# Malgorzata M Szczesniak

## List of Publications by Year in Descending Order



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| 134 papers | 5,161 citations | 37 h-index | 67 g-index |
| 136 ext. papers | 5,297 ext. citations | 4.6 avg, IF | 5.27 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 134 | Reassessing the Role of Holes in Noncovalent Interactions: It is Pauli Repulsion that Counts.. *Frontiers in Chemistry*, **2022**, 10, 858946 | 5 | 2 |
| 133 | Water Soluble Host–Guest Chemistry Involving Aromatic N-Oxides and Sulfonateresorcinarene. *Symmetry*, **2020**, 12, 1751 | 2.7 | 1 |
| 132 | Assessment of SAPT(DFT) with meta-GGA functionals. *Journal of Molecular Modeling*, **2020**, 26, 102 | 2 | 3 |
| 131 | On the Nature of Luminescence Thermochromism of Multinuclear Copper(I) Benzoate Complexes in the Crystalline State. *Crystals*, **2019**, 9, 36 | 2.3 | 5 |
| 130 | Assessment of Newest Meta-GGA Hybrids for Late Transition Metal Reactivity: Fractional Charge and Fractional Spin Perspective. *Journal of Physical Chemistry C*, **2019**, 123, 8047-8056 | 3.8 | 14 |
| 129 | The nature of three-body interactions in DFT: Exchange and polarization effects. *Journal of Chemical Physics*, **2017**, 147, 084106 | 3.9 | 13 |
| 128 | Employing Range Separation on the meta-GGA Rung: New Functional Suitable for Both Covalent and Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2016**, 12, 3662-73 | 6.4 | 9 |
| 127 | Noncovalent interactions determine the conformation of aurophilic complexes with 2-mercapto-4-methyl-5-thiazoleacetic acid ligands. *Dalton Transactions*, **2015**, 44, 13641-50 | 4.3 | 4 |
| 126 | Range-Separated meta-GGA Functional Designed for Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 4297-306 | 6.4 | 17 |
| 125 | Tuned range-separated hybrid functionals in the symmetry-adapted perturbation theory. *Journal of Chemical Physics*, **2014**, 141, 134120 | 3.9 | 13 |
| 124 | Density functional theory approach to gold-ligand interactions: separating true effects from artifacts. *Journal of Chemical Physics*, **2014**, 140, 244313 | 3.9 | 11 |
| 123 | Density-dependent onset of the long-range exchange: a key to donor-acceptor properties. *Journal of Physical Chemistry A*, **2013**, 117, 11580-6 | 2.8 | 18 |
| 122 | A first-principles-based correlation functional for harmonious connection of short-range correlation and long-range dispersion. *Journal of Chemical Physics*, **2012**, 137, 204121 | 3.9 | 6 |
| 121 | Optical absorption spectra of gold clusters Au(n) (n = 4, 6, 8,12, 20) from long-range corrected functionals with optimal tuning. *Journal of Chemical Physics*, **2012**, 137, 114302 | 3.9 | 52 |
| 120 | Ab initio long-range interaction and adiabatic channel capture model for ultracold reactions between the KRb molecules. *Journal of Chemical Physics*, **2012**, 137, 114305 | 3.9 | 14 |
| 119 | Interactions of ThO(X) with He, Ne and Ar from the ab initio coupled cluster and symmetry adapted perturbation theory calculations. *Chemical Physics*, **2012**, 399, 50-58 | 2.3 | 3 |
| 118 | Dispersion-free component of non-covalent interaction via mutual polarization of fragment densities. *Journal of Chemical Physics*, **2012**, 136, 204109 | 3.9 | 8 |

