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	Evaluation of the Density Functional Approximation on the Computation of Hydrogen Bond Interactions. The Journal of Physical Chemistry, 1995, 99, 15837-15845.	2.9	332
2	Choice of Coordination Number in d10Complexes of Group 11 Metals. Journal of the American Chemical Society, 2004, 126, 1465-1477.	13.7	198
3	Strain index, lattice softness and superconductivity of organic donor-molecule salts. Physica C: Superconductivity and Its Applications, 1991, 174, 475-486.	1.2	175
4	Exceptionally Long (â‰¥2.9 Ã…) Câˆ’C Bonds between [TCNE]âˆ’ Ions: Two-Electron, Four-Center Ï€*-Ï€* Câˆ’C Bonding in Ï€-[TCNE]22âˆ’. Angewandte Chemie - International Edition, 2001, 40, 2540-2545.	13.8	164
5	Four-Center Carbonâˆ’Carbon Bonding. Accounts of Chemical Research, 2007, 40, 189-196.	15.6	164
6	The Câ€“Hâ‹¯Ï€ bonds: strength, identification, and hydrogen-bonded nature: a theoretical study. Chemical Physics Letters, 2000, 318, 345-354.	2.6	157
7	Magnetic Coupling in End-to-End Azido-Bridged Copper and Nickel Binuclear Complexes:Â A Theoretical Study. Inorganic Chemistry, 2000, 39, 3221-3229.	4.0	152
8	A theoretical study of the ionic dissociation of HF, HCl, and H2S in water clusters. Journal of Chemical Physics, 1996, 104, 7081-7085.	3.0	148
9	High-Temperature Magnetic Ordering in a New Organic Magnet. Physical Review Letters, 1997, 79, 2336-2339.	7.8	140
10	The Nature of Intermolecular Culâ‹…â‹…â‹…Cul Interactions: A Combined Theoretical and Structural Database Analysis. Chemistry - A European Journal, 2004, 10, 2117-2132.	3.3	139
11	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
12	Synthesis, crystal structures, electronic structure and magnetic behaviour of the trithiatriazapentalenyl radical, C2S3N3. Journal of Materials Chemistry, 2001, 11, 1992-2003.	6.7	123
13	Comparative Analysis of the Multicenter, Long Bond in [TCNE]^{Â·âˆ’}and Phenalenyl Radical Dimers: A Unified Description of Multicenter, Long Bonds. Journal of the American Chemical Society, 2009, 131, 7699-7707.	13.7	122
14	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
15	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
16	Cï£¿Hâ€¦S and Sâ€¦S: Two major forces in organic conductors. Advanced Materials, 1995, 7, 233-237.	21.0	120
17	Ligand Macrocycle Structural Effects on Copperâˆ’Dioxygen Reactivity. Inorganic Chemistry, 2000, 39, 4059-4072.	4.0	116
18	New Îº-phase materials, Îº-(ET)2Cu[N(CN)2]X.X=Cl, Br and I. The synthesis, structure and superconductivity above 11 K in the Cl (Tc = 12.8 K, 0.3 kbar) and Br(Tc = 11.6 K) salts. Synthetic Metals, 1991, 42, 1983-1990.	3.9	108

