Trans-Membrane Proteins. Journal of Physical Chemistry B, 2010, 114, 7047-7055.	1.2	12
90	The Phonon Spectrum of Phase-I Ammonia:â€‰ Reassignment of Lattice Mode Symmetries from Combined Molecular and Lattice Dynamics Calculations. Journal of Physical Chemistry A, 2008, 112, 1322-1329.	1.1	11

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91	Determination of the experimental equilibrium structure of solid nitromethane using path-integral molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 094502.	1.2	11
92	Using molecular-dynamics simulations to understand and improve the treatment of anharmonic vibrations. II. Developing and assessing new Debyeâ€“Waller factors. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, 346-356.	0.3	11
93	Tantalum Recycling by Solvent Extraction: Chloride Is Better than Fluoride. Metals, 2020, 10, 346.	1.0	11
94	Câ€“H Borylation Catalysis of Heteroaromatics by a Rhenium Boryl Polyhydride. ACS Catalysis, 2021, 11, 7394-7400.	5.5	11
95	Molecular structures of tetraborane(10) derivatives: ab initio calculations for H2MB3H8 (Mâ€...=â€...B, Al, Ga) Tj ETQq1 1 0.784314 r Transactions, 1998, , 2147-2154.	1.1	10
96	The synthesis of C[Si(CH3)2X]3SiX3 compounds (Xâ€...=â€...H, Cl, Br and OH) and the molecular structure of C[Si(CH3)2H]3SiH3 in the gas phase; a study by electron diffraction and ab initio molecular orbital calculationsâ€Šâ€. Journal of the Chemical Society Dalton Transactions, 1999, , 2293-2302.	1.1	10
97	Reply to comment on: â€˜A symmetric hydrogen bond revisited: potassium hydrogen maleate by variable temperature, variable pressure neutron diffraction and plane-wave DFT methodsâ€™ [Chem. Phys. Lett. 381 (2003) 102]. Chemical Physics Letters, 2004, 399, 292-293.	1.2	10
98	A New Polymorph of N,Nâ€²-Dimethylurea Characterized by X-ray Diffraction and First-Principles Lattice Dynamics Calculations. Journal of Physical Chemistry A, 2009, 113, 5998-6003.	1.1	10
99	New Route to Local Order Models for Disordered Crystalline Materials: Diffuse Scattering and Computational Modeling of Phloroglucinol Dihydrate. Crystal Growth and Design, 2011, 11, 2045-2049.	1.4	10
100	The Supramolecular and Coordination Chemistry of Cobalt(II) Extraction by Phosphinic Acids. European Journal of Inorganic Chemistry, 2018, 2018, 1511-1521.	1.0	10
101	The molecular structures of 2-, 3- and 4-chloropyridine and chloropyrazine in the gas phase by electron diffraction and ab initio calculationsâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 745-754.	0.9	9
102	Conformational control by halogen substitution and by crystallisation: a study of the molecular structures of CH(SiMe2H)3 and CH(SiMe2Br)3 by gas-phase electron diffraction, and ab initio molecular orbital calculationsâ€Šâ€. Dalton Transactions RSC, 2000, , 4312-4322.	2.3	9
103	Molecular structure of ButCl2SiSiCl2But in the gas phase by electron diffraction and ab initio calculations. Molecular structures of the compounds ButX2SiSiX2But (X = Cl, Br or I) by vibrational spectroscopy, X-ray crystallography and ab initio calculationsâ€. Dalton Transactions RSC, 2001, , 2916-2925.	2.3	9
104	Molecular structures of M(Bu^t)₃(M = Al, Ga, In) using gas-phase electron diffraction and ab initio calculations: experimental and computational evidence for charge-transfer processes leading to photodissociation. Dalton Transactions, 2008, , 404-410.	1.6	9
105	EPR/ENDOR and Computational Study of Outer Sphere Interactions in Copper Complexes of Phenolic Oximes. Inorganic Chemistry, 2015, 54, 8465-8473.	1.9	9
106	High-Pressure Neutron Powder Diffraction Study of Îµ-CL-20: A Gentler Way to Study Energetic Materials. Journal of Physical Chemistry C, 2020, 124, 27985-27995.	1.5	9
107	Neutron powder and ab initio structure of ortho-xylene: the influence of crystal packing on phenyl ring geometry at 2 K. Chemical Communications, 2000, , 539-540.	2.2	8
108	A new, tetragonal, helical phase of plumbocene, Cp2Pb; variations on a molecular string (Cp=C5H5). Journal of Organometallic Chemistry, 2002, 650, 75-76.	0.8	8