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| 117 | Symmetry-adapted perturbation theory based on unrestricted Kohn-Sham orbitals for high-spin open-shell van der Waals complexes. *Journal of Chemical Physics*, **2012**, 137, 164104 | 3.9 | 38 |
| 116 | Aurophilic Interactions from Wave Function, Symmetry-Adapted Perturbation Theory, and Rangehybrid Approaches. *Journal of Chemical Theory and Computation*, **2011**, 7, 2399-407 | 6.4 | 34 |
| 115 | Density functional theory approach to noncovalent interactions via monomer polarization and Pauli blockade. *Physical Review Letters*, **2010**, 104, 163001 | 7.4 | 31 |
| 114 | Electronic structure and spin coupling of the manganese dimer: The state of the art of ab initio approach. *Journal of Chemical Physics*, **2010**, 132, 024312 | 3.9 | 22 |
| 113 | A density functional theory approach to noncovalent interactions via interacting monomer densities. *Physical Chemistry Chemical Physics*, **2010**, 12, 14686-92 | 3.6 | 5 |
| 112 | Derivation of the supermolecular interaction energy from the monomer densities in the density functional theory. *Chemical Physics Letters*, **2010**, 486, 160-165 | 2.5 | 20 |
| 111 | Study of ArO- and ArO via slow photoelectron velocity-map imaging spectroscopy and Ab initio calculations. *Journal of Physical Chemistry A*, **2009**, 113, 4631-8 | 2.8 | 7 |
| 110 | Study of KrO- and KrO via slow photoelectron velocity-map imaging spectroscopy and ab initio calculations. *Journal of Physical Chemistry A*, **2009**, 113, 14439-46 | 2.8 | 7 |
| 109 | The nature of interactions between clusters of Mg and Zn with HCN from symmetry-adapted perturbation theory based of DFT. *Journal of Chemical Physics*, **2009**, 130, 224704 | 3.9 | 4 |
| 108 | Interactions and collisions of cold metal atoms in magnetic traps. *Physica Scripta*, **2009**, 80, 048109 | 2.6 | 5 |
| 107 | Europium dimer: van der Waals molecule with extremely weak antiferromagnetic spin coupling. *Journal of Chemical Physics*, **2009**, 131, 241102 | 3.9 | 10 |
| 106 | Ab initio study of the Br(2P)-HBr van der Waals complex. *Journal of Chemical Physics*, **2009**, 130, 184304 | 3.9 | 6 |
| 105 | Nonadditive interactions in ns2 and spin-polarized ns metal atom trimers. *Journal of Chemical Physics*, **2008**, 129, 134302 | 3.9 | 15 |
| 104 | Interactions of lanthanide atoms: Comparative ab initio study of YbHe, Yb 2 and TmHe, TmYb potentials. *European Physical Journal D*, **2007**, 45, 147-153 | 1.3 | 28 |
| 103 | Diffuse basis functions for small-core relativistic pseudopotential basis sets and static dipole polarizabilities of selected lanthanides La, Sm, Eu, Tm and Yb. *Structural Chemistry*, **2007**, 18, 769-772 | 1.8 | 32 |
| 102 | Interactions of transition metal atoms in high-spin states: Cr2, Sc-Cr, and Sc-Kr. *Journal of Chemical Physics*, **2007**, 127, 244302 | 3.9 | 13 |
| 101 | Interaction potentials for Br(-)-Rg (Rg=He-Rn): spectroscopy and transport coefficients. *Journal of Chemical Physics*, **2006**, 125, 64305 | 3.9 | 16 |
| 100 | Ab initio study of Tm-He interactions and dynamics in a magnetic trap. *Physical Review A*, **2006**, 74, | 2.6 | 13 |

