Janet E Del Bene

List of Publications by Year
in descending order

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240 papers	8,561 citations	44069 48 h-index	69250 77 g-index

241 all docs	241 docs citations	241 times ranked	3028 citing authors

#	Article	IF	Citations
1	IR and NMR properties of N-base:PH2F:BeX2 ternary and corresponding binary complexes stabilised by pnicogen and beryllium bonds. Molecular Physics, 2021, 119, e1905191.	1.7	8
2	Perturbing the Oâ€“Hâ€¦O Hydrogen Bond in 1-oxo-3-hydroxy-2-propene. Molecules, 2021, 26, 3086.	3.8	1
3	Probing the structures, binding energies, and spin-spin coupling constants of halogen-bonded Azine:ClF complexes. Chemical Physics Letters, 2020, 761, 137916.	2.6	12
4	Mutual Influence of Pnicogen Bonds and Beryllium Bonds: Energies and Structures in the Spotlight. Journal of Physical Chemistry A, 2020, 124, 5871-5878.	2.5	13
5	Unusual Complexes of P(CH)3 with FH, ClH, and ClF. Molecules, 2020, 25, 2846.	3.8	1
6	Hydrogen bonds and halogen bonds in complexes of carbones Lâ†'Câ†Ł as electron donors to HF and ClF, for L = CO, N2, HNC, PH3, and SH2. Physical Chemistry Chemical Physics, 2020, 22, 15966-15975.	2.8	5
7	Complexes H2CO:PXH2and HCO2Hâ€‰:â€‰PXH2for X=NC, F, Cl, CN, OH, CCH, CH3, and H: Pnicogen Bonds and Hydrogen Bonds. ChemPhysChem, 2020, 21, 741-748.	2.1	6
8	Calculated coupling constants ¹J(Xâ€“Y) and ¹K(Xâ€“Y), and fundamental relationships among the reduced coupling constants for molecules H_mXâ€“YH_n, with X, Y â••¹H, ⁷Li, ⁹Be, ¹¹B, ¹³C, ¹⁵N, ¹⁷O, ¹⁹F, ³¹P, ³³S, and ³⁵Cl. Magnetic Resonance in Chemistry, 2020, 58, 727-732.	1.9	0
9	Potential Energy Surfaces of HN(CH)SX:CO₂ for X = F, Cl, NC, CN, CCH, and H: NÂ·Â·Â·C Tetrel Bonds and OÂ·Â·Â·S Chalcogen Bonds. Journal of Physical Chemistry A, 2019, 123, 7270-7277.	2.5	23
10	What Types of Noncovalent Bonds Stabilize Dimers (XCP)₂, for X = CN, Cl, F, and H?. Journal of Physical Chemistry A, 2019, 123, 10086-10094.	2.5	6
11	Nâ€¦C and Sâ€¦S Interactions in Complexes, Molecules, and Transition Structures HN(CH)SX:SCO, for X = F, Cl, NC, CCH, H, and CN. Molecules, 2019, 24, 3232.	3.8	4
12	Exploring N C tetrel and O S chalcogen bonds in HN(CH)SX:OCS systems, forâ€¯Xâ€¯=â€¯F, NC, Cl, CN, CCH, and H. Chemical Physics Letters, 2019, 730, 466-471.	2.6	22
13	Can a Clâ€“HÂ·Â·Â·F Hydrogen Bond Replace a ClÂ·Â·Â·F Halogen Bond? H2XP:ClY:ZH versus H2XP:ClY:HZ for Y, Z = F, Cl. Journal of Physical Chemistry A, 2019, 123, 3992-3999.	2.5	1
14	Probing Câ¯S chalcogen bonds in complexes SC:SHX, for Xâ€¯=â€¯NO2, NC, F, Cl, CN, CCH, and NH2. Chemical Physics Letters, 2019, 721, 86-90.	2.6	8
15	Pnicogen bonds in complexes with CO and CS: differentiating properties. Molecular Physics, 2019, 117, 1117-1127.	1.7	14
16	Reaction of ClF and Cl2 with PH2X: The oxidation of P(III) to P(V). Chemical Physics Letters, 2019, 715, 190-194.	2.6	4
17	Hydrogen and Halogen Bonding in Cyclic FH_(4-n):FCl_n Complexes, for n = 0â€“4. Journal of Physical Chemistry A, 2018, 122, 2587-2597.	2.5	16
18	Complexes of O=C=S with Nitrogen Bases: Chalcogen Bonds, Tetrel Bonds, and Other Secondary Interactions. ChemPhysChem, 2018, 19, 1886-1894.	2.1	24

