Juan J Novoa

List of Publications by Year in descending order

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233 papers	8,162 citations	41344 49 h-index	66911 78 g-index
245 all docs	245 docs citations	245 times ranked	6008 citing authors

#	Article	IF	Citations
1	Origin of the magnetic couplings for the weak ferromagnet Li+[TCNE]â€¢- (TCNEÂ=ÂTetracyanoethylene). Polyhedron, 2022, 221, 115871.	2.2	0
2	Insights into the magnetism and phase transitions of organic radical-based materials. Journal of Materials Chemistry C, 2021, 9, 10624-10646.	5.5	27
3	Pitfalls on evaluating pair exchange interactions for modelling molecule-based magnetism. Journal of Materials Chemistry C, 2021, 9, 10647-10660.	5.5	7
4	Low temperature structures and magnetic interactions in the organic-based ferromagnetic and metamagnetic polymorphs of decamethylferrocenium 7,7,8,8-tetracyano-p-quinodimethanide, [FeCp*2]Ë™+[TCNQ]Ë™â^'. Dalton Transactions, 2021, 50, 11228-11242.	3.3	6
5	Assessing Cu2L2X4 dimeric moieties as ferromagnetic building blocks in double halide-bridged polymers (XÂ=ÂClâ^', Brâ^' and LÂ=Âbenzamide). An experimental and computational study. Polyhedron, 2020, 185, 114603.	2.2	2
6	Two different mechanisms of stabilization of regular Ï€-stacks of radicals in switchable dithiazolyl-based materials. Journal of Materials Chemistry C, 2020, 8, 5437-5448.	5.5	7
7	Reorganization of Intermolecular Interactions in the Polymorphic Phase Transition of a Prototypical Dithiazolyl-Based Bistable Material. Crystal Growth and Design, 2019, 19, 2329-2339.	3.0	7
8	The magnetic fingerprint of dithiazolyl-based molecule magnets. Physical Chemistry Chemical Physics, 2018, 20, 20406-20416.	2.8	16
9	Understanding room-temperature Ï€-dimerisation of radical ions: intramolecular Ï€-[TTF]₂²⁺ in functionalised calix[4]arenes. Physical Chemistry Chemical Physics, 2017, 19, 3807-3819.	2.8	7
10	Bistability in Organic Magnetic Materials: A Comparative Study of the Key Differences between Hysteretic and Nonâ€hysteretic Spin Transitions in Dithiazolyl Radicals. Chemistry - A European Journal, 2017, 23, 3479-3489.	3.3	26
11	Ferromagnetic Exchange in Bichloride Bridged Cu(II) Chains: Magnetostructural Correlations between Ordered and Disordered Systems. Inorganic Chemistry, 2017, 56, 5441-5454.	4.0	10
12	Origin of Bistability in the Butylâ€Substituted Spirobiphenalenylâ€Based Neutral Radical Material. Chemistry - A European Journal, 2017, 23, 7772-7784.	3.3	10
13	Formation of Long, Multicenter Ï€â€[TCNE]₂^{2â^'} Dimers in Solution: Solvation and Stability Assessed through Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 17037-17046.	3.3	7
14	The Tetracyanopyridinide Dimer Dianion, Ïƒâ€[TCNPy] 2 2â^'. Chemistry - A European Journal, 2016, 22, 12312-12315.	3.3	3
15	A New Conformation With an Extraordinarily Long, 3.04â€…Ã… Twoâ€Electron, Sixâ€Center Bond Observed for the Ï€â€[TCNE]₂^{2â^'} Dimer in [NMe₄]₂[TCNE]₂ (TCNE=Tetracyanoethylene). Chemistry - A European Journal, 2015, 21, 13240-13245.	3.3	9
16	Orientational Preference of Long, Multicenter Bonds in Radical Anion Dimers: A Case Study of Ï€â€[TCNB]₂^{2â^'} and Ï€â€[TCNP]₂^{2â^'}. Chemistry - A European Journal, 2015, 21, 6420-6432.	3.3	14
17	Electronic Excitation Energies in Dimers between Radical Ions Presenting Long, Multicenter Bonding. Journal of Chemical Theory and Computation, 2015, 11, 2651-2660.	5.3	6
18	The nature of the Câ€“Brâ‹¯Brâ€“C intermolecular interactions found in molecular crystals: a general theoretical-database study. CrystEngComm, 2015, 17, 3354-3365.	2.6	32