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19	On the Bonding Nature of the M.cntdot. .cntdot. .cntdot.M Interactions in Dimers of Square-Planar Pt(II) and Rh(I) Complexes. Journal of the American Chemical Society, 1995, 117, 7169-7171.	13.7	103
20	Structure-Magnetism Relationships inÎ±-Nitronyl Nitroxide Radicals. Chemistry - A European Journal, 1999, 5, 1631-1642.	3.3	103
21	Interaction energies associated with short intermolecular contacts of Câ€“H bonds. Ab initio computational study of the Câ€“Hâ‹…â‹…â‹…â‹…O contact interaction in CH4â‹…â‹…â‹…OH2. Journal of Chemical Physics, 1991, 95, 5179-5186.	3.0	101
22	On the usefulness of the counterpoise method on hydrogen-bonded complexes: a numerical test using near complete basis sets on H2O â€¦ HF, (H2O)2, (HF) 2 and CH4â€¦H2O. Chemical Physics Letters, 1996, 251, 33-46.	2.6	88
23	Inter-anion Oâ€“HâˆÂ·Â·Â·Oâˆ’ hydrogen bond like interactions: the breakdown of the strengthâ€“length analogy. Chemical Communications, 1998, , 1959-1960.	4.1	87
24	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
25	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
26	Structure of the First Solvation Shell of the Hydroxide Anion. A Model Study Using OH-(H2O)n(n= 4, 5,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	79
27	Calculation of microscopic exchange interactions and modelling of macroscopic magnetic properties in molecule-based magnets. Chemical Society Reviews, 2011, 40, 3182.	38.1	77
28	Spin Density Distribution of Î±-Nitronyl Aminoxyl Radicals from Experimental and ab Initio Calculated ESR Isotropic Hyperfine Coupling Constants. Journal of the American Chemical Society, 2000, 122, 11393-11405.	13.7	70
29	Similarities and differences in the structural and electronic properties of .kappa.-phase organic conducting and superconducting salts. Inorganic Chemistry, 1989, 28, 4516-4522.	4.0	68
30	On the Validity of the McConnell-I Model of Ferromagnetic Interactions:â€‰ The [2.2]Paracyclophane Example. Journal of Physical Chemistry A, 1998, 102, 8404-8412.	2.5	68
31	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
32	Kinetics of the Proton Transfer in XÂ·Â·Â·(H2O)4Clusters (X = H2O, NH3, H2S, and HCl):Â Evidence of a Concerted Mechanism. The Journal of Physical Chemistry, 1996, 100, 16495-16501.	2.9	66
33	Determination of the Spin Distribution in Nitronylnitroxides by Solid-State 1H, 2H, and 13C NMR Spectroscopy. Journal of the American Chemical Society, 1999, 121, 9659-9667.	13.7	66
34	Are non-linear Câ€“Hâ‹¯O contacts hydrogen bonds or Van der Waals interactions?. Chemical Physics Letters, 1998, 290, 519-525.	2.6	65
35	Substituted m-phenylene bridges as strong ferromagnetic couplers for Cuiiâ€“bridgeâ€“Cuii magnetic interactions: new perspectives. Chemical Communications, 2005, , 5172.	4.1	65
36	Interactions energies associated with short intermolecular contacts of Câ€“H bonds. II. Ab initio computational study of the Câ€“Hâ‹…â‹…â‹…â‹…Hâ€“C interactions in methane dimer. Journal of Chemical Physics, 1991, 94, 4835-4841.	3.0	62

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37	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
38	A numerical evaluation of the counterpoise method on hydrogen bond complexes using near complete basis sets. Chemical Physics Letters, 1994, 225, 240-246.	2.6	60
39	Ab initio computation of the potential energy surfaces of the waterÂ·hydrocarbon complexes H2OÂ·C2H2, H2OÂ·C2H4 and H2OÂ·CH4: minimum energy structures, vibrational frequencies and hydrogen bond energies. Chemical Physics, 1995, 200, 319-335.	1.9	60
40	First-principles study of the neutral molecular metalNi(tmdt)2. Physical Review B, 2002, 65, .	3.2	60
41	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
42	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
43	Substituent effects in intermolecular C(sp3)-H â‹¯ O(sp3) contacts: how strong can a C(sp3)-H â‹¯ O(sp3) hydrogen bond be?. Chemical Physics Letters, 1997, 266, 23-30.	2.6	57
44	Synthesis, Structure, and Magnetic Behavior of Bis(2-amino-5-fluoropyridinium) Tetrachlorocuprate(II). Inorganic Chemistry, 2007, 46, 11254-11265.	4.0	57
45	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
46	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
47	The key role of vibrational entropy in the phase transitions of dithiazolyl-based bistable magnetic materials. Nature Communications, 2014, 5, 4411.	12.8	55
48	Structure and stability of the X3- systems (X = fluoride, chloride, bromide, iodide) and their interaction with cations. The Journal of Physical Chemistry, 1988, 92, 6561-6566.	2.9	54
49	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
50	Strength and Directionality of the Sâ‹…â‹…â‹…S Intermolecular Interactions Present in TTF-Based Molecular Crystals. A Combined Statistical and Ab Initio Study. Chemistry - A European Journal, 1999, 5, 3689-3697.	3.3	49
51	Evidence of the existence of dissociated water molecules in water clusters. Journal of Chemical Physics, 1995, 103, 4360-4362.	3.0	48
52	Structure-Magnetism Relationships in Î±-Nitronyl Nitroxide Radicals: Pitfalls and Lessons to be Learned. Advanced Materials, 1998, 10, 1461-1466.	21.0	48
53	Are all short Oâ€“HÂ·Â·Â·O contacts hydrogen bonds? A quantitative look at the nature of Oâ€“HÂ·Â·Â·O intermolecular hydrogen bonds. New Journal of Chemistry, 2000, 24, 5-8.	2.8	48
54	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