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19	Using protonation to change a Clâ‹¯N halogen bond in N-Base:ClOH complexes to a Clâ‹¯O halogen bond. Chemical Physics Letters, 2018, 710, 123-128.	2.6	10
20	Complexes of CO2 with the Azoles: Tetrel Bonds, Hydrogen Bonds and Other Secondary Interactions. Molecules, 2018, 23, 906.	3.8	35
21	Lone-Pair Hole on P: PÂ·Â·Â·N Pnicogen Bonds Assisted by Halogen Bonds. Journal of Physical Chemistry A, 2017, 121, 1362-1370.	2.5	31
22	Borylene as an electron-pair donor for Pâ€¦B pnicogen bonds. Structural Chemistry, 2017, 28, 1419-1427.	2.0	16
23	Hydrogen-bonded complexes with carbenes as electron-pair donors. Chemical Physics Letters, 2017, 675, 46-50.	2.6	20
24	Carbenes as Electron-Pair Donors To CO₂ for CÂ·Â·Â·C Tetrel Bonds and Câ€“C Covalent Bonds. Journal of Physical Chemistry A, 2017, 121, 4039-4047.	2.5	48
25	Carbenes as Electronâ€Pair Donors for Pâ‹…â‹…â‹…C Pnicogen Bonds. ChemPhysChem, 2017, 18, 1597-1610.	2.1	24
26	Azines as Electron-Pair Donors to CO₂ for NÂ·Â·Â·C Tetrel Bonds. Journal of Physical Chemistry A, 2017, 121, 8017-8025.	2.5	35
27	The halogen bond in solution: general discussion. Faraday Discussions, 2017, 203, 347-370.	3.2	5
28	Computational approaches and sigma-hole interactions: general discussion. Faraday Discussions, 2017, 203, 131-163.	3.2	17
29	Beyond the halogen bond: general discussion. Faraday Discussions, 2017, 203, 227-244.	3.2	2
30	Solid-state chemistry and applications: general discussion. Faraday Discussions, 2017, 203, 459-483.	3.2	2
31	Carbonâ€“Carbon Bonding between Nitrogen Heterocyclic Carbenes and CO₂. Journal of Physical Chemistry A, 2017, 121, 8136-8146.	2.5	45
32	Using one halogen bond to change the nature of a second bond in ternary complexes with Pâ‹¯Cl and Fâ‹¯Cl halogen bonds. Faraday Discussions, 2017, 203, 29-45.	3.2	17
33	Halogen bonding with carbene bases. Chemical Physics Letters, 2017, 685, 338-343.	2.6	16
34	Halogen Bonding Involving CO and CS with Carbon as the Electron Donor. Molecules, 2017, 22, 1955.	3.8	14
35	H2XP:OH2 Complexes: Hydrogen vs. Pnicogen Bonds. Crystals, 2016, 6, 19.	2.2	21
36	B4H4and B4(CH3)4as Unique Electron Donors in Hydrogen-Bonded and Halogen-Bonded Complexes. Journal of Physical Chemistry A, 2016, 120, 5745-5751.	2.5	18

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37	Using (FH)2 and (FH)3 to Bridge the Ïƒ-Hole and the Lone Pair at P in Complexes with H2 XP, for X=CH3 , OH, H, CCH, F, Cl, NC, and CN. ChemPhysChem, 2016, 17, 1475-1485.	2.1	3
38	Anionic complexes of Fâ˜' and Clâ˜' with substituted methanes: Hydrogen, halogen, and tetrel bonds. Chemical Physics Letters, 2016, 655-656, 115-119.	2.6	40
39	Boron as an Electronâ€Pair Donor for Bâ‹…â‹…â‹…Cl Halogen Bonds. ChemPhysChem, 2016, 17, 3112-3119.	2.1	26
40	Unusual acidâ€"base properties of the P₄ molecule in hydrogen-, halogen-, and pnicogen-bonded complexes. Physical Chemistry Chemical Physics, 2016, 18, 32593-32601.	2.8	19
41	Properties of cationic pnicogen-bonded complexes F₄₋_nH_nP⁺:N-base with Hâ€"PÂ·Â·Â·N linear andn= 1â€"4. Molecular Physics, 2016, 114, 102-117.	1.7	13
