

Stewart F Parker

List of Publications by Year in descending order

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326
papers

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times ranked

8949
citing authors

#	ARTICLE	IF	CITATIONS
1	Water in Deep Eutectic Solvents: New Insights From Inelastic Neutron Scattering Spectroscopy. <i>Frontiers in Physics</i> , 2022, 10, .	2.1	17
2	The characterisation of commercial 2D carbons: graphene, graphene oxide and reduced graphene oxide. <i>Materials Advances</i> , 2022, 3, 2810-2826.	5.4	16
3	Vibrational spectroscopy to study ancient Roman funerary practices at the "Hypogeum of the Garlands" (Italy). <i>Scientific Reports</i> , 2022, 12, 3707.	3.3	3
4	Assignment of the Vibrational Spectra of Diiron Nonacarbonyl, Fe ₂ (CO) ₉ . <i>Physchem</i> , 2022, 2, 108-115.	1.1	1
5	Vibrational Spectroscopy of Hexahalo Complexes. <i>Inorganic Chemistry</i> , 2022, , .	4.0	1
6	Vibrational properties of SrVO_2H with large spin-phonon coupling. <i>Physical Review Materials</i> , 2022, 6, .	2.4	0
7	Neutron spectroscopy studies of methanol to hydrocarbons catalysis over ZSM-5. <i>Catalysis Today</i> , 2021, 368, 20-27.	4.4	7
8	Investigations of Hydrocarbon Species on Solid Catalysts by Inelastic Neutron Scattering. <i>Topics in Catalysis</i> , 2021, 64, 593-602.	2.8	3
9	Characterisation of hydration water in Nafion membrane. <i>RSC Advances</i> , 2021, 11, 9381-9385.	3.6	9
10	Structure and spectroscopy of methionyl-methionine for aquaculture. <i>Scientific Reports</i> , 2021, 11, 458.	3.3	2
11	Profiling of human burned bones: oxidising versus reducing conditions. <i>Scientific Reports</i> , 2021, 11, 1361.	3.3	24
12	Studies of propene conversion over H-ZSM-5 demonstrate the importance of propene as an intermediate in methanol-to-hydrocarbons chemistry. <i>Catalysis Science and Technology</i> , 2021, 11, 2924-2938.	4.1	7
13	Control of zeolite microenvironment for propene synthesis from methanol. <i>Nature Communications</i> , 2021, 12, 822.	12.8	23
14	An Inelastic Neutron Scattering Investigation of the Temporal Behaviour of the Hydrocarbonaceous Overlayer of a Prototype Fischer-Tropsch to Olefins Catalyst. <i>Topics in Catalysis</i> , 2021, 64, 631-637.	2.8	1
15	Applications of Neutron Scattering in Technical Catalysis: Characterisation of Hydrogenous Species on/in Unsupported and Supported Palladium. <i>Topics in Catalysis</i> , 2021, 64, 603-613.	2.8	3
16	Looking for Minor Phenolic Compounds in Extra Virgin Olive Oils Using Neutron and Raman Spectroscopies. <i>Antioxidants</i> , 2021, 10, 643.	5.1	5
17	New Spectroscopic Insight into the Deactivation of a ZSM-5 Methanol-to-Hydrocarbons Catalyst. <i>ChemCatChem</i> , 2021, 13, 2625-2633.	3.7	7
18	The Characterisation of Hydrogen on Nickel and Cobalt Catalysts. <i>Topics in Catalysis</i> , 2021, 64, 644-659.	2.8	6