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19	Unravelling the Key Driving Forces of the Spin Transition in Ï€-Dimers of Spiro-biphenalenyl-Based Radicals. Journal of the American Chemical Society, 2015, 137, 12843-12855.	13.7	20
20	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. Chemical Science, 2015, 6, 2371-2381.	7.4	34
21	Elucidating the 2D Magnetic Topology of the â€˜Metalâ€“Radicalâ€™ TTTAâ‹…Cu(hfac)₂ System. Chemistry - A European Journal, 2014, 20, 7083-7090.	3.3	16
22	On the Importance of Thermal Effects and Crystalline Disorder in the Magnetism of Benzotriazinylâ€Derived Organic Radicals. Chemistry - an Asian Journal, 2014, 9, 3612-3622.	3.3	14
23	S=1/2 Oneâ€Dimensional Randomâ€Exchange Ferromagnetic Zigzag Ladder, Which Exhibits Competing Interactions in a Critical Regime. Chemistry - A European Journal, 2014, 20, 8355-8362.	3.3	15
24	Multistep Ï€ Dimerization of Tetrakis(nâ€decyl)heptathienoacene Radical Cations: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 10351-10359.	3.3	12
25	Insights into the crystal-packing effects on the spin crossover of [Fe^{II}(1-bpp)]²⁺-based materials. Physical Chemistry Chemical Physics, 2014, 16, 27012-27024.	2.8	57
26	Diradicals acting through diamagnetic phenylene vinylene bridges: Raman spectroscopy as a probe to characterize spin delocalization. Journal of Chemical Physics, 2014, 140, 164903.	3.0	6
27	The nature of the Câ€“Clâ‹¯Clâ€“C intermolecular interactions found in molecular crystals: a general theoretical-database study covering the 2.75â€“4.0 Ã… range. CrystEngComm, 2014, 16, 8232-8242.	2.6	34
28	The polymorphism of a triarylphosphine oxide: a case of missing isomers. CrystEngComm, 2014, 16, 8214-8223.	2.6	1
29	Assessing the Performance of CASPT2 and DFT Methods for the Description of Long, Multicenter Bonding in Dimers between Radical Ions. Journal of Chemical Theory and Computation, 2014, 10, 650-658.	5.3	29
30	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	12.8	55
31	Structure and Properties of Nitrogen-Rich 1,4-Dicyanotetrazine, C₄N₆: A Comparative Study with Related Tetracyano Electron Acceptors. Journal of Organic Chemistry, 2014, 79, 8189-8201.	3.2	5
32	The Origin of the Room-Temperature Stability of [TTF].+â‹…â‹…â‹…[TTF].+Long, Multicenter Bonds Found in Functionalized Ï€-[R-TTF]22+Dimers Included in the Cucurbit[8]uril Cavity. Chemistry - A European Journal, 2014, 20, 7784-7795.	3.3	12
33	A theoretical analysis of the magnetic properties of the low-dimensional copper(II)X2(2-X-3-methylpyridine)2 (X = Cl and Br) complexes. Highlights in Theoretical Chemistry, 2014, , 219-230.	0.0	0
34	Preface to the ESPA-2012 special issue. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	0
35	Keys for the Existence of Stable Dimers of Bis-tetrathiafulvalene (bis-TTF)-Functionalized Molecular Clips Presenting [TTF]â€¢+Â·Â·[TTF]â€¢+ Long, Multicenter Bonds at Room Temperature. Journal of the American Chemical Society, 2013, 135, 13814-13826.	13.7	30
36	Dividing the Spoils: Role of Pyrazine Ligands and Perchlorate Counterions in the Magnetic Properties of Bis(pyrazine)diperchloratecopper(II), [Cu(pz)₂](ClO₄)₂. Inorganic Chemistry, 2013, 52, 12923-12932.	4.0	22

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37	A theoretical analysis of the magnetic properties of the low-dimensional copper(II)X2(2-X-3-methylpyridine)2 (XÂ=ÂCl and Br) complexes. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	4