42	The Pnicogen Bond in Review: Structures, Binding Energies, Bonding Properties, and Spin-Spin Coupling Constants of Complexes Stabilized by Pnicogen Bonds. Challenges and Advances in Computational Chemistry and Physics, 2015, , 191-263.	0.6	59
43	Properties of Cationic Pnicogen-Bonded Complexes F4â€"nHnP+:N-Base with Fâ€"PÂ·Â·Â·N Linear andn= 0â€"3. Journal of Physical Chemistry A, 2015, 119, 5853-5864.	2.5	44
44	PÂ·Â·Â·N Pnicogen Bonds in Cationic Complexes of F4P+and F3HP+with Nitrogen Bases. Journal of Physical Chemistry A, 2015, 119, 3125-3133.	2.5	38
45	Can HNî€NH, FNî€NH, or HNî€CHOH bridge the Ïƒ-hole and the lone pair at P in binary complexes with H2XP, for X = F, Cl, NC, OH, CN, CCH, CH3, and H?. Physical Chemistry Chemical Physics, 2015, 17, 30729-30735.	2.8	16
46	Exploring the PX3:NCH and PX3:NH3 potential surfaces, with X = F, Cl, and Br. Chemical Physics Letters, 2015, 641, 84-89.	2.6	29
47	Exploring the (H₂Câ€¢PH₂)⁺:N-Base Potential Surfaces: Complexes Stabilized by Pnicogen, Hydrogen, and Tetrel Bonds. Journal of Physical Chemistry A, 2015, 119, 11701-11710.	2.5	26
48	Using beryllium bonds to change halogen bonds from traditional to chlorine-shared to ion-pair bonds. Physical Chemistry Chemical Physics, 2015, 17, 2259-2267.	2.8	49
49	Substituent Effects on the Properties of Pnicogen-Bonded Complexes H₂XP:PYH₂, for X, Y = F, Cl, OH, NC, CCH, CH₃, CN, and H. Journal of Physical Chemistry A, 2015, 119, 224-233.	2.5	37
50	Pnicogen-Bonded Complexes H_nF_{5â€"n}P:N-Base, for n = 0â€"5. Journal of Physical Chemistry A, 2014, 118, 10144-10154.	2.5	35
51	Ïƒâ€"Ïƒ and Ïƒâ€"Ï€ pnicogen bonds in complexes H2XP:PCX, for XÂ=ÂF, Cl, OH, NC, CN, CCH, CH3, and H. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	25
52	Ramsey terms for two-, three-, and four-bond coupling involving¹⁵N and¹⁷O in hydrogen-bonded and nonhydrogen-bonded systems: are coupling constants sensitive to RAHBs?. Molecular Physics, 2014, 112, 107-116.	1.7	12
53	Pnicogen-Bonded Anionic Complexes. Journal of Physical Chemistry A, 2014, 118, 3386-3392.	2.5	68
54	Characterizing Traditional and Chlorine-Shared Halogen Bonds in Complexes of Phosphine Derivatives with ClF and Cl₂. Journal of Physical Chemistry A, 2014, 118, 4222-4231.	2.5	34

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55	Pnicogen Bonds between Xâ•PH₃ (X = O, S, NH, CH₂) and Phosphorus and Nitrogen Bases. Journal of Physical Chemistry A, 2014, 118, 1527-1537.	2.5	77
56	Influence of Substituent Effects on the Formation of PÂ·Â·Â·Cl Pnicogen Bonds or Halogen Bonds. Journal of Physical Chemistry A, 2014, 118, 2360-2366.	2.5	75
57	Characterizing Complexes with Pnicogen Bonds Involving sp² Hybridized Phosphorus Atoms: (H₂Câ•PX)₂ with X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂. Journal of Physical Chemistry A, 2013, 117, 6893-6903.	2.5	65
58	Pnicogen Bonded Complexes of PO₂X (X = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2013, 117, 10497-10503.	2.5	129
59	Exploring (NH₂F)₂, H₂FP:NFH₂, and (PH₂F)₂ Potential Surfaces: Hydrogen Bonds or Pnicogen Bonds?. Journal of Physical Chemistry A, 2013, 117, 183-191.	2.5	81
