# Ajit J Thakkar

List of Publications by Year
in descending order

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| 272 | 7,624 | 47006 | 88630 |
|---|---|---|---|
| papers | citations | 47 h-index | 70 g-index |

| 286 | 286 | 286 | 2625 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Intermolecular forces via hybrid Hartreeâ€“Fockâ€“SCF plus damped dispersion (HFD) energy calculations. An improved spherical model. Journal of Chemical Physics, 1982, 76, 3057-3063. | 3.0 | 298 |
| 2 | Compact and accurate integral-transform wave functions. I. The1S1state of the helium-like ions fromHâ^'throughMg10+. Physical Review A, 1977, 15, 1-15. | 2.5 | 269 |
| 3 | The generator coordinate method applied to variational perturbation theory. Multipole polarizabilities, spectral sums, and dispersion coefficients for helium. Journal of Chemical Physics, 1981, 75, 4496-4501. | 3.0 | 140 |
| 4 | A new generalized expansion for the potential energy curves of diatomic molecules. Journal of Chemical Physics, 1975, 62, 1693-1701. | 3.0 | 138 |
| 5 | Abinitiodispersion coefficients for interactions involving rareâ€gas atoms. Journal of Chemical Physics, 1992, 97, 3252-3257. | 3.0 | 132 |
| 6 | Multipole moments, polarizabilities, and hyperpolarizabilities for N2from fourthâ€order manyâ€body perturbation theory calculations. Journal of Chemical Physics, 1988, 88, 7623-7632. | 3.0 | 131 |
| 7 | Improved Roothaanâ€“Hartreeâ€“Fock wave functions for atoms and ions with Nâ‰54. Journal of Chemical Physics, 1995, 103, 3000-3005. | 3.0 | 130 |
| 8 | The electronâ€”electron cusp condition for the spherical average of the intracule matrix. Chemical Physics Letters, 1976, 42, 476-481. | 2.6 | 120 |
| 9 | Analytical Hartree-Fock wave functions subject to cusp and asymptotic constraints: He to Xe, Li+ to Cs+, H? to I?. International Journal of Quantum Chemistry, 1999, 71, 491-497. | 2.0 | 117 |
| 10 | Double and quadruple zeta contracted Gaussian basis sets for hydrogen through neon. International Journal of Quantum Chemistry, 1993, 48, 343-354. | 2.0 | 100 |
| 11 | Comparison of kinetic-energy density functionals. Physical Review A, 1992, 46, 6920-6924. | 2.5 | 99 |
| 12 | Analytical Hartree-Fock wave functions for the atoms Cs to Lr. Theoretical Chemistry Accounts, 2000, 104, 411-413. | 1.4 | 96 |
| 13 | Oscillator strengths forS-PandP-Dtransitions in heliumlike ions. Physical Review A, 1992, 46, 5397-5405. | 2.5 | 95 |
| 14 | Higher dispersion coefficients: Accurate values for hydrogen atoms and simple estimates for other systems. Journal of Chemical Physics, 1988, 89, 2092-2098. | 3.0 | 94 |
| 15 | Polarizabilities and hyperpolarizabilities of carbon dioxide. Journal of Chemical Physics, 1990, 93, 4164-4171. | 3.0 | 90 |
| 16 | Ground-state energies for the helium isoelectronic series. Physical Review A, 1994, 50, 854-856. | 2.5 | 89 |
| 17 | Compact and accurate integral-transform wave functions. II. The2S1,2S3,2P1, and2P3states of the helium-like ions from He throughMg10+. Physical Review A, 1977, 15, 16-22. | 2.5 | 86 |
| 18 | Roothaan-Hartree-Fock wave functions for atoms withZâ‰54. Physical Review A, 1993, 47, 4510-4512. | 2.5 | 76 |

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|---|---|---|---|
| 19 | Hyperpolarizabilities and polarizabilities of neon: Discrepancy between theory and experiment. Chemical Physics Letters, 1989, 156, 87-90. | 2.6 | 74 |
| 20 | Statistical electron correlation coefficients for the five lowest states of the heliumlike ions. Physical Review A, 1981, 23, 473-478. | 2.5 | 70 |
| 21 | Internally folded densities. Chemical Physics, 1981, 63, 175-183. | 1.9 | 69 |
| 22 | Intramolecular bond length dependence of the anisotropic dispersion coefficients for interactions of rare gas atoms with N2, CO, Cl2, HCl and HBr. Molecular Physics, 1993, 80, 533-548. | 1.7 | 68 |
| 23 | Accurate charge densities and two-electron intracule functions for the heliumlike ions. Journal of Chemical Physics, 1977, 67, 1191. | 3.0 | 64 |
| 24 | Quadrupole and Octopole Moments of Heteroaromatic Rings. Journal of Physical Chemistry A, 1999, 103, 10009-10014. | 2.5 | 64 |
| 25 | Rapid basin-hopping. TIP4P water clusters. <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" display="inline" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mi) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 492.7 Td (mathvariant="i | 2.6 | 60 |
| 26 | Anisotropic electronic intracule densities for diatomics. International Journal of Quantum Chemistry, 1984, 26, 157-166. | 2.0 | 59 |
| 27 | Polarizabilities and hyperpolarizabilities of F2. