

Simon J. Coles

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718
papers

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h-index

91
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820
ext. papers

16,189
ext. citations

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avg, IF

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L-index

#	Paper	IF	Citations
718	Superconducting and Semiconducting Magnetic Charge Transfer Salts: (BEDT-TTF) ₄ Fe(C ₂ O ₄) ₃ ·nH ₂ O (A = H ₂ O, K, NH ₄). <i>Journal of the American Chemical Society</i> , 1995 , 117, 12209-12217	16.4	517
717	Changing and challenging times for service crystallography. <i>Chemical Science</i> , 2012 , 3, 683-689	9.4	394
716	The catalytic intermolecular orthoarylation of phenols. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 112-4	16.4	280
715	Applying Hot-Stage Microscopy to Co-Crystal Screening: A Study of Nicotinamide with Seven Active Pharmaceutical Ingredients. <i>Crystal Growth and Design</i> , 2008 , 8, 1697-1712	3.5	258
714	Novel Expanded Ring N-Heterocyclic Carbenes: Free Carbenes, Silver Complexes, And Structures. <i>Organometallics</i> , 2008 , 27, 3279-3289	3.8	204
713	Quadratic Nonlinear Optical Properties of N-Aryl Stilbazolium Dyes. <i>Advanced Functional Materials</i> , 2002 , 12, 110-116	15.6	197
712	Squaramides as potent transmembrane anion transporters. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 4426-30	16.4	185
711	Lewis acidity of tris(pentafluorophenyl)borane: crystal and molecular structure of B(C ₆ F ₅) ₃ ·DPEt ₃ . <i>Inorganic Chemistry Communication</i> , 2000 , 3, 530-533	3.1	163
710	Chiral 2,6-lutidinyl-biscarbene complexes of palladium. <i>Chemical Communications</i> , 2001 , 1270-1271	5.8	160
709	Luminescent, enantiopure, phenylatopyridine iridium-based coordination capsules. <i>Journal of the American Chemical Society</i> , 2012 , 134, 19334-7	16.4	159
708	Synthesis and characterisation of infinite co-ordination networks from flexible dipyriddy ligands and cadmium salts. <i>Dalton Transactions RSC</i> , 2000 , 3065-3073		153
707	High-Activity Catalysts for Suzuki Coupling and Amination Reactions with Deactivated Aryl Chloride Substrates: Importance of the Palladium Source. <i>Organometallics</i> , 2003 , 22, 987-999	3.8	147
706	Thiophene and Selenophene Copolymers Incorporating Fluorinated Phenylene Units in the Main Chain: Synthesis, Characterization, and Application in Organic Field-Effect Transistors. <i>Chemistry of Materials</i> , 2005 , 17, 6567-6578	9.6	145
705	Quadratic Optical Nonlinearities of N-Methyl and N-Aryl Pyridinium Salts. <i>Advanced Functional Materials</i> , 2003 , 13, 347-357	15.6	141
704	Anion-directed assembly: the first fluoride-directed double helix. <i>Chemical Communications</i> , 2003 , 568-95.8		141
703	Luminescent Pt(II)(bipyridyl)(diacetylde) chromophores with pendant binding sites as energy donors for sensitised near-infrared emission from lanthanides: structures and photophysics of Pt(II)/Ln(III) assemblies. <i>Chemistry - A European Journal</i> , 2006 , 12, 9299-313	4.8	130
702	Orthopalladated and -platinated bulky triarylphosphite complexes: synthesis, reactivity and application as high-activity catalysts for Suzuki and Stille coupling reactions. <i>Chemistry - A European Journal</i> , 2003 , 9, 3216-27	4.8	128