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55	Pyramidality and metal-metal multiple bonding: structural correlations and theoretical study. Journal of the American Chemical Society, 1993, 115, 6216-6229.	13.7	44
56	Electrostatic compression on non-covalent interactions: the case of Ï€ stacks involving ions. New Journal of Chemistry, 1999, 23, 577-579.	2.8	44
57	Interanionic(â^')Oâ^'Hâ‹…â‹…â‹…O(â^') Interactions: A Solid-State and Computational Study of the Ring and Chain Motifs. Chemistry - A European Journal, 2000, 6, 4536-4551.	3.3	44
58	The nature of intramolecular hydrogen-bonded and non-hydrogen-bonded conformations of simple di- and triamides. Journal of the American Chemical Society, 1991, 113, 9017-9026.	13.7	42
59	Ionization of Bases in Water:Â Structure and Stability of the NH4+Â·Â·Â·OH-Ionic Forms in Ammoniaâ^'Water Clusters. The Journal of Physical Chemistry, 1996, 100, 7398-7404.	2.9	41
60	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
61	The mechanism for the reversible oxygen addition to heme. A theoretical CASPT2 study. Chemical Communications, 2007, , 3160.	4.1	40
62	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
63	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
64	Theoretical Study of the Electronic Structure of [TCNQ]₂^{2â^'}(TCNQ =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 3 Solution and the Solid State. Journal of Physical Chemistry A, 2009, 113, 7124-7132.	2.5	39
65	A new tetrameric CuIIcluster with square topology exhibiting ferro- and antiferromagnetic magnetic pathways : which is which?. Chemical Communications, 2004, , 1102-1103.	4.1	38
66	Câ€“HÂ·Â·Â·O Hydrogen bonds in the mixed-valence salt [(Î·6-C6H6)2Cr]+[CrO3(OCH3)]- and the breakdown of the length/strength analogy. New Journal of Chemistry, 1998, 22, 755-757.	2.8	37
67	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
68	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
69	Density functional computations on the structure and stability of OHâ^'(H2O)n (n = 1â^'3) clusters. A test study. Chemical Physics Letters, 1997, 269, 401-407.	2.6	36
70	Framework Bonding and Coordination Sphere Rearrangement in the M2X2Cores of Synthetic Analogues of Oxyhemocyanin and Related Cu and Pt Complexes. Inorganic Chemistry, 1998, 37, 1202-1212.	4.0	35
71	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
72	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

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73	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
74	Stereochemistry of PhenylÎ±-Nitronyl Nitroxide Radicals. Chemistry - A European Journal, 2000, 6, 2350-2361.	3.3	34
75	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
76	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
77	Dynamical effects on the magnetic properties of dithiazolyl bistable materials. Chemical Science, 2015, 6, 2371-2381.	7.4	34
78	A density functional study of crystalline acetic acid and its proton transfer polymorphic forms. Journal of Chemical Physics, 2000, 113, 9208-9216.	3.0	33
79	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
80	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
81	Evidence for Multicenter Bonding in Dianionic Tetracyanoethylene Dimers by Raman Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 6421-6425.	13.8	33
82	Strength and directionality of the C(sp3)î—¸Hâ‹¯S(sp3) interaction. An ab initio study using the H2Sâ‹¯CH4 model complex. Chemical Physics Letters, 1997, 279, 140-150.	2.6	32
83	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
84	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
85	[Cyanil]22â^' dimers possess long, two-electron ten-center (2eâ^'/10c) multicenter bonding. Physical Chemistry Chemical Physics, 2008, 10, 4106.	2.8	31
86	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
87	Keys for the Existence of Stable Dimers of Bis-tetrathiafulvalene (bis-TTF)-Functionalized Molecular Clips Presenting [TTF]â€¢+Â·Â·Â·[TTF]â€¢+ Long, Multicenter Bonds at Room Temperature. Journal of the American Chemical Society, 2013, 135, 13814-13826.	13.7	30
88	The Mechanism of the Through-Space Magnetic Interactions in Purely Organic Molecular Magnets. , 2001, , 33-60.		30
89	Accurate calculation of the electron affinities of the group-13 atoms. Chemical Physics, 1992, 166, 77-84.	1.9	29
90	Ab Initio Study of the Intermolecular Interactions in the Hofmann Clathrates. The Journal of Physical Chemistry, 1995, 99, 2296-2306.	2.9	29

