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	Extensive theoretical studies of the hydrogenâ€bonded complexes (H2O)2, (H2O)2H+, (HF)2, (HF)2H+, F2Hâ", and (NH3)2. Journal of Chemical Physics, 1986, 84, 2279-2289.	3.0	666
2	Proton affinities of ammonia, water, and hydrogen fluoride and their anions: a quest for the basis-set limit using the Dunning augmented correlation-consistent basis sets. The Journal of Physical Chemistry, 1993, 97, 107-110.	2.9	190
3	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
4	Ab initio computation of the enthalpies of some gas-phase hydration reactions. The Journal of Physical Chemistry, 1983, 87, 3279-3282.	2.9	139
5	31Pâ€"31P spinâ€"spin coupling constants for pnicogen homodimers. Chemical Physics Letters, 2011, 512, 184-187.	2.6	132
6	Pnicogen Bonded Complexes of PO₂X (X = F, Cl) with Nitrogen Bases. Journal of Physical Chemistry A, 2013, 117, 10497-10503.	2.5	129
7	Coupled-cluster calculations of the excitation energies of benzene and the azabenzenes. Journal of Chemical Physics, 1997, 106, 6051-6060.	3.0	126
8	Do coupling constants and chemical shifts provide evidence for the existence of resonance-assisted hydrogen bonds?. Molecular Physics, 2004, 102, 2563-2574.	1.7	126
9	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
10	Selfâ€Consistent Molecular Orbital Methods. X. Molecular Orbital Studies of Excited States with Minimal and Extended Basis Sets. Journal of Chemical Physics, 1971, 55, 2236-2241.	3.0	120
11	Theory of molecular interactions. III. A comparison of studies of H2O polymers using different molecularâ€orbital basis sets. Journal of Chemical Physics, 1973, 58, 3605-3608.	3.0	120
12	Theoretical Study of Open Chain Dimers and Trimers Containing CH3OH and H2O. Journal of Chemical Physics, 1971, 55, 4633-4636.	3.0	115
13	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
14	Predicted NMR Coupling Constants Across Hydrogen Bonds:â€‰ A Fingerprint for Specifying Hydrogen Bond Type?. Journal of the American Chemical Society, 2000, 122, 3560-3561.	13.7	100
15	Unraveling Environmental Effects on Hydrogen-Bonded Complexes:Â Matrix Effects on the Structures and Proton-Stretching Frequencies of Hydrogenâ"Halide Complexes with Ammonia and Trimethylamine. Journal of the American Chemical Society, 2000, 122, 2101-2115.	13.7	96
16	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
17	Theory of Molecular Interactions. II. Molecular Orbital Studies of HF Polymers Using a Minimal Slaterâ€Type Basis. Journal of Chemical Physics, 1971, 55, 2296-2299.	3.0	93
18	Ab Initio Study of the Structural, Energetic, Bonding, and IR Spectroscopic Properties of Complexes with Dihydrogen Bonds. Journal of Physical Chemistry A, 2002, 106, 9325-9330.	2.5	90

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19	Interplay of Fâ€“H^{...}F Hydrogen Bonds and P^{...}N Pnicogen Bonds. Journal of Physical Chemistry A, 2012, 116, 9205-9213.	2.5	90
20	Vibrational spectroscopy of the hydrogen bond: An ab initio quantum-chemical perspective. International Reviews in Physical Chemistry, 1999, 18, 119-162.	2.3	88
21	Molecular orbital study of the complexes (AHn)2H+ formed from ammonia, water, hydrogen fluoride, phosphine, hydrogen sulfide, and hydrogen chloride. The Journal of Physical Chemistry, 1985, 89, 3669-3674.	2.9	87
22	Hydrogen bonds between firstâ€row hydrides and acetylene. Journal of Chemical Physics, 1983, 78, 4063-4065.	3.0	84
23	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
24	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