38	A theoretical analysis of the magnetic properties of the low dimensional bis(2-chloropyrazine)dichlorocopper(II) molecule-based magnet. Polyhedron, 2013, 64, 163-171.	2.2	2
39	Assigning the dimensionality in low-dimensional materials: A rigorous study of the dimensionality of (2,5-dimethylpyrazine)CuCl2. Polyhedron, 2013, 52, 699-705.	2.2	6
40	Impact of short and long-range effects on the magnetic interactions in neutral organic radical-based materials. Physical Chemistry Chemical Physics, 2013, 15, 6982.	2.8	18
41	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 6421-6425.	13.8	33
42	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. Angewandte Chemie, 2013, 125, 6549-6553.	2.0	13
43	Are the phenyl embrace motifs between Ph₄P⁺cations in crystals attractive? An accurate theoretical evaluation. CrystEngComm, 2012, 14, 792-798.	2.6	9
44	Synthesis, Structure, Magnetic Behavior, and Theoretical Analysis of Diazine-Bridged Magnetic Ladders: Cu(quinoxoline)X2 and Cu(2,3-dimethylpyrazine)X2 (X = Cl, Br). Inorganic Chemistry, 2012, 51, 6315-6325.	4.0	27
45	Tracing the Sources of the Different Magnetic Behavior in the Two Phases of the Bistable (BDTA)₂[Co(mnt)₂] Compound. Inorganic Chemistry, 2012, 51, 8646-8648.	4.0	12
46	The Nature of the [TTF]^{.+}â‹…â‹…â‹…[TTF]^{.+} Interactions in the [TTF]₂²⁺ Dimers Embedded in Charged [3]Catenanes: Roomâ€Temperature Multicenter Long Bonds. Chemistry - A European Journal, 2012, 18, 5335-5344.	3.3	22
47	Substituent and counterion effects on the formation of Ï€-dimer dications of end-capped heptathienoacenes. Chemical Communications, 2011, 47, 12622.	4.1	14
48	Tunneling versus Hopping in Mixed-Valence Oligo-p-phenylenevinylene Polychlorinated Bis(triphenylmethyl) Radical Anions. Journal of the American Chemical Society, 2011, 133, 5818-5833.	13.7	81
49	Cationâ€“Anion Hydrogen Bonds: A New Class of Hydrogen Bonds That Extends Their Strength beyond the Covalent Limit. A Theoretical Characterization. Journal of Physical Chemistry A, 2011, 115, 13114-13123.	2.5	23
50	Calculation of microscopic exchange interactions and modelling of macroscopic magnetic properties in molecule-based magnets. Chemical Society Reviews, 2011, 40, 3182.	38.1	77
51	Theoretical evaluation of the nature and strength of the FÂ·Â·Â·F intermolecular interactions present in fluorinated hydrocarbons. Theoretical Chemistry Accounts, 2011, 128, 541-553.	1.4	58
52	Unusually Long, Multicenter, Cation^{Î´+}â‹…â‹…â‹…Anion^{Î´â^'}Bonding Observed for Several Polymorphs of [TTF][TCNE]. Chemistry - A European Journal, 2011, 17, 9326-9341.	3.3	18
53	Design and Preparation of Coâ€crystals Utilizing the ${{f R}{{ f 2hfill atop f 4hfill}}}$(8) Hydrogenâ€Bonding Motif. Chemistry - A European Journal, 2010, 16, 9047-9055.	3.3	12
54	Studying the Origin of the Antiferromagnetic to Spinâ€Canting Transition in the Î²â€pâ€NCC₆F₄CNSSN[.]Molecular Magnet. Chemistry - A European Journal, 2010, 16, 2741-2750.	3.3	51

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55	First-Principles Bottom-Up Study of 1D to 3D Magnetic Transformation in the Copper Pyrazine Dinitrate S = 1/2 Antiferromagnetic Crystal. Inorganic Chemistry, 2010, 49, 1750-1760.	4.0	33
56	The Magnetism of (5MAP)₂CuBr₄ [5MAP = 5-Methyl-2-aminopyridinium]: A Quasi-2D or a 3D Magnetic System?. Inorganic Chemistry, 2010, 49, 8017-8024.	4.0	13
57	Origin of the Magnetic Bistability in Molecule-Based Magnets: A First-Principles Bottom-Up Study of the TTTA Crystal. Journal of the American Chemical Society, 2010, 132, 17817-17830.	13.7	61