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91	An analytical representation of the ground potential energy surface (2Aâ€²) of the H+Cl2â†'HCl+Cl and Cl+HClâ†'HCl+Cl reactions, based on ab initio calculations. Journal of Chemical Physics, 1998, 108, 3168-3177.	3.0	29
92	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
93	Association of two-coordinate copper(I) complexes: switching on and off CuÂ·Â·Â·Cu, ligandÂ·Â·Â·ligand and Cuâ€“ligand interactions. Chemical Communications, 1998, , 1149-1150.	4.1	28
94	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
95	Insights into the magnetism and phase transitions of organic radical-based materials. Journal of Materials Chemistry C, 2021, 9, 10624-10646.	5.5	27
96	The large range of chromium-chromium quadruple bond distances: structural and theoretical analysis. Journal of the American Chemical Society, 1990, 112, 8998-9000.	13.7	26
97	Bis(ethylenethio)tetrathiafulvalene (BET-TTF), an organic donor with high electrical conductivity. Advanced Materials, 1995, 7, 1023-1027.	21.0	26
98	The Hydrogen Bonding Strategy. A New Approach Towards Purely Organic/Molecular Ferromagnets. Molecular Crystals and Liquid Crystals, 1995, 271, 1-12.	0.3	26
99	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
100	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
101	The symmetry breaking problem in the triflouride anion: A multireference approach. Journal of Chemical Physics, 1996, 105, 8777-8784.	3.0	25
102	Theoretical analysis of the crystal packing of nitronyl nitroxide radicals: the packing of the Î±-2-hydro nitronyl nitroxide radical. Chemical Physics Letters, 1997, 265, 190-199.	2.6	25
103	Interaction energies associated with short intermolecular contacts of carbon-hydrogen bonds. 1. Ab initio computational study of C-H.cntdot..cntdot..cntdot.anion interactions, C-H.cntdot..cntdot..cntdot.X-(X- = I3-, IBr2-, ICl2-). Inorganic Chemistry, 1991, 30, 54-58.	4.0	24
104	The strengthâ€“length relationship at the light of ab initio computations: does it really hold?. CrystEngComm, 2004, 6, 367-376.	2.6	24
105	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
106	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
107	Supramolecular Photomagnetic Materials: Photoinduced Dimerization of Ferrocene-Based Polychlorotriphenylmethyl Radicals. Chemistry - A European Journal, 2004, 10, 603-616.	3.3	22
108	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

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109	The Nature of the [TTF]^{.+}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
110	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
111	Interaction energies associated with short intermolecular contacts of Cî—¸H bonds. 4. Ab initio computational study of Cî—¸Hâ€¦anion interactions in CH4â€¦Xâ¯ (X=F, Cl, Br, I). Chemical Physics Letters, 1991, 180, 241-248.	2.6	20
112	An ab initio analytical potential energy surface for the O(3P)+CS(Xâ€‰1Î£+)â†’CO(Xâ€‰1Î£+)+S(3P) reaction useful for kinetic and dynamical studies. Journal of Chemical Physics, 1996, 105, 10999-11006.	3.0	20
113	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
114	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
115	Convergence of a multireference second-order mbpt method (CIPSI) using a zero-order wavefunction derived from an MS SCF calculation. Chemical Physics Letters, 1986, 126, 98-102.	2.6	19
116	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
117	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
118	Hydrogen bonding and collective proton modes in clusters and periodic layers of squaric acid: A density functional study. Journal of Chemical Physics, 2001, 115, 6406-6417.	3.0	19
119	Theoretical Analysis of the Packing and Polimorphism of Molecular Crystals Using Quantum Mechanical Methods: The Packing of the 2-Hydro Nitronyl Nitroxide. Molecular Crystals and Liquid Crystals, 1997, 305, 143-156.	0.3	18
120	Theoretical Study of the Mechanism of Carbonyl Insertion Reactions Catalyzed by Nickel Complexes. Organometallics, 2000, 19, 2170-2178.	2.3	18
121	Unusually Long, Multicenter, Cation^{Î´+}â‹…â‹…Anion^{Î´â¯}Bonding Observed for Several Polymorphs of [TTF][TCNE]. Chemistry - A European Journal, 2011, 17, 9326-9341.	3.3	18
122	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
123	Organic Ferromagnets. Hydrogen Bonded Supramolecular Magnetic Organizations Derived from Hydroxylated Phenyl ?-Nitronyl Nitroxide Radicals. Journal De Physique, I, 1996, 6, 1967-1986.	1.2	18
124	Structure and stability of tetraatomic bromine and ion, Br4 and Br42-, and their interaction with cations and transition metals. Journal of the American Chemical Society, 1987, 109, 6586-6591.	13.7	17
125	On the Strength of the Cï£¿Hâ€¦O Hydrogen Bond and the Eclipsed Arrangement of the Methyl Group in a Tricyclic Orthoamide Trihydrate. Angewandte Chemie International Edition in English, 1993, 32, 588-589.	4.4	17
126	Ab Initio Computation of the Spin Population of Substituted Î±-Nitronyl Nitroxide Radicals. Molecular Crystals and Liquid Crystals, 1995, 271, 79-90.	0.3	17

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127	The Origin of the Magnetic Moments in Compressed Crystals of Polymeric C60. Angewandte Chemie - International Edition, 2004, 43, 577-580.	13.8	17
128	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
129	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
130	Oxidation of Endâ€Capped Pentathienoacenes and Characterization of Their Radical Cations. Chemistry - A European Journal, 2009, 15, 12346-12361.	3.3	17
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