701	Syntheses and properties of two-dimensional charged nonlinear optical chromophores incorporating redox-switchable cis-tetraammineruthenium(II) centers. <i>Journal of the American Chemical Society</i> , 2005 , 127, 4845-59	16.4	123
700	Carbon Monoxide and Isocyanide Complexes of Trivalent Uranium Metallocenes. <i>Chemistry - A European Journal</i> , 1999 , 5, 3000-3009	4.8	114
699	Fluoride-selective binding in a new deep cavity calix[4]pyrrole: experiment and theory. <i>Journal of the American Chemical Society</i> , 2002 , 124, 8644-52	16.4	113
698	Crystal structure and magnetic properties of the layer ferrimagnet N(n-C ₅ H ₁₁) ₄ MnIIIFeIII(C ₂ O ₄) ₃ . <i>Journal of the Chemical Society Dalton Transactions</i> , 1996 , 1839-1843		113
697	First Examples of Diazepanylidene Carbenes and Their Late-Transition-Metal Complexes. <i>Organometallics</i> , 2007 , 26, 4800-4809	3.8	112
696	Synthesis and Single Crystal X-ray Diffraction Study on the First Isolable Carbonyl Complex of an Actinide, (C ₅ Me ₄ H) ₃ U(CO). <i>Journal of the American Chemical Society</i> , 1995 , 117, 2649-2650	16.4	111
695	Syntheses and Quadratic Nonlinear Optical Properties of Salts Containing Benzothiazolium Electron-Acceptor Groups. <i>Chemistry of Materials</i> , 2006 , 18, 5907-5918	9.6	100
694	Synthesis and Characterization of the First Sandwich Complex of Trivalent Thorium: A Structural Comparison with the Uranium Analogue. <i>Journal of the American Chemical Society</i> , 1999 , 121, 6867-6871	16.4	90
693	Chiral palladium bis(phosphite)PCP-pincer complexes via ligand C-H activation. <i>Chemical Communications</i> , 2006 , 3880-2	5.8	88
692	A versatile indium trichloride mediated Prins-type reaction to unsaturated heterocycles. <i>Journal of Organic Chemistry</i> , 2003 , 68, 7880-3	4.2	88
691	2-amidopyrroles and 2,5-diamidopyrroles as simple anion binding agents. <i>Journal of Organic Chemistry</i> , 2001 , 66, 7849-53	4.2	85
690	Ditopic ligands for the simultaneous solvent extraction of cations and anions. <i>Chemical Communications</i> , 1999 , 2077-2078	5.8	84
689	The first direct experimental comparison between the hugely contrasting properties of PEDOT and the all-sulfur analogue PEDTT by analogy with well-defined EDTT/PEDOT copolymers. <i>Journal of Materials Chemistry</i> , 2005 , 15, 4783		82
688	A chiral ferromagnetic molecular metal. <i>Journal of the American Chemical Society</i> , 2010 , 132, 9271-3	16.4	81
687	Synthesis and Biological Evaluation of JAHAs: Ferrocene-Based Histone Deacetylase Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2011 , 2, 358-362	4.3	80
686	A novel ditopic receptor and reversal of anion binding selectivity in the presence and absence of bound cation. <i>Organic Letters</i> , 2003 , 5, 4971-4	6.2	77
685	Reaction of naphthoquinones with substituted nitromethanes. Facile synthesis and antifungal activity of naphtho[2,3-d]isoxazole-4,9-diones. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010 , 20, 193-5	3.9	76
684	Intra- and intermolecular N-H...F-C hydrogen-bonding interactions in amine adducts of tris(pentafluorophenyl)borane and -alane. <i>Inorganic Chemistry</i> , 2005 , 44, 5921-33	5.1	76

683	Pharmaceutical co-crystals $\bar{\Delta}$ are we there yet?. <i>CrystEngComm</i> , 2014 , 16, 5753-5761	3.3	74
682	Ultra-fast co-sensitization and tri-sensitization of dye-sensitized solar cells with N719, SQ1 and triarylamine dyes. <i>Journal of Materials Chemistry</i> , 2012 , 22, 13318		73
681	Enhancement of the chemical semantic web through the use of InChI identifiers. <i>Organic and Biomolecular Chemistry</i> , 2005 , 3, 1832-4	3.9	70
680	Binding and Electrochemical Recognition of Barbiturate and Urea Derivatives by a Regioisomeric Series of Hydrogen-Bonding Ferrocene Receptors. <i>Organometallics</i> , 2004 , 23, 946-951	3.8	70
679	Synthesis and Reactivity of New Mono(cyclopentadienyl)zirconium and -hafnium Alkyl Complexes. Crystal and Molecular Structure of $[\{C_5H_3(SiMe_3)_2\}HfMe_2(\eta\text{-}6\text{-toluene})][BMe(C_6F_5)_3]$. <i>Organometallics</i> , 1995 , 14, 2456-2462	3.8	70
678	FAIR Principles: Interpretations and Implementation Considerations. <i>Data Intelligence</i> , 2020 , 2, 10-29	3	66
677	The Role of Ligand Transformations on the Performance of Phosphite- and Phosphinite-Based Palladium Catalysts in the Suzuki Reaction. <i>Organometallics</i> , 2003 , 22, 1364-1371	3.8	66
676	Fluoride anion binding by cyclic boronic esters: influence of backbone chelate on receptor integrity. <i>Dalton Transactions</i> , 2006 , 3660-7	4.3	65
675	Solution phase, solid state, and theoretical investigations on the MacMillan imidazolidinone. <i>Organic Letters</i> , 2009 , 11, 133-6	6.2	64
674	Phosphine and arsine adducts of N-donor palladacycles as catalysts in the Suzuki coupling of aryl bromides. <i>Dalton Transactions</i> , 2003 , 3350	4.3	64
673	Multidentate Lewis acids: synthesis, structure and mode of action of a redox-based fluoride ion sensor. <i>Chemical Communications</i> , 2002 , 740-1	5.8	62
672	To bend or not to bend $\bar{\Delta}$ are heteroatom interactions within conjugated molecules effective in dictating conformation and planarity?. <i>Materials Horizons</i> , 2016 , 3, 333-339	14.4	62
671	Further evidence for spontaneous solid-state polymerisation reactions in 2,5-dibromothiophene derivatives. <i>Journal of Materials Chemistry</i> , 2003 , 13, 2075		60
670	Anabolic steroids detected in bodybuilding dietary supplements - a significant risk to public health. <i>Drug Testing and Analysis</i> , 2015 , 7, 609-18	3.5	59
669	Anomalous NMR behavior of meso compounds with remote stereogenic centers on addition of chiral shift reagent or chiral solvating agent. <i>Journal of the American Chemical Society</i> , 2003 , 125, 4943-50 ^{16.4}		59
668	Hexyl-substituted oligothiophenes with a central tetrafluorophenylene unit: crystal engineering of planar structures for p-type organic semiconductors. <i>Chemical Communications</i> , 2005 , 1465-7	5.8	58
667	Simple Palladacyclic and Platinacyclic Catalysts for the 1,4-Conjugate Addition of Arylboronic Acids and Arylsiloxanes to Enones. <i>Organometallics</i> , 2007 , 26, 6346-6353	3.8	57
666	The effect of protonation on the spectroscopic and redox properties of a series of ferrocenoyl derivatives. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999 , 57-62		56