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| 99 | van der Waals interactions and dipole polarizabilities of lanthanides: Tm(2F)-He and Yb(1S)-He potentials. *Journal of Chemical Physics*, **2006**, 124, 114301 | 3.9 | 23 |
| 98 | Interactions in open-shell clusters: ab initio study of pre-reactive complex O(3P) + HCl. *Journal of Physical Chemistry A*, **2005**, 109, 11484-94 | 2.8 | 7 |
| 97 | Interaction potentials of the RG-I anions, neutrals, and cations (RG = He, Ne, Ar). *Journal of Chemical Physics*, **2005**, 122, 194311 | 3.9 | 35 |
| 96 | Suppression of angular forces in collisions of non-S-state transition metal atoms. *Physical Review Letters*, **2005**, 94, 013202 | 7.4 | 51 |
| 95 | Paradigm pre-reactive van der Waals complexes: XHX and XH2 (X = F, Cl, Br). *International Reviews in Physical Chemistry*, **2004**, 23, 541-571 | 7 | 35 |
| 94 | Interactions of transition metal atoms with He. *European Physical Journal D*, **2004**, 31, 429-437 | 1.3 | 20 |
| 93 | Counterpoise-corrected geometries and harmonic frequencies of N-body clusters: Application to (HF)n (n=3,4). *Journal of Chemical Physics*, **2003**, 118, 537-549 | 3.9 | 46 |
| 92 | Ab initio potential energy and dipole moment surfaces, infrared spectra, and vibrational predissociation dynamics of the 35Cl2H2/D2 complexes. *Journal of Chemical Physics*, **2003**, 119, 12931-12945 | 3.9 | 43 |
| 91 | Characterization of ArnO2 clusters from ab initio and diffusion Monte Carlo calculations. *Journal of Chemical Physics*, **2003**, 118, 2748 | 3.9 | 8 |
| 90 | Modeling of the three-body effects in the Ar2O2 trimer from ab initio calculations. *Journal of Chemical Physics*, **2003**, 118, 2731 | 3.9 | 6 |
| 89 | Modeling of the Three-Body Effects in the Neutral Trimers in the Quartet State by ab initio Calculations. H3, Na3, and Na2B. *Collection of Czechoslovak Chemical Communications*, **2003**, 68, 587-626 | | 2 |
| 88 | Ab initio calculations and modeling of three-body forces in Ar2H2O. *International Journal of Quantum Chemistry*, **2002**, 90, 1215-1231 | 2.1 | |
| 87 | Ab initio calculations and modeling of three-dimensional adiabatic and diabatic potential energy surfaces of F(2P)H2(1) Van der Waals complex. *International Journal of Quantum Chemistry*, **2002**, 90, 1038-1048 | 2.1 | 11 |
| 86 | Dynamics of O(3Pj)+Rg collisions on ab initio and scattering potentials. *Journal of Chemical Physics*, **2002**, 116, 1457-1467 | 3.9 | 20 |
| 85 | Modeling of adiabatic and diabatic potential energy surfaces of Cl(2P)?H2(1+) prereactive complex from ab initio calculations. *Journal of Chemical Physics*, **2002**, 117, 4709-4719 | 3.9 | 16 |
| 84 | Ab initio simulations of the KrO2 anion photoelectron spectra. *Journal of Chemical Physics*, **2002**, 117, 2629-2634 | 3.9 | 15 |
| 83 | Ab Initio Calculations and Modeling of Three-Dimensional Adiabatic and Diabatic Potential Energy Surfaces of Br(2P)H2(1) Pre-Reactive Complex. *Journal of Physical Chemistry A*, **2002**, 106, 7362-7368 | 2.8 | 7 |
| 82 | Theoretical prediction of the ArO2 anion ZEKE photoelectron spectrum. *Chemical Physics Letters*, **2001**, 347, 415-420 | 2.5 | 4 |

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| 81 | Ab initio calculations of adiabatic and diabatic potential energy surfaces of Cl(2P)?HCl(1Σ+) van der Waals complex. *Journal of Chemical Physics*, **2001**, 115, 3085-3098 | 3.9 | 41 |