58	A theoretical investigation of the oxidation states of palladium complexes and their role in the carbonylation reaction. Molecular Physics, 2010, 108, 1619-1640.	1.7	5
59	Oxidation of Endâ€Capped Pentathienoacenes and Characterization of Their Radical Cations. Chemistry - A European Journal, 2009, 15, 12346-12361.	3.3	17
60	Long, multicenter bonding in Ï€-[terthiophene] 2 2+ dimers. Theoretical Chemistry Accounts, 2009, 123, 137-143.	1.4	8
61	The origin of the bistability in the thiazyl radical 1,3,5-trithia-2,4,6-triazapentalenyl (TTTA): A first principles bottom-up investigation of the magnetic properties of its high temperature polymorph. Polyhedron, 2009, 28, 1614-1619.	2.2	10
62	On the existence of temperature induced changes in the magnetic topology of crystals that show no first-order crystallographic phase transitions. Polyhedron, 2009, 28, 1965-1971.	2.2	17
63	Theoretical Study of the Electronic Structure of [TCNQ]₂^{2â^’}(TCNQ =) Tj ETQq1 1 0.784314 rgBT /Overlock Solution and the Solid State. Journal of Physical Chemistry A, 2009, 113, 7124-7132.	2.5	39
64	Structure and Magnetic Interactions in the Organic-Based Ferromagnet Decamethylferrocenium Tetracyanoethenide, [FeCp*2]â€¢+[TCNE]â€¢â^’. Inorganic Chemistry, 2009, 48, 3296-3307.	4.0	34
65	The Tetracyanopyrazinide Dimer Dianion, [TCNP]₂^{2â^’}. 2-Electron 8-Center Bonding. Journal of the American Chemical Society, 2009, 131, 9070-9075.	13.7	41
66	Comparative Analysis of the Multicenter, Long Bond in [TCNE]^{Â·â^’}and Phenalenyl Radical Dimers: A Unified Description of Multicenter, Long Bonds. Journal of the American Chemical Society, 2009, 131, 7699-7707.	13.7	122
67	Theoretical Study of the Electronic Structure of [Tetrathiafulvalene]22+ Dimers and Their Long, Intradimer Multicenter Bonding in Solution and the Solid State. Journal of Physical Chemistry A, 2009, 113, 484-492.	2.5	55
68	Strong through-space two-halide magnetic exchange of â^’234 K in (2,5-dimethylpyrazine)copper(ii) bromide. Chemical Communications, 2009, , 1359.	4.1	35
69	Metallocenium Salts of Nickel Bis(Î±-thiophenedithiolate) [M(Cp*)2][Ni(Î±-tpdt)2] (M = Fe, Mn, Cr) - Metamagnetism and Magnetic Frustration. European Journal of Inorganic Chemistry, 2008, 2008, 5327-5337.	2.0	14
70	Study of the magnetic exchange within the cluster polymer [NaCu6(gly)8(ClO4)3(H2O)]n(ClO4)2n. Inorganica Chimica Acta, 2008, 361, 3919-3925.	2.4	10
71	A first-principles bottom-up study of the magnetic interaction mechanism in the bulk ferromagnet p-O2N-C6F4-CNSSN. Inorganica Chimica Acta, 2008, 361, 3586-3592.	2.4	7
72	On the hydrogen bond nature of the Câ€“Hâ‹¯F interactions in molecular crystals. An exhaustive investigation combining a crystallographic database search and ab initio theoretical calculations. CrystEngComm, 2008, 10, 423.	2.6	121

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73	[Cyanil]22â^' dimers possess long, two-electron ten-center (2eâ^'/10c) multicenter bonding. Physical Chemistry Chemical Physics, 2008, 10, 4106.	2.8	31
74	From Bonds to Packing: An Energy-Based Crystal Packing Analysis for Molecular Crystals Packing Analysis for Molecular Crystals. NATO Science for Peace and Security Series B: Physics and Biophysics, 2008, , 307-332.	0.3	2
75	Synthesis, Structure, and Magnetic Properties of an Antiferromagnetic Spin-Ladder Complex:Â Bis(2,3-dimethylpyridinium) Tetrabromocuprate. Journal of the American Chemical Society, 2007, 129, 952-959.	13.7	121