665	Noncovalent functional-group-arene interactions. <i>Angewandte Chemie - International Edition</i> , 2007 , 46, 7823-6	16.4	54
664	Fluorescent rhenium-naphthalimide conjugates as cellular imaging agents. <i>Inorganic Chemistry</i> , 2014 , 53, 3788-97	5.1	51
663	Halide titanium(IV) Schiff base complexes; fluoride and bromide derivatives and evidence for a new seven-coordinate chloride intermediate. <i>Journal of the Chemical Society Dalton Transactions</i> , 1998 , 3489-3494	5.1	51
662	Isolation of the reactive intermediate in palladium-catalysed coupling of secondary phosphineboranes with aryl halides. <i>Chemical Communications</i> , 1999 , 63-64	5.8	50
661	A switchable self-assembling and disassembling chiral system based on a porphyrin-substituted phenylalanine-phenylalanine motif. <i>Nature Communications</i> , 2016 , 7, 12657	17.4	49
660	Synthesis and structural characterization of an unprecedented nonmetal cation polyborate salt containing two different "isolated" polyborate anions: [H ₂ en] ₂ [B ₄ O ₅ (OH) ₄][B ₇ O ₉ (OH) ₅]·BH ₂ O (en = H ₂ NCH ₂ CH ₂ NH ₂). <i>Inorganic Chemistry</i> , 2011 , 50, 12215-8	5.1	49
659	Poly(3,4-ethylenediselena)thiophene The Selenium Equivalent of PEDOT. <i>Chemistry of Materials</i> , 2007 , 19, 301-307	9.6	48
658	Polymorphism based on molecular stereoisomerism in tris(oxalato) Cr(III) salts of bedt-ttf [bis(ethylenedithio)tetrathiafulvalene]. <i>Chemical Communications</i> , 1999 , 513-514	5.8	48
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656	On the choice of Lewis acids for the Prins reaction; two total syntheses of (E)-Civet. <i>Tetrahedron</i> , 2011 , 67, 5107-5124	2.4	46
655	The synthesis, structure and ethene polymerisation catalysis of mono(salicylaldiminato) titanium and zirconium complexes. <i>Dalton Transactions</i> , 2005 , 561-71	4.3	46
654	Photoinduced formation of a cryptand from a coronand: an unexpected switch in cation binding affinity. <i>Chemistry - A European Journal</i> , 2002 , 8, 3331-42	4.8	46
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652	Synergistic catalysis: enantioselective addition of alkylbenzoxazoles to enals. <i>Chemistry - A European Journal</i> , 2014 , 20, 16853-7	4.8	45
651	Anion complexation via C-H...X interactions using a palladacyclic receptor. <i>Chemical Communications</i> , 2008 , 2429-31	5.8	45
650	The electroactivity of tetrathiafulvalene vs. polythiophene: synthesis and characterisation of a fused thieno[3,4-b]TF polymer. <i>Journal of Materials Chemistry</i> , 2004 , 14, 1964-1969		45
649	Efficient Ni(II)2Ln(III)2 Electrocyclization Catalysts for the Synthesis of trans-4,5-Diaminocyclopent-2-enones from 2-Furaldehyde and Primary or Secondary Amines. <i>Inorganic Chemistry</i> , 2016 , 55, 6988-94	5.1	45
648	Tetranuclear Zn/4f coordination clusters as highly efficient catalysts for Friedel-Crafts alkylation. <i>Chemical Communications</i> , 2016 , 52, 7866-9	5.8	45