60	John Pople: The Man and His Science. ACS Symposium Series, 2013, , 301-315.	0.5	0
61	Phosphorus As a Simultaneous Electron-Pair Acceptor in Intermolecular PÂ·Â·Â·N Pnicogen Bonds and Electron-Pair Donor to Lewis Acids. Journal of Physical Chemistry A, 2013, 117, 3133-3141.	2.5	66
62	Pnicogen-Bonded Cyclic Trimers (PH₂X)₃ with X = F, Cl, OH, NC, CN, CH₃, H, and BH₂. Journal of Physical Chemistry A, 2013, 117, 4981-4987.	2.5	94
63	Properties of Complexes H₂Câ•(X)P:PXH₂, for X = F, Cl, OH, CN, NC, CCH, H, CH₃, and BH₂: PÂ·Â·Â·P Pnicogen Bonding at Ïƒ-Holes and Ï€-Holes. Journal of Physical Chemistry A, 2013, 117, 11592-11604.	2.5	67
64	Multinuclear NMR Characterization of Cyanuric Fluoride (2,4,6â€Trifluoroâ€1,3,5â€triazine). Journal of Heterocyclic Chemistry, 2012, 49, 1257-1259.	2.6	25
65	Interplay of Fâ€“H^{...}F Hydrogen Bonds and P^{...}N Pnicogen Bonds. Journal of Physical Chemistry A, 2012, 116, 9205-9213.	2.5	90
66	Structures, Binding Energies, and Spinâ€“Spin Coupling Constants of Geometric Isomers of Pnicogen Homodimers (PHFX)₂, X = F, Cl, CN, CH₃, NC. Journal of Physical Chemistry A, 2012, 116, 3056-3060.	2.5	79
67	Influence of Hydrogen Bonds on the PÂ·Â·Â·P Pnicogen Bond. Journal of Chemical Theory and Computation, 2012, 8, 2320-2327.	5.3	106
68	FCl:PCX Complexes: Old and New Types of Halogen Bonds. Journal of Physical Chemistry A, 2012, 116, 2300-2308.	2.5	51
69	Variations in the structures and binding energies of binary complexes with HBO. Chemical Physics Letters, 2012, 538, 5-9.	2.6	5
70	Homo- and heterochiral dimers (PHFX)2, X=Cl, CN, CH3, NC: To what extent do they differ?. Chemical Physics Letters, 2012, 538, 14-18.	2.6	58
71	Proton-bound homodimers involving second-row atoms. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	7
72	The boronâ€“boron single bond in diborane(4) as a non-classical electron donor for hydrogen bonding. Physical Chemistry Chemical Physics, 2011, 13, 14026.	2.8	33

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73	Structures, Energies, Bonding, and NMR Properties of Pnicogen Complexes H₂XP:NXH₂(X â••H, CH₃, NH₂, OH, F, Cl). Journal of Physical Chemistry A, 2011, 115, 13724-13731.	2.5	170
74	Ab Initio Study of Ternary Complexes X:(HCNH)⁺:Z with X, Z = NCH, CNH, FH, ClH, and FCl: Diminutive Cooperative Effects on Structures, Binding Energies, and Spinâ€“Spin Coupling Constants Across Hydrogen Bonds. Journal of Physical Chemistry A, 2011, 115, 12677-12687.	2.5	22
75	Structures, Energies, and Spinâ€“Spin Coupling Constants of Methyl-Substituted 1,3-Diborata-2,4-diphosphoniocyclobutanes: Four-member Bâ€“Pâ€“Bâ€“P Rings B2P2(CH3)nH8â€“n, withn= 0, 1, 2, 4. Journal of Physical Chemistry A, 2011, 115, 10502-10510.	2.5	1
76	Structures, Energies, and Spinâ^'Spin Coupling Constants of Fluoro-Substituted 1,3-Diborata-2,4-diphosphoniocyclobutanes: Four-Member Bâ^'Pâ^'Bâ^'P Rings B2P2FnH8â^'nwithn= 0, 1, 2, 4. Journal of Physical Chemistry A, 2011, 115, 4511-4520.	2.5	5
77	An ab initio study of cooperative effects in ternary complexes X:CNH:Z with X, Z=CNH, FH, ClH, FCl, and HLi: structures, binding energies, and spinâ€“spin coupling constants across intermolecular bonds. Physical Chemistry Chemical Physics, 2011, 13, 13951.	2.8	40