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19	Net Zero and Catalysis: How Neutrons Can Help. <i>Physchem</i> , 2021, 1, 95-120.	1.1	3
20	The effect of cation substitution on the local coordination of protons in Ba ₂ In _{1.85} Mo _{0.15} O ₆ H ₂ (M ^A =Al _n) Tj ETQq0,0,0 rgBT /Overlock 1	2.7	5
21	A Spectroscopic Paradox: The Interaction of Methanol with ZSM-5 at Room Temperature. <i>Topics in Catalysis</i> , 2021, 64, 672-684.	2.8	5
22	The impact of moderate heating on human bones: an infrared and neutron spectroscopy study. <i>Royal Society Open Science</i> , 2021, 8, 210774.	2.4	10
23	How Many Molecules Can Fit in a Zeolite Pore? Implications for the Hydrocarbon Pool Mechanism of the Methanol-to-Hydrocarbons Process. <i>Catalysts</i> , 2021, 11, 1204.	3.5	3
24	Spectroscopic Signatures of Hydrogen-Bonding Motifs in Protonic Ionic Liquid Systems: Insights from Diethylammonium Nitrate in the Solid State. <i>Journal of Physical Chemistry C</i> , 2021, 125, 24463-24476.	3.1	4
25	Exploiting the flexibility of the pyrochlore composition for acid-resilient iridium oxide electrocatalysts in proton exchange membranes. <i>Journal of Materials Chemistry A</i> , 2021, 9, 25114-25127.	10.3	8
26	Understanding the Surface Characteristics of Biochar and Its Catalytic Activity for the Hydrodeoxygenation of Guaiacol. <i>Catalysts</i> , 2021, 11, 1434.	3.5	6
27	Perspectives on the effect of sulfur on the hydrocarbonaceous overlayer on iron Fischer-Tropsch catalysts. <i>Catalysis Today</i> , 2020, 339, 32-39.	4.4	11
28	Hydrogen Partitioning as a Function of Time-on-Stream for an Unpromoted Iron-Based Fischer-Tropsch Synthesis Catalyst Applied to CO Hydrogenation. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 52-60.	3.7	7
29	A Python Algorithm to Analyze Inelastic Neutron Scattering Spectra Based on the γ -Scale Formalism. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7671-7680.	5.3	5
30	Chemosteometric regression models of heat exposed human bones to determine their pre-burnt metric dimensions. <i>American Journal of Physical Anthropology</i> , 2020, 173, 734-747.	2.1	19
31	Structure and vibrational spectroscopy of lithium and potassium methanesulfonates. <i>Royal Society Open Science</i> , 2020, 7, 200776.	2.4	3
32	Investigation of MoO _x /Al ₂ O ₃ under Cyclic Operation for Oxidative and Non-Oxidative Dehydrogenation of Propane. <i>Catalysts</i> , 2020, 10, 1370.	3.5	5
33	The application of inelastic neutron scattering to investigate iron-based Fischer-Tropsch to olefins catalysis. <i>Journal of Catalysis</i> , 2020, 392, 197-208.	6.2	9
34	The Interaction of Hydrogen with Iron Benzene-1,3,5-Tricarboxylate (Fe-BTC). <i>Catalysts</i> , 2020, 10, 1255.	3.5	2
35	Investigation of Commercial Graphenes. <i>ChemistryOpen</i> , 2020, 9, 1060-1064.	1.9	5
36	Octane isomer dynamics in H-ZSM-5 as a function of Si/Al ratio: a quasi-elastic neutron scattering study. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2020, 378, 20200063.	3.4	2