25	What a difference a decade makes: progress in ab initio studies of the hydrogen bond. Computational and Theoretical Chemistry, 2001, 573, 11-23.	1.5	80
26	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
27	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
28	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
29	Basis set and correlation effects on computed hydrogen bond energies of the dimers (AHn)2: AHn=NH3, OH2, and FH. Journal of Chemical Physics, 1987, 86, 2110-2113.	3.0	70
30	Pnicogen-Bonded Anionic Complexes. Journal of Physical Chemistry A, 2014, 118, 3386-3392.	2.5	68
31	Nâ^'N Spinâ^'Spin Coupling Constants [2hJ(15Nâ^'15N)] Across Nâ^'HÂ·Â·Â·N Hydrogen Bonds in Neutral Complexes:Â To What Extent Does the Bonding at the Nitrogens Influence2hJN-N?. Journal of the American Chemical Society, 2000, 122, 10480-10481.	13.7	67
32	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
33	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
34	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
35	Vibrational Spectroscopic and NMR Properties of Hydrogen-Bonded Complexes:Â Do They Tell Us the Same Thing?. Journal of the American Chemical Society, 2000, 122, 4794-4797.	13.7	63
36	Molecular orbital theory of the hydrogen bond. PI electrons as proton acceptors. Chemical Physics Letters, 1974, 24, 203-207.	2.6	62

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37	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
38	Vibrational Effects on the Fâ^'F Spinâ^'Spin Coupling Constant (2hJF-F) in FHF- and FDF-. Journal of Physical Chemistry A, 2001, 105, 8399-8402.	2.5	58
39	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
40	Hydrogen bonds between hydrogen halides and unsaturated hydrocarbons. Chemical Physics Letters, 1982, 91, 185-189.	2.6	57
41	Interpreting2hJ(F,N),1hJ(H,N) and1J(F,H) in the hydrogen-bonded FH-collidine complex. Magnetic Resonance in Chemistry, 2002, 40, 767-771.	1.9	54
42	Molecular orbital theory of the hydrogen bond. XII. Amide hydrogen bonding in formamideâ€“water and formamideâ€formaldehyde systems. Journal of Chemical Physics, 1975, 62, 1961-1970.	3.0	53
43	On the Relationship between the Preferred Site of Hydrogen Bonding and Protonation. Journal of Physical Chemistry A, 2005, 109, 5509-5517.	2.5	53
44	FCl:PCX Complexes: Old and New Types of Halogen Bonds. Journal of Physical Chemistry A, 2012, 116, 2300-2308.	2.5	51
45	Cooperativity and Proton Transfer in Hydrogen-Bonded Triads. ChemPhysChem, 2005, 6, 1411-1418.	2.1	50
46	Anab initio molecular orbital study of substituted carbonyl compounds. Theoretica Chimica Acta, 1975, 36, 195-206.	0.8	49
47	15N,15N spin-spin coupling constants across N?H?N and N?H+?N hydrogen bonds: can coupling constants provide reliable estimates of N?N distances in biomolecules?. Magnetic Resonance in Chemistry, 2001, 39, S109-S114.	1.9	49
48	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
49	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
50	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
51	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
52	Hydrogen bonding: Methodology and applications to complexes of HF and HCl with HCN and CH3CN. International Journal of Quantum Chemistry, 1992, 44, 527-541.	2.0	47
53	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
54	Molecular Orbital Theory of the Hydrogen Bond. III. Dimers Containing NH2OH, H2O, HOF, and H2O. Journal of Chemical Physics, 1972, 57, 1899-1908.	3.0	45

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55	Molecular orbital theory of the hydrogen bond. X. Monosubstituted carbonyls as proton acceptors. Journal of Chemical Physics, 1975, 62, 1314-1322.	3.0	45