78	31Pâ€“31P spinâ€“spin coupling constants for pnicogen homodimers. Chemical Physics Letters, 2011, 512, 184-187.	2.6	132
79	Do nitrogen bases form chlorine-shared and ion-pair halogen bonds?. Chemical Physics Letters, 2011, 508, 6-9.	2.6	24
80	Ab Initio EOM-CCSD Investigation of One-Bond Câ^'C, Nâ^'C, and Nâ^'N Spinâ^'Spin Coupling Constants in Fluoroazines. Journal of Physical Chemistry A, 2010, 114, 5205-5210.	2.5	7
81	Prebiotic Selection of the AT Base-Pair?. ACS Symposium Series, 2010, , 95-107.	0.5	1
82	An ab initio investigation of the properties of H2:HX hydrogen-bonded complexes. Chemical Physics Letters, 2010, 489, 159-163.	2.6	24
83	New Insights into Factors Influencing Bi¿N Bonding in X:BH₃â^'n</sub>F_nand X:BH₃â^'n</sub>Cl_nfor X=N₂, HCN, LiCN, H₂CNH, NF₃, NH₃andn=0â€“3: The Importance of Deformation. Chemistry - A European Journal, 2010, 16, 11897-11905.	3.3	39
84	Difluorobenzenes revisited: an experimental and theoretical study of spinâ€“spin coupling constants for 1,2â€; 1,3â€; and 1,4â€difluorobenzene. Magnetic Resonance in Chemistry, 2010, 48, 68-73.	1.9	14
85	Do Traditional, Chlorine-shared, and Ion-pair Halogen Bonds Exist? An ab Initio Investigation of FCl:CNX Complexes. Journal of Physical Chemistry A, 2010, 114, 12958-12962.	2.5	81
86	Probing ¹J(Câ^'F) and ⁿJ(Fâ^'F) Spinâ^'Spin Coupling Constants for Fluoroazines: An Ab Initio Theoretical Investigation. Journal of Physical Chemistry A, 2010, 114, 2637-2643.	2.5	19
87	Two-, three-, and four-bond Nâ€“F spinâ€“spin coupling constants in fluoroazines. Molecular Physics, 2010, 108, 1367-1373.	1.7	9
88	Ab Initio Study of Nonadditivity Effects: Spinâ^'Spin Coupling Constants for Tetrafluoroethene in Ternary Ï€ Complexes. Journal of Physical Chemistry A, 2010, 114, 3713-3717.	2.5	4
89	Ab Initio Study of Ternary Complexes AÂ·Â·Â·NCHÂ·Â·Â·C with A,C = HCN, HF, HCl, ClF, and LiH: Energetics and Spinâ^'Spin Coupling Constants across Intermolecular Bonds. Journal of Physical Chemistry A, 2010, 114, 8463-8473.	2.5	26
90	Structural and Electronic Effects on One-Bond Spinâ^'Spin Coupling Constants1J(Bâ^'N),1J(Bâ^'H), and1J(Bâ^'F) for Complexes of Nitrogen Bases with BH3and Its Fluoro-Substituted Derivatives. Journal of Physical Chemistry A, 2010, 114, 12775-12779.	2.5	8

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91	Do corresponding coupling constants in hydrogen-bonded homo- and hetero-chiral dimers differ?. Canadian Journal of Chemistry, 2010, 88, 694-699.	1.1	7
92	A theoretical study of diborenes HLB=BLH for L=CO, NH3, OH2, PH3, SH2, ClH: structures, energies, and spinâ€“spin coupling constants. Theoretical Chemistry Accounts, 2009, 124, 187-195.	1.4	10
93	Comparison of methods for determining the correlation contribution to hydrogen bond energies. International Journal of Quantum Chemistry, 2009, 36, 445-452.	2.0	1
94	An Ab Initio Study of the Structures and Selected Properties of 1,2-Dihydro-1,2-azaborine and Related Molecules. Journal of Chemical Theory and Computation, 2009, 5, 2239-2247.	5.3	46