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37	Toward Sustained Product Formation in the Liquid-Phase Hydrogenation of Mandelonitrile over a Pd/C Catalyst. <i>Organic Process Research and Development</i> , 2020, 24, 1112-1123.	2.7	7
38	The Effect of Co-feeding Methyl Acetate on the H-ZSM5 Catalysed Methanol-to-Hydrocarbons Reaction. <i>Topics in Catalysis</i> , 2020, 63, 370-377.	2.8	6
39	Differences in the morphology and vibrational dynamics of crystalline, glassy and amorphous silica â€“ commercial implications. <i>Materials Advances</i> , 2020, 1, 749-759.	5.4	7
40	Structure and Dynamics of the Superprotonic Conductor Caesium Hydrogen Sulfate, CsHSO ₄ . <i>Molecules</i> , 2020, 25, 1271.	3.8	4
41	The role of oxygen vacancies on the vibrational motions of hydride ions in the oxyhydride of barium titanate. <i>Journal of Materials Chemistry A</i> , 2020, 8, 6360-6371.	10.3	9
42	Effect of steam de-alumination on the interactions of propene with H-ZSM-5 zeolites. <i>RSC Advances</i> , 2020, 10, 23136-23147.	3.6	15
43	The structure and vibrational spectroscopy of cryolite, Na ₃ AlF ₆ . <i>RSC Advances</i> , 2020, 10, 25856-25863.	3.6	7
44	The Methyl Torsion in Unsaturated Compounds. <i>ACS Omega</i> , 2020, 5, 2755-2765.	3.5	11
45	Neutrons for Cultural Heritageâ€”Techniques, Sensors, and Detection. <i>Sensors</i> , 2020, 20, 502.	3.8	19
46	Volatile Hydrogen Intermediates of CO ₂ Methanation by Inelastic Neutron Scattering. <i>Catalysts</i> , 2020, 10, 433.	3.5	9
47	Computational and Spectroscopic Studies of Carbon Disulfide. <i>Molecules</i> , 2020, 25, 1901.	3.8	3
48	Onset of Propene Oligomerization Reactivity in ZSM-5 Studied by Inelastic Neutron Scattering Spectroscopy. <i>ACS Omega</i> , 2020, 5, 7762-7770.	3.5	9
49	Local Coordination Environments and Vibrational Dynamics of Protons in Hexagonal and Cubic Sc-Doped BaTiO ₃ Proton-Conducting Oxides. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8643-8651.	3.1	6
50	High-Pressure Neutron Powder Diffraction Study of Î¼-CL-20: A Gentler Way to Study Energetic Materials. <i>Journal of Physical Chemistry C</i> , 2020, 124, 27985-27995.	3.1	9
51	Hydrodeoxygenation of Guaiacol as a Bio-Oil Model Compound over Pillared Clay-Supported Nickelâ€“Molybdenum Catalysts. <i>Journal of Physical Chemistry C</i> , 2019, 123, 21429-21439.	3.1	24
52	First analysis of ancient burned human skeletal remains probed by neutron and optical vibrational spectroscopy. <i>Science Advances</i> , 2019, 5, eaaw1292.	10.3	19
53	Local Coordination of Protons in In- and Sc-Doped BaZrO ₃ . <i>Journal of Physical Chemistry C</i> , 2019, 123, 26065-26072.	3.1	10
54	Characterisation of fac-tris [2-phenylpyridinato-C ² , N]iridium(III) by inelastic neutron scattering spectroscopy and periodic density functional theory. <i>Journal of Physics Communications</i> , 2019, 3, 065010.	1.2	3