| 80 | Ab initio zero electron kinetic energy spectroscopy of the ArCl− and KrCl− anions. *Journal of Chemical Physics*, **2001**, 114, 9929-9937 | 3.9 | 20 |
| 79 | Collision and transport properties of Rg+Cl(2P) and Rg+Cl−(1S) (Rg=Ar, Kr) from ab initio potentials. *Journal of Chemical Physics*, **2001**, 114, 9919-9928 | 3.9 | 35 |
| 78 | Ab initio potential energy surface for the Ar(1S)+OH(X2Π) interaction and bound rovibrational states. *Journal of Chemical Physics*, **2000**, 112, 4952-4958 | 3.9 | 46 |
| 77 | State of the Art and Challenges of the ab Initio Theory of Intermolecular Interactions. *Chemical Reviews*, **2000**, 100, 4227-4252 | 68.1 | 451 |
| 76 | Ab initio based study of the ArO− photoelectron spectra: Selectivity of spin–orbit transitions. *Journal of Chemical Physics*, **2000**, 112, 5852-5865 | 3.9 | 31 |
| 75 | Structure and energetics of ArnNO+ clusters from ab initio calculations. *Journal of Chemical Physics*, **2000**, 112, 10895-10904 | 3.9 | 7 |
| 74 | The nature of Van der Waals bond. *Theoretical and Computational Chemistry*, **1999**, 6, 665-699 | | 1 |
| 73 | A three-dimensional potential energy surface for He+Cl2 (B 3Πu+): Ab initio calculations and a multiproperty fit. *Journal of Chemical Physics*, **1999**, 111, 997-1007 | 3.9 | 41 |
| 72 | Many-body exchange effects in clusters of rare gases with a chromophore: He2CO2. *Chemical Physics*, **1998**, 239, 573-591 | 2.3 | 6 |
| 71 | RG+Cl(2P) (RG=He, Ne, Ar) interactions: Ab initio potentials and collision properties. *Journal of Chemical Physics*, **1998**, 109, 2144-2154 | 3.9 | 36 |
| 70 | Ab initio study of the van der Waals interaction of NH(X 3Σ−) with Ar(1S). *Journal of Chemical Physics*, **1998**, 108, 3235-3242 | 3.9 | 37 |
| 69 | From Intermolecular Interactions to Incipient Chemical Bond. *Collection of Czechoslovak Chemical Communications*, **1998**, 63, 1473-1484 | | 10 |
| 68 | The effect of two- and three-body interactions in ArnCO2 (n=1,2) on the asymmetric stretching CO2 coordinate: An ab initio study. *Journal of Chemical Physics*, **1997**, 106, 10215-10221 | 3.9 | 20 |
| 67 | Ab initio calculations of the interaction of He with the B 3Πu+ state of Cl2 as a function of the Cl2 internuclear separation. *Journal of Chemical Physics*, **1997**, 106, 2685-2694 | 3.9 | 37 |
| 66 | Origins and modeling of many-body exchange effects in van der Waals clusters. *Journal of Chemical Physics*, **1997**, 106, 3301-3310 | 3.9 | 20 |
| 65 | Ab initio study of the O2(X 3Σg−)+Ar(1S) van der Waals interaction. *Journal of Chemical Physics*, **1997**, 106, 7731-7737 | 3.9 | 24 |
| 64 | Ar?C2H2: a challenging system for ab initio calculations. *Journal of Molecular Structure*, **1997**, 436-437, 387-400 | 3.4 | 14 |

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| 63 | Ab Initio Study of Nonadditive Effects in the (H2O)2H2 Cluster. *The Journal of Physical Chemistry*, **1996**, 100, 10875-10881 | | 4 |
| 62 | Ab initio study of van der Waals interaction of formamide with a nonpolar partner. Ar???H2NCOH complex. *Journal of Chemical Physics*, **1996**, 105, 8213-8222 | 3.9 | 5 |