95	What factors determine whether a proton-bound homodimer has a symmetric or an asymmetric hydrogen bond?. Molecular Physics, 2009, 107, 1095-1105.	1.7	28
96	Characterizing Complexes with Fâ^'LiÂ·Â·Â·N, Hâ^'LiÂ·Â·Â·N, and CH3LiÂ·Â·Â·N Lithium Bonds: Structures, Binding Energies, and Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2009, 113, 10327-10334.	2.5	18
97	Characterizing Complexes with Fâ^'Li⁺â^'F Lithium Bonds: Structures, Binding Energies, and Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2009, 113, 8359-8365.	2.5	8
98	Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spinâ^'Spin Coupling Constants for Molecules with C, N, and O Double and Triple Bonds and Selected F-Substituted Derivatives. Journal of Chemical Theory and Computation, 2009, 5, 208-216.	5.3	41
99	A Systematic Comparison of Second-Order Polarization Propagator Approximation and Equation-of-Motion Coupled Cluster Singles and Doubles Câ^'C, Câ^'N, Nâ^'N, Câ^'H, and Nâ^'H Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2009, 113, 12411-12420.	2.5	29
100	Spinâ€“spin coupling across intramolecular Nï£¿H⁺ï£¿N hydrogen bonds in models for proton sponges: an ab initio investigation. Magnetic Resonance in Chemistry, 2008, 46, 457-463.	1.9	18
101	Resolving an apparent discrepancy between theory and experiment: spinâ€“spin coupling constants for FCCF. Magnetic Resonance in Chemistry, 2008, 46, 1003-1006.	1.9	27
102	19Fâ€“19F and 19Fâ€“1H spinâ€“spin coupling constants in cyclic FH polymers (FH)n, n=2â€“6. Solid State Nuclear Magnetic Resonance, 2008, 34, 86-92.	2.3	14
103	Spinâ^'Spin Coupling across Intermolecular Fâ^'ClÂ·Â·Â·N Halogen Bonds. Journal of Physical Chemistry A, 2008, 112, 7925-7929.	2.5	40
104	Ab Initio EOM-CCSD Spinâ^'Spin Coupling Constants for Hydrogen-Bonded Formamide Complexes: Bridging Complexes with NH3, (NH3)2, H2O, (H2O)2, FH, and (FH)2. Journal of Physical Chemistry A, 2008, 112, 6338-6343.	2.5	18
105	A Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOMâ^'CCSD) Spinâ^'Spin Coupling Constants for Selected Singly Bonded Molecules, and the Hydrides NH₃, H₂O, and HF and Their Protonated and Deprotonated Ions and Hydrogen-Bonded Complexes. Journal of Chemical Theory and Computation, 2008, 4, 967-973.	5.3	48
106	Structures, Bonding, and One-Bond Bâ^'N and Bâ^'H Spinâ^'Spin Coupling Constants for a Series of Neutral and Anionic Five-Membered Rings Containing BN Bonds. Journal of Chemical Theory and Computation, 2008, 4, 1869-1876.	5.3	5
107	Spin-spin coupling constants for water polymers and hydronium ion complexes with water. Molecular Physics, 2008, 106, 1461-1471.	1.7	5
108	HCâ‹®P and H₃Câ^'Câ‹®P as Proton Acceptors in Protonated Complexes Containing Two Phosphorus Bases:â€‰ Structures, Binding Energies, and Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2007, 111, 9924-9930.	2.5	14

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109	Spinâ^'Spin Coupling Constants for Iminoboranes RBNH, HBNR, and RBNR and Comparisons with Corresponding Isoelectronic Acetylenes RCCH and RCCR, for R = H, CH3, NH2, OH, and F. Journal of Chemical Theory and Computation, 2007, 3, 549-556.	5.3	8