76	Structure and Stability of the [TCNE]₂²⁻Dimers in Dichloromethane Solution:â€‰ A Computational Study. Journal of Physical Chemistry A, 2007, 111, 8020-8027.	2.5	39
77	Four-Center Carbonâ^'Carbon Bonding. Accounts of Chemical Research, 2007, 40, 189-196.	15.6	164
78	The mechanism for the reversible oxygen addition to heme. A theoretical CASPT2 study. Chemical Communications, 2007, , 3160.	4.1	40
79	Synthesis, Structure, and Magnetic Behavior of Bis(2-amino-5-fluoropyridinium) Tetrachlorocuprate(II). Inorganic Chemistry, 2007, 46, 11254-11265.	4.0	57
80	Control of Two-Electron Four-Center (2e-/4c) Câ^'C Bond Formation Observed for Tetracyanoethenide Dimerization, [TCNE]22-. Inorganic Chemistry, 2007, 46, 103-107.	4.0	17
81	The origin of the two-electron/four-centers Cï£¿C bond in Ï€-TCNE22â^' dimers: Electrostatic or dispersion?. Journal of Computational Chemistry, 2007, 28, 326-334.	3.3	37
82	A theoretical study of the magnetism of the Î±-p-cyano-tetrafluorophenyl-dithiadiazolyl radical using a first principles bottom-up procedure. Polyhedron, 2007, 26, 1949-1958.	2.2	32
83	Theoretical study of the magnetism in molecular crystals using a first-principles bottom-up methodol. Progress in Theoretical Chemistry and Physics, 2007, , 271-289.	0.2	15
84	The Nature of the Câ€“HÂ·ÂÂ·ÂÂ·X Intermolecular Interactions in Molecular Crystals. A Theoretical Perspective. , 2006, , 193-244.		12
85	A DFT computational study of the mechanism of butadiene carbonylation catalyzed by palladium complexes. Molecular Physics, 2006, 104, 805-831.	1.7	2
86	Analysis of the magneto-structural correlations in the meso-tetraphenylporphyrinatomanganese(iii) tetracyanoethenide family of molecule-based magnets. Journal of Materials Chemistry, 2006, 16, 2600-2611.	6.7	33
87	Bulk ferromagnetism in nitronyl nitroxide crystals: a first principles bottom-up comparative study of four bulk nitronyl nitroxide ferromagnets (KAXHAS, YOMYII, LICMIT and YUJNEW). Molecular Physics, 2006, 104, 857-873.	1.7	20
88	The mechanism of transition metal catalyzed carbonylation of allyl halides: A theoretical investigation. Journal of Organometallic Chemistry, 2006, 691, 4498-4507.	1.8	9
89	The nature of the AuI ... AuI Interactions between Cationic [AuL2]+ Complexes in the Solid State. Theoretical Chemistry Accounts, 2006, 116, 472-479.	1.4	12
90	Direct versus Mediated Through-Space Magnetic Interactions: A First Principles, Bottom-Up Reinvestigation of the Magnetism of the Pyridyl-Verdazyl:Hydroquinone Molecular Co-Crystal. Chemistry - A European Journal, 2006, 12, 3995-4005.	3.3	59

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91	Generalized Stone-Wales transformation as the possible origin of ferromagnetism in polymeric C60: A density-functional theory study. Journal of Chemical Physics, 2006, 125, 174312.	3.0	4
92	Ferromagnetism in pressed polymerizedC60solids induced byC60cage vacancies: A density-functional study. Physical Review B, 2006, 73, .	3.2	9
93	Quantitative analysis of the magnetism of the meta-(methoxy)phenyl nitronyl nitroxide crystal: A bottomâ€“up analysis of a crystal presenting competing ferro and antiferromagnetic interactions. Polyhedron, 2005, 24, 2368-2376.	2.2	5
94	Solvent-mediated intermolecular bonds: cationâ€“cation and anionâ€“anion interactions in solution showing the signature of chemical bonds. Computational and Theoretical Chemistry, 2005, 727, 181-189.	1.5	15
95	The Mechanism of Magnetic Interaction in Spin-Ladder Molecular Magnets: A First-Principles, Bottom-Up, Theoretical Study of the Magnetism in the Two-Legged Spin-Ladder Bis(2-amino-5-nitropyridinium) Tetrabromocuprate Monohydrate. European Journal of Inorganic Chemistry, 2005, 2005, 4697-4706.	2.0	35
96	Towards a Better Understanding of Magnetic Interactions withinm-Phenylene ?-Nitronyl Nitroxide and Imino Nitroxide Based Radicals, Part III: Magnetic Exchange in a Series of Triradicals and Tetraradicals Based on the Phenyl Acetylene and Biphenyl Coupling Units. Chemistry - A European Journal, 2005, 11, 2440-2454.	3.3	30
97	Substituted m-phenylene bridges as strong ferromagnetic couplers for Cuiiâ€“bridgeâ€“Cuii magnetic interactions: new perspectives. Chemical Communications, 2005, , 5172.	4.1	65
98	Broken Inter-C60Bonds as the Cause of Magnetism in Polymeric C60:Â A Density Functional Study Using C60Dimers. Journal of Physical Chemistry A, 2005, 109, 4979-4982.	2.5	2
99	DFT Computational Study of the Mechanism of Allyl Chloride Carbonylation Catalyzed by Palladium Complexes. Organometallics, 2005, 24, 2086-2096.	2.3	16
100	A First-Principles Analysis of the Magnetism of CuII Polynuclear Coordination Complexes: the Case of [Cu4(bpy)4(aspartate)2(H2O)3](ClO4)4â€¢2.5H2O. Molecules, 2004, 9, 757-770.	3.8	12
101	The Origin of the Magnetic Moments in Compressed Crystals of Polymeric C60. Angewandte Chemie - International Edition, 2004, 43, 577-580.	13.8	17
102	The Origin of the Magnetic Moments in Compressed Crystals of Polymeric C60.. ChemInform, 2004, 35, no.	0.0	0
103	Supramolecular Photomagnetic Materials: Photoinduced Dimerization of Ferrocene-Based Polychlorotriphenylmethyl Radicals. Chemistry - A European Journal, 2004, 10, 603-616.	3.3	22
104	The Nature of Intermolecular CuIâ‹…â‹…â‹…CuI Interactions: A Combined Theoretical and Structural Database Analysis. Chemistry - A European Journal, 2004, 10, 2117-2132.	3.3	139
105	Magneto-Structural Characterization of Metallocene-Bridged Nitronyl Nitroxide Diradicals by X-Ray, Magnetic Measurements, Solid-state NMR Spectroscopy, and Ab Initio Calculations. Chemistry - A European Journal, 2004, 10, 1355-1365.	3.3	22
106	The Mechanism of Magnetic Interactions in the Bulk Ferromagnetpara-(Methylthio)Phenyl Nitronyl Nitroxide (YUJNEW): A First Principles, Bottom-Up, Theoretical Study. Chemistry - A European Journal, 2004, 10, 6422-6432.	3.3	37
107	Magneto-Structural Characterization of Metallocene-Bridged Nitronyl Nitroxide Diradicals by X-Ray, Magnetic Measurements, Solid-state NMR Spectroscopy, and Ab Initio Calculations. Chemistry - A European Journal, 2004, 10, 3354-3354.	3.3	0
108	Evaluation of the capability of C60-fullerene to act as a magnetic coupling unit. Journal of Physics and Chemistry of Solids, 2004, 65, 787-791.	4.0	17

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109	The strengthâ€“length relationship at the light of ab initio computations: does it really hold?. CrystEngComm, 2004, 6, 367-376.	2.6	24
110	A new tetrameric CuIIcluster with square topology exhibiting ferro- and antiferromagnetic magnetic pathways : which is which?. Chemical Communications, 2004, , 1102-1103.	4.1	38
111	Choice of Coordination Number in d10Complexes of Group 11 Metals. Journal of the American Chemical Society, 2004, 126, 1465-1477.	13.7	198
112	The mechanism of the magnetic interaction in the Î² phase of the p -(nitro)phenyl nitronyl nitroxide (KAXHAS). A bottom-up study using only ab initio data. Polyhedron, 2003, 22, 1935-1944.	2.2	23
113	Through space magnetic exchange in tetrabromocuprates: theoretical considerations. Polyhedron, 2003, 22, 2235-2239.	2.2	15