56	Carbonâ€“Carbon Bonding between Nitrogen Heterocyclic Carbenes and CO₂. Journal of Physical Chemistry A, 2017, 121, 8136-8146.	2.5	45
57	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
58	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
59	Two-Bond 19Fâˆ’15N Spinâˆ’Spin Coupling Constants (2hJF-N) across Fâˆ’HÂ·Â·Â·N Hydrogen Bonds. Journal of Physical Chemistry A, 2003, 107, 3121-3125.	2.5	42
60	Anab initio molecular orbital study of the structures and energies of neutral and charged bimolecular complexes of NH3 with the hydrides AHn (A = N, O, F, P, S, and Cl). Journal of Computational Chemistry, 1989, 10, 603-615.	3.3	41
61	Matrix Isolation and ab Initio Study of the Hydrogen-Bonded Complex between H2O2 and (CH3)2O. Journal of Physical Chemistry A, 2000, 104, 2033-2037.	2.5	41
62	Systematic Comparison of Second-Order Polarization Propagator Approximation (SOPPA) and Equation-of-Motion Coupled Cluster Singles and Doubles (EOM-CCSD) Spinâˆ’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
63	Molecular orbital theory of the hydrogen bond. 24. Ground-state water-uracil complexes. Journal of Computational Chemistry, 1981, 2, 188-199.	3.3	40
64	4hJ(31Pâˆ’31P) Coupling Constants through Nâˆ’H+âˆ’N Hydrogen Bonds:Â A Comparsion of Computed ab Initio and Experimental Data. Journal of Physical Chemistry A, 2000, 104, 7165-7166.	2.5	40
65	Spinâˆ’Spin Coupling across Intermolecular Fâˆ’ClÂ·Â·Â·N Halogen Bonds. Journal of Physical Chemistry A, 2008, 112, 7925-7929.	2.5	40
66	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
67	Anionic complexes of Fâˆ’ and Clâˆ’ with substituted methanes: Hydrogen, halogen, and tetrel bonds. Chemical Physics Letters, 2016, 655-656, 115-119.	2.6	40
68	Molecular orbital theory of the hydrogen bond. IV. The dimers ROHÂ·Â·Â·OCH2. Journal of Chemical Physics, 1973, 58, 3139-3145.	3.0	39
69	Basis set and correlation effects on computed positive ion hydrogen bond energies of the complexes AHnÂ· AHn+ 1+1: AHn= NH3, OH2, and FH. Journal of Computational Chemistry, 1987, 8, 810-815.	3.3	39
70	One-Bond Spinâˆ’Spin Coupling Constants of Xâˆ’1H Proton Donors in Complexes with Xâˆ’Hâˆ’Y Hydrogen Bonds, for X =13C,15N,17O, and19F:Â Predictions, Comparisons, and Relationships among1JX-H,1KX-H, and Xâˆ’H Distances. Journal of the American Chemical Society, 2004, 126, 15624-15631.	13.7	39
71	New Insights into Factors Influencing BIΣ¿N Bonding in X:BH_{3âˆ’n}F_nand X:BH_{3âˆ’n}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
72	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding: vibrational consequences of proton position in 1:1 complexes of HCl and 4-X-pyridines. Chemical Physics Letters, 1995, 247, 89-94.	2.6	38

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73	What determines the sign of the Fermi-contact contribution to the NMR spinâ€“spin coupling constant?. Chemical Physics Letters, 2003, 382, 100-105.	2.6	38
74	Systematic ab Initio Study of15Nâˆ’15N and15Nâˆ’1H Spinâˆ’Spin Coupling Constants Across Nâˆ’H+âˆ’N Hydrogen Bonds:Â Predicting Nâˆ’N and Nâˆ’H Coupling Constants and Relating Them to Hydrogen Bond Type. Journal of Physical Chemistry A, 2006, 110, 7496-7502.	2.5	38
75	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
76	Basis-set effects on computed acid-base interaction energies using the Dunning correlation-consistent polarized split-valence basis sets. Computational and Theoretical Chemistry, 1994, 307, 27-34.	1.5	37
77	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
78	Molecular orbital theory of the hydrogen bond.. Chemical Physics, 1976, 15, 463-472.	1.9	35