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55	Structure and spectroscopy of the supercapacitor material hydrous ruthenium oxide, RuO ₂ ·xH ₂ O, by neutron scattering*. Molecular Physics, 2019, 117, 3417-3423.	1.7	9
56	Examining the temporal behavior of the hydrocarbonaceous overlayer on an iron based Fischer-Tropsch catalyst. RSC Advances, 2019, 9, 2608-2617.	3.6	16
57	The effect of particle size, morphology and support on the formation of palladium hydride in commercial catalysts. Chemical Science, 2019, 10, 480-489.	7.4	43
58	Local structure and vibrational dynamics in indium-doped barium zirconate. Journal of Materials Chemistry A, 2019, 7, 7360-7372.	10.3	24
59	Band vs. polaron: vibrational motion and chemical expansion of hydride ions as signatures for the electronic character in oxyhydride barium titanate. Journal of Materials Chemistry A, 2019, 7, 16211-16221.	10.3	22
60	Low-temperature studies of propene oligomerization in ZSM-5 by inelastic neutron scattering spectroscopy. RSC Advances, 2019, 9, 18785-18790.	3.6	8
61	Breaking the Limit of Lignin Monomer Production via Cleavage of Interunit Carbon-Carbon Linkages. Chem, 2019, 5, 1521-1536.	11.7	167
62	Integrated Theoretical and Empirical Studies for Probing Substrate-Framework Interactions in Hierarchical Catalysts. Chemistry - A European Journal, 2019, 25, 9938-9947.	3.3	7
63	Adsorbed States of Hydrogen on Platinum: A New Perspective. Chemistry - A European Journal, 2019, 25, 6496-6499.	3.3	23
64	Spectroscopic characterisation of centropolyindanes. Physical Chemistry Chemical Physics, 2019, 21, 4568-4577.	2.8	2
65	Assignment of the solid state spectra of the group VI hexacarbonyls by inelastic neutron scattering spectroscopy. Physical Chemistry Chemical Physics, 2019, 21, 24950-24955.	2.8	5
66	Human bone probed by neutron diffraction: the burning process. RSC Advances, 2019, 9, 36640-36648.	3.6	6
67	Synthesis, Computational Studies, Inelastic Neutron Scattering, Infrared and Raman Spectroscopy of Ruthenocene. European Journal of Inorganic Chemistry, 2019, 2019, 1142-1146.	2.0	7
68	Investigation of the Dynamics of 1-Octene Adsorption at 293 K in a ZSM-5 Catalyst by Inelastic and Quasielastic Neutron Scattering. Journal of Physical Chemistry C, 2019, 123, 417-425.	3.1	12
69	Investigation of ZSM-5 catalysts for dimethylether conversion using inelastic neutron scattering. Applied Catalysis A: General, 2019, 569, 1-7.	4.3	17
70	Vibrational Spectroscopy with Neutrons. , 2019, , 1-8.		0
71	The neutron guide upgrade of the TOSCA spectrometer. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2018, 896, 68-74.	1.6	84
72	AbINS: The modern software for INS interpretation. Physica B: Condensed Matter, 2018, 551, 443-448.	2.7	51

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73	Electron-Phonon Coupling in Luminescent Europium-Doped Hydride Perovskites Studied by Luminescence Spectroscopy, Inelastic Neutron Scattering, and First-Principles Calculations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10501-10509.	3.1	26
74	Understanding the Interactions between Vibrational Modes and Excited State Relaxation in $\text{Y}_3\text{Ce}_2\text{Al}_5\text{O}_{12}$: Design Principles for Phosphors Based on f^4 Transitions. <i>Chemistry of Materials</i> , 2018, 30, 1865-1877.	6.7	59
75	Hydrogen Bonding in Amorphous Calcium Carbonate and Molecular Reorientation Induced by Dehydration. <i>Journal of Physical Chemistry C</i> , 2018, 122, 3591-3598.	3.1	42
76	Novel platinum-based anticancer drug: a complete vibrational study. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2018, 74, 628-634.	0.5	10
77	Vibrational spectroscopy with neutrons: Recent developments. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 190, 518-523.	3.9	22
78	Structure and vibrational spectroscopy of methanesulfonic acid. <i>Royal Society Open Science</i> , 2018, 5, 181363.	2.4	27
79	Comparison of two multifunctional catalysts $[\text{M}/\text{Nb}_2\text{O}_5]$ ($\text{M} = \text{Pd}, \text{Pt}$) for one-pot hydrodeoxygenation of lignin. <i>Catalysis Science and Technology</i> , 2018, 8, 6129-6136.	4.1	26
80	Fractal dimension as a scaling law for nuclear quantum effects: a neutron Compton scattering study on carbon allotropes. <i>Journal of Physics: Conference Series</i> , 2018, 1055, 012007.	0.4	3
81	Observation of the stretch mode in H_2 and D_2 by inelastic neutron scattering spectroscopy. <i>Journal of Physics: Conference Series</i> , 2018, 1055, 012001.	0.4	1
82	Comprehensive Vibrational Spectroscopic Characterization of Nylon-6 Precursors for Precise Tracking of the Beckmann Rearrangement. <i>ChemPhysChem</i> , 2018, 19, 3196-3203.	2.1	4
83	Vibrational spectroscopy of metal methanesulfonates: $\text{M} = \text{Na}, \text{Cs}, \text{Cu}, \text{Ag}, \text{Cd}$. <i>Royal Society Open Science</i> , 2018, 5, 171574.	2.4	15
84	Mutual interactions in a ternary protein/bioprotectant/water system. <i>Vibrational Spectroscopy</i> , 2018, 99, 190-195.	2.2	1
85	Heat-induced Bone Diagenesis Probed by Vibrational Spectroscopy. <i>Scientific Reports</i> , 2018, 8, 15935.	3.3	67
86	Potential of Bioapatite Hydroxyls for Research on Archeological Burned Bone. <i>Analytical Chemistry</i> , 2018, 90, 11556-11563.	6.5	27
87	Spectroscopic Characterization of Model Compounds, Reactants, and Byproducts Connected with an Isocyanate Production Chain. <i>Industrial & Engineering Chemistry Research</i> , 2018, 57, 7355-7362.	3.7	4
88	Biomaterials from human bone - probing organic fraction removal by chemical and enzymatic methods. <i>RSC Advances</i> , 2018, 8, 27260-27267.	3.6	13
89	Deactivation of a Single-Site Gold-on-Carbon Acetylene Hydrochlorination Catalyst: An X-ray Absorption and Inelastic Neutron Scattering Study. <i>ACS Catalysis</i> , 2018, 8, 8493-8505.	11.2	63
90	Complete assignment of the vibrational spectra of borazine: the inorganic benzene. <i>RSC Advances</i> , 2018, 8, 23875-23880.	3.6	6