| 61 | Ab initio study of the He(1S)+CH(X 2) interaction. *Journal of Chemical Physics*, **1996**, 105, 9525-9535 | 3.9 | 23 |
| 60 | Ab initio study of van der Waals interaction of CO2 with Ar. *Journal of Chemical Physics*, **1996**, 104, 6569-6576 | 3.9 | 67 |
| 59 | Ab initio study of the O2(X 3g)+He(1S) van der Waals cluster. *Journal of Chemical Physics*, **1996**, 104, 7997-8002 | 3.9 | 34 |
| 58 | Partitioning of interaction energy in van der Waals complexes involving excited state species: The He(1S)+Cl2(B 3u) interaction. *Journal of Chemical Physics*, **1995**, 103, 10116-10127 | 3.9 | 46 |
| 57 | Towards an analytical three-body potential of Ar2Cl *Journal of Chemical Physics*, **1995**, 103, 299-308 | 3.9 | 22 |
| 56 | On the role of bond functions in interaction energy calculations: Ar???HCl, Ar???H2O, (HF)2. *Journal of Chemical Physics*, **1995**, 103, 1498-1507 | 3.9 | 78 |
| 55 | Comment on A possible definition of basis set superposition error *Chemical Physics Letters*, **1995**, 241, 140-145 | 2.5 | 23 |
| 54 | Ab initio study of He(1S)+Cl2(X 1g,3u) potential energy surfaces. *Journal of Chemical Physics*, **1994**, 101, 6800-6809 | 3.9 | 33 |
| 53 | Supermolecular approach to many-body dispersion interactions in weak van der Waals complexes: He, Ne, and Ar trimers. *Journal of Chemical Physics*, **1994**, 101, 8860-8869 | 3.9 | 54 |
| 52 | On the nature of the interaction energy in the Ar-Cl2 complex. *Computational and Theoretical Chemistry*, **1994**, 307, 187-199 | | 24 |
| 51 | Origins of Structure and Energetics of van der Waals Clusters from ab Initio Calculations. *Chemical Reviews*, **1994**, 94, 1723-1765 | 68.1 | 736 |
| 50 | The complex of N2 with H2O, D2O, and HDO: A combined ab initio and diffusion Monte Carlo study. *Journal of Chemical Physics*, **1994**, 101, 1378-1391 | 3.9 | 60 |
| 49 | Ab initio study of nonadditive interactions in the Ar2HF and Ar2HCl clusters. II. Analysis of exchange and induction effects. *Journal of Chemical Physics*, **1994**, 101, 10708-10716 | 3.9 | 30 |
| 48 | Ab initio study of the potential energy surface of CH4-H2O. *Journal of Chemical Physics*, **1993**, 98, 3078-3089 | 3.9 | 95 |
| 47 | Ab initio study of the H2COAr complex. *Journal of Chemical Physics*, **1993**, 99, 5211-5218 | 3.9 | 10 |
| 46 | The nonadditive interactions in the Ar2HF and Ar2HCl clusters: An ab initio study. *Journal of Chemical Physics*, **1993**, 99, 6732-6741 | 3.9 | 46 |

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| 45 | On the nature of the interaction energy in the Ar□ClF complex. *Journal of Chemical Physics*, **1993**, 99, 3700-3706 | 3.9 | 22 |
| 44 | Proton-donor properties of water and ammonia in van der Waals complexes. Be□H2O and Be□NH3. *Journal of Chemical Physics*, **1993**, 98, 7020-7028 | 3.9 | 4 |
| 43 | Helium atom as a probe of molecular shape and properties: He?H2O complex. *Journal of Molecular Structure*, **1993**, 297, 313-325 | 3.4 | 17 |
| 42 | Intermolecular potential of H2O???H2 in the van der Waals region. An ab initio study. *Journal of Chemical Physics*, **1992**, 96, 6039-6047 | 3.9 | 36 |
| 41 | Proton□donor properties of water and ammonia in van der Waals complexes with rare-gas atoms. Kr□H2O and Kr□NH3. *Journal of Chemical Physics*, **1992**, 97, 8181-8187 | 3.9 | 28 |