79	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
80	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
81	Complexes of CO2 with the Azoles: Tetrel Bonds, Hydrogen Bonds and Other Secondary Interactions. Molecules, 2018, 23, 906.	3.8	35
82	Geometry, basis set, and correlation energy dependence of computed protonation energies of carbonyl bases. Chemical Physics Letters, 1983, 94, 213-217.	2.6	34
83	An ab Initio Study of Anharmonicity and Field Effects in Hydrogen-Bonded Complexes of the Deuterated Analogues of HCl and HBr with NH3and N(CH3)3. Journal of Physical Chemistry A, 2001, 105, 3371-3378.	2.5	34
84	Computed Spinâˆ’Spin Coupling Constants (1JX-Y) in Molecules HmXâˆ’YHnfor X and Y =13C,15N, and31P:Â Comparisons with Experiment and Insights into the Signs of1JX-Y. Journal of Physical Chemistry A, 2004, 108, 3662-3667.	2.5	34
85	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
86	Predicted signs of reduced two-bond spinâ€“spin coupling constants(2hKXâ€“Y) across Xâ€”Hâ€”Y hydrogen bonds. Magnetic Resonance in Chemistry, 2004, 42, 421-423.	1.9	33
87	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
88	Molecular orbital theory of the hydrogen bond. Computational and Theoretical Chemistry, 1985, 124, 201-212.	1.5	32
89	Basis Set and Correlation Effects on Computed Lithium Ion Affinities. The Journal of Physical Chemistry, 1996, 100, 6284-6287.	2.9	32
90	3hJ(15Nâˆ’31P) Spinâˆ’Spin Coupling Constants across Nâˆ’HÂ·Â·Â·Oâˆ’P Hydrogen Bonds. Journal of the American Chemical Society, 2002, 124, 6393-6397.	13.7	32

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91	Molecular orbital theory of the hydrogen bond. XIV. Disubstituted carbonyl compounds as proton acceptors. Journal of Chemical Physics, 1975, 63, 4666-4671.	3.0	31
92	Basis set dependence of correlation corrections to protonation energies. Chemical Physics Letters, 1981, 83, 240-242.	2.6	31
93	The electronic absorption spectra of Clî—¸Oî—¸Cl and Clî—¸Clî—¸O. An ab initio EOM-CCSD(T) investigation. Chemical Physics Letters, 1995, 246, 541-545.	2.6	31
94	Relating Environmental Effects and Structures, IR, and NMR Properties of Hydrogen-Bonded Complexes:Â ClH:Pyridine. Journal of Physical Chemistry A, 2001, 105, 5442-5449.	2.5	31
95	19Fâ€“19F spinâ€“spin coupling constant surfaces for (HF)2 clusters: The orientation and distance dependence of the sign and magnitude of JFâ€“F. Journal of Chemical Physics, 2004, 120, 3237-3243.	3.0	31
96	Unusual substituent effects on the bonding of iminoboranes. Physical Chemistry Chemical Physics, 2007, 9, 3970-3977.	2.8	31
97	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
98	Molecular orbital theory of the hydrogen bond. XXIX. Waterâ€“thymine complexes. Journal of Chemical Physics, 1982, 76, 1058-1063.	3.0	30
99	Characterizing Hydrogen Bonding and Proton Transfer in 2:1 FH:NH3 and FH:Collidine Complexes through One- and Two-Bond Spinâ^'Spin Coupling Constants across Hydrogen Bonds. Journal of Physical Chemistry A, 2005, 109, 10759-10769.	2.5	30
100	Basis set and correlation effects on computed proton affinities of some oxygen and nitrogen bases. Journal of Computational Chemistry, 1985, 6, 296-301.	3.3	29
101	To What Extent Do External Fields and Vibrational and Isotopic Effects Influence NMR Coupling Constants Across Hydrogen Bonds? Two-Bond Clâ^'N Spinâ^'Spin Coupling Constants (2hJCl-N) in Model ClH:NH3Complexes. Journal of Physical Chemistry A, 2002, 106, 5385-5392.	2.5	29
102	One-Bond (1dJH-H) and Three-Bond (3dJX-M) Spinâ^'Spin Coupling Constants Across Xâ^'HÂ·Â·Â·Hâ^'M Dihydrogen Bonds. Journal of Physical Chemistry A, 2002, 106, 9331-9337.	2.5	29
103	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
104	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
105	Theoretical study of the diâ€imide (N2H2) molecule in ground andnâ†'Ï€* excited states. Journal of Chemical Physics, 1992, 96, 7573-7579.	3.0	28
106	Predicted Signs of One-Bond Spinâ^'Spin Coupling Constants (1hJH-Y) across Xâ^'Hâ^'Y Hydrogen Bonds for Complexes with Y = 15N, 17O, and 19F. Journal of Physical Chemistry A, 2004, 108, 11762-11767.	2.5	28
107	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
108	Ab initio theoretical and matrix isolation experimental studies of hydrogen bonding. IV. The HBr:pyridine complex. Journal of Molecular Structure, 1997, 436-437, 367-386.	3.6	27

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109	Base Properties of H2CO in the Excited1nâ†'Ï€* State. Journal of Physical Chemistry A, 1998, 102, 5124-5127.	2.5	27
110	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
111	Geometry, basis set, and correlation energy dependence of computed protonation energies of imino bases. Journal of Computational Chemistry, 1984, 5, 381-386.	3.3	26
112	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H2O2with Phosphorus and Sulfur Bases. Journal of Physical Chemistry A, 2001, 105, 11365-11370.	2.5	26
113	Vibrational averaging of NMR properties for an Nâ€“Hâ€“N hydrogen bond. Chemical Physics Letters, 2001, 346, 288-292.	2.6	26
114	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
115	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
116	Boron as an Electronâ€Pair Donor for Bâ‹…â‹…â‹…Cl Halogen Bonds. ChemPhysChem, 2016, 17, 3112-3119.	2.1	26
117	A quantum chemical mechanism for the water-initiated decomposition of silica. Computational Materials Science, 2003, 27, 102-108.	3.0	25
118	Two-Bond13Câ^'15N Spinâ^'Spin Coupling Constants (2hJC-N) Across Câ^'Hâ^'N Hydrogen Bondsâ€. Journal of Physical Chemistry A, 2003, 107, 3222-3227.	2.5	25
119	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
120	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
121	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H2O2with NH3and N(CH3)3. Journal of Physical Chemistry A, 2001, 105, 6430-6435.	2.5	24
122	An ab initio investigation of the properties of H2:HX hydrogen-bonded complexes. Chemical Physics Letters, 2010, 489, 159-163.	2.6	24
123	Do nitrogen bases form chlorine-shared and ion-pair halogen bonds?. Chemical Physics Letters, 2011, 508, 6-9.	2.6	24
124	Carbenes as Electronâ€Pair Donors for Pâ‹…â‹…â‹…C Pnicogen Bonds. ChemPhysChem, 2017, 18, 1597-1610.	2.1	24
125	Complexes of O=C=S with Nitrogen Bases: Chalcogen Bonds, Tetrel Bonds, and Other Secondary Interactions. ChemPhysChem, 2018, 19, 1886-1894.	2.1	24
126	Molecular orbital theory of the hydrogen bond. XI. The effect of hydrogen bonding on the nâ†'Ï€â^— transition in dimers HOHâ‹…â‹…â‹…OCHR. Journal of Chemical Physics, 1975, 62, 666.	3.0	23

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127	Matrix Isolation and ab Initio Study of 1:1 Hydrogen-Bonded Complexes of H2O2 with HF, HCl, and HBr. Journal of Physical Chemistry A, 2002, 106, 6406-6414.	2.5	23
128	Two-Bond 15Nâˆ’19F Spinâˆ’Spin Coupling Constants (2hJN-F) across Nâˆ’H+...F Hydrogen Bonds. Journal of Physical Chemistry A, 2003, 107, 3126-3131.	2.5	23
129	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
130	Intermolecular interaction in formaldehyde dimers. Journal of Chemical Physics, 1974, 60, 3812-3816.	3.0	22
131	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
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