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91	The effects of MTG catalysis on methanol mobility in ZSM-5. <i>Catalysis Science and Technology</i> , 2018, 8, 3304-3312.	4.1	23
92	Structure/activity relationships applied to the hydrogenation of $\hat{1}\pm, \hat{1}^2$ -unsaturated carbonyls: The hydrogenation of 3-butyne-2-one over alumina-supported palladium catalysts. <i>Catalysis Today</i> , 2017, 283, 110-118.	4.4	7
93	Unravelling exceptional acetylene and carbon dioxide adsorption within a tetra-amide functionalized metal-organic framework. <i>Nature Communications</i> , 2017, 8, 14085.	12.8	193
94	An assessment of hydrocarbon species in the methanol-to-hydrocarbon reaction over a ZSM-5 catalyst. <i>Faraday Discussions</i> , 2017, 197, 447-471.	3.2	34
95	Topological triplon modes and bound states in a Shastryâ€Sutherland magnet. <i>Nature Physics</i> , 2017, 13, 736-741.	16.7	70
96	Understanding the Role of Designed Solid Acid Sites in the Lowâ€Temperature Production of ϵ -Caprolactam. <i>ChemCatChem</i> , 2017, 9, 1897-1900.	3.7	15
97	Inelastic neutron scattering study of reline: shedding light on the hydrogen bonding network of deep eutectic solvents. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17998-18009.	2.8	132
98	Understanding the Role of Molecular Diffusion and Catalytic Selectivity in Liquid-Phase Beckmann Rearrangement. <i>ACS Catalysis</i> , 2017, 7, 2926-2934.	11.2	30
99	Neutron spectroscopy as a tool in catalytic science. <i>Chemical Communications</i> , 2017, 53, 12164-12176.	4.1	44
100	Selective production of arenes via direct lignin upgrading over a niobium-based catalyst. <i>Nature Communications</i> , 2017, 8, 16104.	12.8	346
101	Vibrational spectra of buta-1,3-diene iron tricarbonyl: comparison to surface species. <i>Journal of Lithic Studies</i> , 2017, 3, 119-127.	0.5	2
102	Molecular orientational melting within a lead-halide octahedron framework: The order-disorder transition in $\text{CH}_3\text{NH}_3\text{PbBr}_3$. <i>Physical Review B</i> , 2017, 96, .	3.2	23
103	Raman and inelastic neutron scattering spectra of $(\text{NH}_4)_2\text{SO}_3$, an intermediate for solar hydrogen production. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 30216-30222.	7.1	1
104	Assignment of the vibrational spectra of the parent polysilsesquioxane (POSS): Octahydrosilasequioxane, $\text{H}_8\text{Si}_8\text{O}_{12}$. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 171, 222-228.	3.9	0
105	Structure and Vibrational Spectra of 2,5-Diodothiophene: A Model for Polythiophene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12636-12642.	3.1	11
106	Frontispiece: Metastable Nitric Acid Trihydrate in Ice Clouds. <i>Angewandte Chemie - International Edition</i> , 2016, 55, .	13.8	1
107	The adsorbed state of a thiol on palladium nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17265-17271.	2.8	6
108	Methanol diffusion in zeolite HY: a combined quasielastic neutron scattering and molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17294-17302.	2.8	38