| 40 | Analysis of the intermolecular potential of Ar□CH4: An ab initio study. *Journal of Chemical Physics*, **1992**, 96, 463-469 | 3.9 | 37 |
| 39 | Ab initio study of intermolecular potential for ArHCl. *Journal of Chemical Physics*, **1991**, 94, 6677-6685 | 3.9 | 57 |
| 38 | Ab initio study of the nonadditive effects in the trimer of ammonia. *Journal of Chemical Physics*, **1991**, 95, 5169-5178 | 3.9 | 35 |
| 37 | Ab initio study of the intermolecular potential of Ar□H2O. *Journal of Chemical Physics*, **1991**, 94, 2807-2816 | 3.9 | 78 |
| 36 | Ab initio study of intermolecular potential of H2O trimer. *Journal of Chemical Physics*, **1991**, 94, 2873-2883 | 3.9 | 138 |
| 35 | Intermolecular potential of the methane dimer and trimer. *Journal of Chemical Physics*, **1990**, 93, 4243-4253 | 3.9 | 81 |
| 34 | Calculations of nonadditive effects by means of supermolecular Mo/ller□lesset perturbation theory approach: Ar3 and Ar4. *Journal of Chemical Physics*, **1990**, 92, 2481-2487 | 3.9 | 97 |
| 33 | Potential energy surface for dispersion interaction in water dimer and hydrogen fluoride dimer. *The Journal of Physical Chemistry*, **1990**, 94, 1781-1788 | | 44 |
| 32 | Nonadditive effects in HF and HCl trimers. *Journal of Chemical Physics*, **1989**, 91, 7048-7056 | 3.9 | 113 |
| 31 | Analysis of the potential energy surface of Ar□NH3. *Journal of Chemical Physics*, **1989**, 91, 7809-7817 | 3.9 | 74 |
| 30 | Anisotropy of correlation effects in hydrogen-bonded systems: the HF dimer. *Chemical Physics Letters*, **1989**, 161, 532-538 | 2.5 | 6 |
| 29 | Structures and energies of the lithiated silanes. *Journal of the Chemical Society Perkin Transactions II*, **1989**, 131-135 | | 3 |
| 28 | Vibrational frequencies and intensities of H-bonded and Li-bonded complexes. H3N??HCl and H3N??LiCl. *Journal of Chemical Physics*, **1988**, 89, 3131-3138 | 3.9 | 39 |

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|---|---|---|---|
| 27 | Theoretical vibrational study of the FX???O(CH3)2 hydrogen-bonded complex. *Journal of Chemical Physics*, **1988**, 88, 4861-4866 | 3.9 | 18 |
| 26 | On the connection between the supermolecular Møller-Plesset treatment of the interaction energy and the perturbation theory of intermolecular forces. *Molecular Physics*, **1988**, 63, 205-224 | 1.7 | 291 |
| 25 | Accurate evaluation of SCF and MP2 components of interaction energies. Complexes of HF, OH2, and NH3 with Li+. *Collection of Czechoslovak Chemical Communications*, **1988**, 53, 2214-2229 | | 26 |
| 24 | Vibrational frequencies and intensities of H-bonded systems. 1:1 and 1:2 complexes of NH3 and PH3 with HF. *Journal of Chemical Physics*, **1987**, 87, 2214-2224 | 3.9 | 28 |
| 23 | Effect of secondary basis-set superposition error upon calculated vibrational intensities. *Chemical Physics Letters*, **1986**, 131, 230-236 | 2.5 | 16 |
| 22 | Ab initio study of structure and cooperativity in ammonia-hydrogen fluoride-hydrogen fluoride and phosphine-hydrogen fluoride-hydrogen fluoride. *The Journal of Physical Chemistry*, **1986**, 90, 4253-4258 | | 46 |