110	Can Changes in One-bond Spinâ^'spin Coupling Constants in Acids Be Related to Gas-Phase Proton Affinities of Bases?. Journal of Physical Chemistry A, 2007, 111, 6443-6448.	2.5	7
111	Variation of One-bond Xâ^'Y Coupling Constants1J(Xâ^'Y) and the Components of1J(Xâ^'Y) with Rotation about the Xâ^'Y Bond for Molecules HmXâ^'YHn, with X, Y =15N,17O,31P,33S:Â The Importance of Nonbonding Pairs of Electrons. Journal of Physical Chemistry A, 2007, 111, 2517-2526.	2.5	7
112	Proton-Bound Homodimers:Â How Are the Binding Energies Related to Proton Affinities?. Journal of the American Chemical Society, 2007, 129, 12197-12199.	13.7	43
113	Complexes with Nâ^'H+â^'P Hydrogen Bonds:Â Structures, Binding Energies, and Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2007, 111, 5509-5514.	2.5	3
114	Does the AÂ·T or GÂ·C Base-Pair Possess Enhanced Stability? Quantifying the Effects of CHÂ·Â·Â·O Interactions and Secondary Interactions on Base-Pair Stability Using a Phenomenological Analysis and ab Initio Calculations. Journal of the American Chemical Society, 2007, 129, 934-941.	13.7	126
115	Probing Pâ^'H+â^'P Hydrogen Bonds:Â Structures, Binding Energies, and Spinâ^'Spin Coupling Constants. Journal of Physical Chemistry A, 2007, 111, 3416-3422.	2.5	21
116	Attacking Boron Nucleophiles:â€‰ NMR Properties of Five-Membered Diazaborole Rings. Journal of Physical Chemistry A, 2007, 111, 419-421.	2.5	14
117	Unusual substituent effects on the bonding of iminoboranes. Physical Chemistry Chemical Physics, 2007, 9, 3970-3977.	2.8	31
118	Solvent effects on one-bond Bï£¿Li coupling constants in boryllithium compounds. Magnetic Resonance in Chemistry, 2007, 45, 484-487.	1.9	12
119	Probing the protonâ€transfer coordinate of complexes with Fï£¿Hâ€¦P hydrogen bonds using oneâ€•and twoâ€bond spinâ€“spin coupling constants. Magnetic Resonance in Chemistry, 2007, 45, 714-719.	1.9	20
120	An ab Initio Study of15Nâ^'11B Spinâ^'Spin Coupling Constants for Borazine and Selected Derivatives. Journal of Physical Chemistry A, 2006, 110, 9959-9966.	2.5	49
121	Karplus-Type Equations for1J(Xâ^'Y) in Molecules HmXâ^'YHn:Â (X, Y = N, O, P, S). Journal of Physical Chemistry A, 2006, 110, 12543-12545.	2.5	12
122	Systematic ab Initio Study of15Nâ^'15N and15Nâ^'1H Spinâ^'Spin Coupling Constants Across Nâ^'H+â^'N Hydrogen Bonds:Â Predicting Nâ^'N and Nâ^'H Coupling Constants and Relating Them to Hydrogen Bond Type. Journal of Physical Chemistry A, 2006, 110, 7496-7502.	2.5	38
123	Ab Initio Study of Hydrogen Bonding and Proton Transfer in 3:1 FH:NH3and FH:Collidine Complexes:Â Structures and One- and Two-Bond Coupling Constants across Hydrogen Bonds. Journal of Physical Chemistry A, 2006, 110, 1128-1133.	2.5	15
124	The structure of protonated HCP: A classical or non-classical ion?. Chemical Physics Letters, 2006, 429, 23-26.	2.6	7
125	Computed coupling constants in X(CH3)nH(4â€“n) moieties whereX =13C and15N+, andn = 0â€“4: comparisons with experimental data. Magnetic Resonance in Chemistry, 2006, 44, 698-707.	1.9	14
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