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109	Metastabiles SalpetersÄuretrihydrat in Eiswolken. <i>Angewandte Chemie</i> , 2016, 128, 3334-3338.	2.0	0
110	Different routes to methanol: inelastic neutron scattering spectroscopy of adsorbates on supported copper catalysts. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17253-17258.	2.8	26
111	An investigation of the effect of carbon support on ruthenium/carbon catalysts for lactic acid and butanone hydrogenation. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17259-17264.	2.8	19
112	The reaction of formic acid with Raney TM copper. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , 2016, 472, 20160126.	2.1	2
113	Amides Do Not Always Work: Observation of Guest Binding in an Amide-Functionalized Porous Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2016, 138, 14828-14831.	13.7	44
114	Osteometrics in burned human skeletal remains by neutron and optical vibrational spectroscopy. <i>RSC Advances</i> , 2016, 6, 68638-68641.	3.6	21
115	Hydrogen motions in defective graphene: the role of surface defects. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 24820-24824.	2.8	16
116	The application of inelastic neutron scattering to investigate the interaction of methyl propanoate with silica. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17210-17216.	2.8	6
117	Direct hydrodeoxygenation of raw woody biomass into liquid alkanes. <i>Nature Communications</i> , 2016, 7, 11162.	12.8	359
118	Applications of neutron scattering to heterogeneous catalysis. <i>Journal of Physics: Conference Series</i> , 2016, 746, 012066.	0.4	11
119	An in-depth understanding of the bimetallic effects and coked carbon species on an active bimetallic Ni(Co)/Al ₂ O ₃ dry reforming catalyst. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17311-17319.	2.8	27
120	Adsorption of formate species on Cu(h,k,l) low index surfaces. <i>Surface Science</i> , 2016, 653, 45-54.	1.9	25
121	Application of Inelastic Neutron Scattering to the Methanol-to-Gasoline Reaction Over a ZSM-5 Catalyst. <i>Catalysis Letters</i> , 2016, 146, 1242-1248.	2.6	16
122	Neutron scattering in catalysis and energy materials. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17140-17140.	2.8	7
123	Room temperature methoxylation in zeolites: insight into a key step of the methanol-to-hydrocarbons process. <i>Chemical Communications</i> , 2016, 52, 2897-2900.	4.1	58
124	Stabilization of 3d Transition Metal Hydrido Complexes in SrH ₂ Mg ₂ [Co(I)H ₅], BaH ₂ Mg ₅ [Co(II)H ₄] ₂ , and RbH ₂ Mg ₅ [Co(II)H ₄ Ni(O)H ₄] via Easily Polarizable Hydride Ligands. <i>Inorganic Chemistry</i> , 2016, 55, 3576-3582.	4.0	4
125	Frontispiz: Metastabiles SalpetersÄuretrihydrat in Eiswolken. <i>Angewandte Chemie</i> , 2016, 128, .	2.0	0
126	Metastable Nitric Acid Trihydrate in Ice Clouds. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 3276-3280.	13.8	12