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109	Synthesis, structure and spectroscopic properties of a new class of polymerisable nickel dithiolenes. Journal of Materials Chemistry, 2009, 19, 6194.	6.7	8
110	Describing the chemical bonding in C70 and C70O3 â€“ A quantum chemical topology study. Chemical Physics, 2014, 433, 22-30.	0.9	8
111	Towards understanding the catalytic properties of lead-based ballistic modifiers in double base propellants. Physical Chemistry Chemical Physics, 2020, 22, 25502-25513.	1.3	8
112	Pressure-induced non-innocence in bis(1,2-dionedioximato)Pt(<scp>ii</scp>) complexes: an experimental and theoretical study of their insulatorâ€“metal transitions. Physical Chemistry Chemical Physics, 2020, 22, 6677-6689.	1.3	8
113	Nitric acid monohydrates at high pressure: An experimental and computational study. Physical Review B, 2005, 72, .	1.1	7
114	Constrained dynamics and extraction of normal modes fromab initiomolecular dynamics: Application to ammonia. Journal of Chemical Physics, 2006, 125, 064707.	1.2	7
115	Hybrid functional study of the magnetism and electronic structure of a novel coordination polymer: [Cu(HF2)(pyz)2]BF4. Chemical Physics Letters, 2008, 459, 119-123.	1.2	7
116	Molecular structures of tetraborane(10) derivatives: ab initio calculations for (CH3)2MB3H8 (Mâ€…=â€…B, Al,) Tj ETQq0 0 0 rgBT /Over Chemical Society Dalton Transactions, 1998, , 2155-2162.	1.1	6
117	Investigating anharmonicity using molecular dynamics calculations: the TM hydride series (PH3)3MH4, (M = Os, Ru and Fe). Dalton Transactions, 2010, 39, 5527.	1.6	6
118	Inter- versus Intramolecular Structural Manipulation of a Dichromium(II) Pacman Complex through Pressure Variation. Inorganic Chemistry, 2016, 55, 214-220.	1.9	6
119	Carbon dioxide binary crystals via the thermal decomposition of RDX at high pressure. Chemical Science, 2017, 8, 4872-4878.	3.7	6
120	Evaluating the high-pressure structural response and crystal lattice interactions of the magnetically-bistable organic radical TTTA. CrystEngComm, 2021, 23, 4444-4450.	1.3	6
121	Selective recovery of nickel from obsolete mobile phone PCBs. Hydrometallurgy, 2022, 210, 105843.	1.8	6
122	High pressure studies of metal organic framework materials. International Journal of Nanotechnology, 2012, 9, 18.	0.1	5
123	Density functional theory based molecular dynamics simulations of C70O3 doped with light molecules. Chemical Physics, 2014, 428, 121-126.	0.9	5
124	Reducing the Competition: A Dual-Purpose Ionic Liquid for the Extraction of Gallium from Iron Chloride Solutions. Molecules, 2020, 25, 4047.	1.7	5
125	Simple Amides and Amines for the Synergistic Recovery of Rhodium from Hydrochloric Acid by Solvent Extraction. Chemistry - A European Journal, 2021, 27, 8714-8722.	1.7	5
126	Conformational Analysis with Both Experimental and Computational Data for Both Gaseous and Crystalline Phases:â€‰ Unexpected Interactions in N-Methyldichloroacetamide. Journal of Physical Chemistry A, 2004, 108, 185-193.	1.1	4

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127	A new high pressure phase of sodium formate dihydrate; an experimental and computational study. Dalton Transactions, 2007, , 2014.	1.6	4
128	Study of the stability of aluminium trimeric clusters in aqueous solutions. Molecular Simulation, 2012, 38, 934-943.	0.9	4
129	Co-extraction of Iron and Sulfate by Bis(2,4,4-trimethylpentyl)phosphinic Acid, CYANEXÂ®272. Solvent Extraction and Ion Exchange, 2020, 38, 328-339.	0.8	4
130	Towards Computational Screening for New Energetic Molecules: Calculation of Heat of Formation and Determination of Bond Strengths by Local Mode Analysis. Frontiers in Chemistry, 2021, 9, 726357.	1.8	4
131	Highly Asymmetric Coordination in Alkenes:Â Gas-Phase Structures oftrans-1,2-Dichloro-1,2-disilylethene and 1-Bromo-1-silylethene. Inorganic Chemistry, 2003, 42, 6539-6544.	1.9	3
132	First principles static and dynamic calculations for the transition metal hydride series MH₄L₃ (M = Fe, Ru and Os; L = NH₃,) Tj ET Q q 0 0 0 rgBT /Overl	1.6	3
133	Tetrachloropyrimidine: molecular structure by electron diffraction, vibrational analysis by infrared, Raman and inelastic neutron scattering spectroscopies, and quantum mechanical calculations. Physical Chemistry Chemical Physics, 1999, 1, 3453-3460.	1.3	2
134	Electron transfer modifies chemical properties of C70 fullerene surface: An ab initio molecular dynamics study of C70O3 molozonides doped with light atoms. Chemical Physics Letters, 2014, 605-606, 93-97.	1.2	2
135	Pressure-induced structural changes in Methylamine borane and dimethylamine borane. Journal of Alloys and Compounds, 2017, 722, 953-961.	2.8	2
136	Tuning the optical bandgap and piezoresistance in iridium-based molecular semiconductors through ligand modification. Materials Advances, 2021, 2, 5135-5143.	2.6	2
137	Aluminiumâ€Catalyzed C(sp)â^'H Borylation of Alkynes. Angewandte Chemie, 2021, 133, 20840-20845.	1.6	2
138	From lattice vibrations to molecular dissociation. Theoretical and Computational Chemistry, 2022, , 215-232.	0.2	1
139	Dihydrogen Bonds in Solid BH3NH3. ChemInform, 2004, 35, no.	0.1	0
140	Femtosecond Electron Diffraction Study of the Cyclization Reaction in Crystalline Diarylethene. EPJ Web of Conferences, 2013, 41, 05033.	0.1	0
141	Celebrating 300 years of chemistry at Edinburgh. Dalton Transactions, 2014, , .	1.6	0
142	Evaluating the crystalline orbital hierarchy and high-pressure structureâ€"property response of an extended-ligand platinum(<scp>II</scp>) bis(1,2-dioximato) complex. CrystEngComm, 2021, 23, 6359-6364.	1.3	0
143	Locating hydrogen positions in the autunite mineral metatorbernite [Cu(UO₂)₂(PO₄)₂Â·8H₂O]: a combined approach using neutron powder diffraction and computational modelling. IUCrJ, 2021, 8, 963-972.	1.0	0
144	Towards Atomically-Resolved Structural Changes during a Solid State Geminate Recombination Reaction. , 2016, , .		0