114	Chemical Reduction of 2,4,6-Tricyano-1,3,5-triazine and 1,3,5-Tricyanobenzene. Formation of Novel 4,4â€˜,6,6â€˜-Tetracyano-2,2â€˜-bitriazine and Its Radical Anionâ€. Journal of Organic Chemistry, 2003, 68, 3367-3379.	3.2	46
115	DFT Computational Study of the Mechanism of Allyl Halides Carbonylation Catalyzed by Nickel Tetracarbonyl. Journal of the American Chemical Society, 2003, 125, 10412-10419.	13.7	26
116	First-principles study of the neutral molecular metalNi(tmdt)2. Physical Review B, 2002, 65, .	3.2	60
117	Magnetic Properties of Organic Molecular Crystals via an Algebraic Heisenberg Hamiltonian. Applications to WILVIW, TOLKEK, and KAXHAS Nitronyl Nitroxide Crystals. Journal of Physical Chemistry A, 2002, 106, 1299-1315.	2.5	87
118	On the existence of long Câ€“C bonds between pairs of anions which repel: when and why? A test case on the [TCNE]22â^'dimers found in ionic crystals. CrystEngComm, 2002, 4, 373-377.	2.6	39
119	Synthesis and structure of an asymmetric copper(i) dimer with two-coordinate and four-coordinate copper(i) sitesElectronic supplementary information (ESI) available: synthesis, NMR, computational details. See http://www.rsc.org/suppdata/cc/b2/b208865g/. Chemical Communications, 2002, , 3008-3009.	4.1	14
120	Oâ^'Hâ‹…â‹…â‹…O Interactions Involving Doubly Charged Anions: Charge Compression in Carbonateâ€“Bicarbonate Crystals Queries on the theoretical part should be addressed to Professor J. J. Novoa.. Chemistry - A European Journal, 2002, 8, 1173.	3.3	35
121	Exceptionally Long (â‰¥2.9 Ã…) CC Bonding Interactions in Ï€-[TCNE]22 Dimers: Two-Electron Four-Center Cation-Mediated CC Bonding Interactions Involving Ï€* Electrons. Chemistry - A European Journal, 2002, 8, 4894-4908.	3.3	134
122	Ligand effects and dimer formation in dicoordinated copper(I) complexes. International Journal of Quantum Chemistry, 2002, 86, 100-105.	2.0	14
123	A general study of the spin population of Î±-nitronyl nitroxide radicals: radicals with crystals presenting dominant ferro or antiferromagnetic behavior. Synthetic Metals, 2001, 122, 477-483.	3.9	15
124	On the charge delocalisation in partially deprotonated polycarboxylic acid anions and zwitterions forming (â^')Oâ€“HÂ·Â·Â·O(â^') interactions in the solid state. New Journal of Chemistry, 2001, 25, 226-230.	2.8	19
125	Synthesis, crystal structures, electronic structure and magnetic behaviour of the trithiatriazapentalenyl radical, C2S3N3. Journal of Materials Chemistry, 2001, 11, 1992-2003.	6.7	123
126	A First-Principles Computation of the Low-Energy Polymorphic Forms of the Acetic Acid Crystal. A Test of the Atomâ^'Atom Force Field Predictions. Journal of Physical Chemistry B, 2001, 105, 1710-1719.	2.6	12

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127	A CW-EPR and ESEEM spectroscopic study of the dithiadiazolyl radicals p-XC6F4CNSSN (X = CN, Br). Applied Magnetic Resonance, 2001, 20, 231-247.	1.2	19
128	Towards a Better Understanding of the Magnetic Interactions withinm-PhenyleneÎ±-Nitronyl Imino Nitroxide Based Biradicals. Chemistry - A European Journal, 2001, 7, 2466-2480.	3.3	68
129	Exceptionally Long (â‰¥2.9 Ã...) Câˆ'C Bonds between [TCNE]â˜ Ions: Two-Electron, Four-Center Ï€*-Ï€* Câˆ'C Bonding in Ï€-[TCNE]22â˜. Angewandte Chemie - International Edition, 2001, 40, 2540-2545.	13.8	164
130	Metamagnetism in linear chain electron-transfer salts based on decamethylferrocenium and metalâ€"bis(dichalcogenate) acceptors. Inorganica Chimica Acta, 2001, 326, 89-100.	2.4	13
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