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127	Characterisation of the surface of freshly prepared precious metal catalysts. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17196-17201.	2.8	7
128	Structure and dehydration mechanism of the proton conducting oxide $\text{Ba}_2\text{In}_2\text{O}_5(\text{H}_2\text{O})_x$. <i>Journal of Materials Chemistry A</i> , 2016, 4, 1224-1232.	10.3	24
129	Evidence for a surface gold hydride on a nanostructured gold catalyst. <i>Chemical Communications</i> , 2016, 52, 533-536.	4.1	45
130	Methyl tunnelling of adsorbed methoxy on alumina catalysts. <i>Chemical Communications</i> , 2016, 52, 366-369.	4.1	2
131	Structural and spectroscopic characterisation of C4 oxygenates relevant to structure/activity relationships of the hydrogenation of 1,2-unsaturated carbonyls. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 153, 289-297.	3.9	1
132	Assignment of the Internal Vibrational Modes of C_{70} by Inelastic Neutron Scattering Spectroscopy and Periodic DFT. <i>ChemistryOpen</i> , 2015, 4, 620-625.	1.9	10
133	From soft harmonic phonons to fast relaxational dynamics in CH_3COOH . <i>Physical Review B</i> , 2015, 92, .	3.2	108
134	Monte carlo simulations of the TOSCA spectrometer: Assessment of current performance and future upgrades. <i>EPJ Web of Conferences</i> , 2015, 83, 03013.	0.3	19
135	The application of inelastic neutron scattering to explore the significance of a magnetic transition in an iron based Fischer-Tropsch catalyst that is active for the hydrogenation of CO. <i>Journal of Chemical Physics</i> , 2015, 143, 174703.	3.0	17
136	Structure and spectroscopy of CuH prepared via borohydride reduction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 608-612.	1.1	11
137	Direct Spectroscopic Evidence of the Mechanism behind the Phase Transition of [2,2]Paracyclophane. <i>Chemistry - A European Journal</i> , 2015, 21, 4556-4560.	3.3	3
138	Conformational insights and vibrational study of a promising anticancer agent: the role of the ligand in Pd(amine) complexes. <i>New Journal of Chemistry</i> , 2015, 39, 6274-6283.	2.8	23
139	The application of inelastic neutron scattering to investigate a hydrogen pre-treatment stage of an iron Fischer-Tropsch catalyst. <i>Applied Catalysis A: General</i> , 2015, 489, 209-217.	4.3	14
140	How the Surface Structure Determines the Properties of CuH. <i>Inorganic Chemistry</i> , 2015, 54, 2213-2220.	4.0	27
141	High-Pressure Experimental and DFT-D Structural Studies of the Energetic Material FOX-7. <i>Journal of Physical Chemistry C</i> , 2015, 119, 2322-2334.	3.1	69
142	($\text{C}_4\text{H}_{12}\text{N}_2$)[CoCl_4]: tetrahedrally coordinated Co^{2+} without the orbital degeneracy. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2015, 71, 20-24.	1.1	14
143	The fine structure of Pearlman's catalyst. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5274-5278.	2.8	22
144	A molecular view of cisplatin's mode of action: interplay with DNA bases and acquired resistance. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5155-5171.	2.8	39

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145	The distribution of isotopomers in crystals. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 140, 462-464.	3.9	1
146	Comment on "Assessment of new DFT methods for predicting vibrational spectra and structure of cisplatin: Which density functional should we choose for studying platinum(II) complexes?" [Spectrochim. Acta A125 (2014) 431-439]. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 347.	3.9	1
147	The use of direct geometry spectrometers in molecular spectroscopy. <i>Journal of Physics: Conference Series</i> , 2014, 554, 012004.	0.4	10
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