- 647 Kinetics of iminium ion catalysis. *Angewandte Chemie - International Edition*, **2008**, 47, 2820-3 16.4 43
- 646 [FeFe]-Hydrogenase Synthetic Mimics Based on Peri-Substituted Dichalcogenides. *Organometallics*, **2014**, 33, 4449-4460 3.8 42
- 645 Click JAHA: conformationally restricted ferrocene-based histone deacetylase inhibitors. *MedChemComm*, **2012**, 3, 61-64 5 42
- 644 Structural and Electronic Effects of 1,3,4-Thiadiazole Units Incorporated into Polythiophene Chains. *Macromolecules*, **2007**, 40, 6585-6593 5.5 42
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- 642 Contrasting linear and quadratic nonlinear optical behavior of dipolar pyridinium chromophores with 4-(dimethylamino)phenyl or ruthenium(II) ammine electron donor groups. *Journal of the American Chemical Society*, **2004**, 126, 10418-27 16.4 42
- 641 Investigating the generation of hydrogen sulfide from the phosphonamidodithioate slow-release donor GYY4137. *MedChemComm*, **2015**, 6, 1649-1655 5 41
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- 638 Enhancement of Tb(III) -Cu(II) Single-Molecule Magnet Performance through Structural Modification. *Chemistry - A European Journal*, **2016**, 22, 12839-48 4.8 40
- 637 Mixed valence Mn(II)/Mn(III) [3 x 3] grid complexes: structural, electrochemical, spectroscopic, and magnetic properties. *Inorganic Chemistry*, **2004**, 43, 7605-16 5.1 39
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- 634 Synthesis of 2-substituted 1-benzyl-2,3,4,5-tetrahydro-1-benzazepines by palladium catalysis: *ta*, Observation of a competitive β -hydride elimination pathway. *Tetrahedron Letters*, **2003**, 44, 3675-3678 2 38
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- 631 CO₂ as a reaction ingredient for the construction of metal cages: a carbonate-panelled [Gd₆Cu₃] tridiminished icosahedron. *Chemical Communications*, **2014**, 50, 3498-500 5.8 37
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- 628 Synergistic catalysis: highly diastereoselective benzoxazole addition to Morita-Baylis-Hillman carbonates. *Chemical Communications*, **2014**, 50, 7447-50 5.8 36
- 627 A study of dye anchoring points in half-squarylium dyes for dye-sensitized solar cells. *Journal of Materials Chemistry A*, **2014**, 2, 4055-4066 13 36
- 626 Synthesis of a class of core-modified aza-BODIPY derivatives. *Journal of Organic Chemistry*, **2014**, 79, 8932-6 4.2 36
- 625 Pentacoordinate silicon complexes with dynamic motion resembling a pendulum on the S(N)2 reaction pathway. *Dalton Transactions*, **2013**, 42, 10971-81 4.3 36
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- 622 Hydrogen bonded supramolecular assemblies based on neutral square-planar palladium(II) complexes. *CrystEngComm*, **2007**, 9, 165 3.3 36
- 621 Tandem Michael/Michael reactions mediated by phosphines or aryl thiolates. *Tetrahedron*, **2007**, 63, 1100-1106 3.6 36
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- 618 Pentaborate(1-) salts templated by substituted pyrrolidinium cations: synthesis, structural characterization, and modelling of solid-state H-bond interactions by DFT calculations. *Dalton Transactions*, **2015**, 44, 7032-40 4.3 35
- 617 Synthesis and Electropolymerization of Hexadecyl Functionalized Bithiophene and Thieno[3,2-b]thiophene End-Capped with EDOT and EDTT Units. *Chemistry of Materials*, **2010**, 22, 3000-3008 3.6 35
- 616 A catalytic asymmetric protocol for the enantioselective synthesis of 3(2H)-furanones. *Chemical Communications*, **2007**, 2494-6 5.8 35
- 615 Synthesis and electropolymerisation of 3,4-bis(alkylsulfanyl)terthiophenes and the significance of the fused dithiin ring in 2,5-dithienyl-3,4-ethylenedithiothiophene (DT-EDTT). *Journal of Materials Chemistry*, **2002**, 12, 500-510 35
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- 613 The Same but Different: Isostructural Polymorphs and the Case of 3-Chloromandelic Acid. *Crystal Growth and Design*, **2014**, 14, 1623-1628 3.5 34
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- 609 The Synthesis, Molecular Structures, and Supramolecular Architecture of Amine Adducts of Bis(pentafluorophenyl)zinc. *Organometallics*, **2006**, 25, 3837-3847 3.8 33
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- 604 Influence of Ligand Steric Bulk in the Synthesis of Transition-Metal Borylene Complexes. *Organometallics*, **2003**, 22, 4213-4217 3.8 32
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