| 21 | Correction of the basis set superposition error in SCF and MP2 interaction energies. The water dimer. *Journal of Chemical Physics*, **1986**, 84, 6328-6335 | 3.9 | 124 |
| 20 | Effects of external ions on the energetics of proton transfers across hydrogen bonds. *The Journal of Physical Chemistry*, **1985**, 89, 262-266 | | 49 |
| 19 | Theoretical studies of lithium bonding in lithium chloride/aliphatic amine complexes. *Chemical Physics*, **1985**, 94, 55-63 | 2.3 | 18 |
| 18 | Effects of external ions on the dynamics of proton transfer across a hydrogen bond. *The Journal of Physical Chemistry*, **1985**, 89, 1835-1840 | | 33 |
| 17 | Contribution of dispersion to the properties of H2S--HF and H2S--HCl. *Journal of Chemical Physics*, **1985**, 83, 1778-1783 | 3.9 | 17 |
| 16 | Interactions between aromatic systems: dimers of benzene and s-tetrazine. *The Journal of Physical Chemistry*, **1984**, 88, 1726-1730 | | 83 |
| 15 | The methylation effect in amine...HF hydrogen-bonded systems. Quantum chemical and statistical thermodynamic study. *The Journal of Physical Chemistry*, **1984**, 88, 5923-5927 | | 14 |
| 14 | Studies of dispersion energy in hydrogen-bonded systems. H2O⋯HOH, H2O⋯HF, H3N⋯HF, HF⋯HF. *Journal of Chemical Physics*, **1984**, 80, 1535-1542 | 3.9 | 34 |
| 13 | Theoretical study of H2O⋯HF and H2O⋯HCl: Comparison with experiment. *Journal of Chemical Physics*, **1984**, 81, 5024-5030 | 3.9 | 79 |
| 12 | Ab initio study of proton transfers including effects of electron correlation. *International Journal of Quantum Chemistry*, **1983**, 23, 739-751 | 2.1 | 56 |
| 11 | Search for simplified procedure for the evaluation of the Gibbs free energy of hydrogen-bond formation. *The Journal of Physical Chemistry*, **1983**, 87, 2608-2614 | | 7 |
| 10 | Møller⋯Plesset treatment of electron correlation effects in (HOHOH)□ *Journal of Chemical Physics*, **1982**, 77, 4586-4593 | 3.9 | 58 |

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| 9 | HF-ClF: minima on the 4-31G and 4-31G* energy hypersurfaces and thermodynamics of formation. *Chemical Physics Letters*, **1981**, 82, 469-472 | 2.5 | 17 |
| 8 | Nonadditivity of the SCF interaction energy in the (LiH)3 complex. *International Journal of Quantum Chemistry*, **1980**, 17, 1069-1074 | 2.1 | 3 |
| 7 | Properties of strong hydrogen-bonded systems. *Chemical Physics Letters*, **1980**, 72, 115-118 | 2.5 | 12 |
| 6 | SCF ab initio study of lithium-bonded complexes. *Chemical Physics Letters*, **1980**, 74, 243-247 | 2.5 | 24 |
| 5 | HF-HCl: stationary points on the scf energy hypersurface and thermodynamics of formation. *Chemical Physics Letters*, **1980**, 74, 248-251 | 2.5 | 23 |
| 4 | Properties of strong hydrogen-bonded systems. II. Ab initioSCF-MO study of the hydrogen bond between nitric acid and ammonia. *Journal of Computational Chemistry*, **1980**, 1, 417-419 | 3.5 | 17 |
| 3 | Ab initio calculations on the lithium fluoride–ethylene complex. *Journal of Chemical Physics*, **1977**, 67, 5400-5401 | 3.9 | 13 |
| 2 | Studies on the lithium bond. *Chemical Physics Letters*, **1976**, 44, 465-467 | 2.5 | 20 |
| 1 | Hydrogen bonding of water, hydrogen sulphide and related acceptors with electron donors. *Journal of Molecular Structure*, **1976**, 30, 271-290 | 3.4 | 11 |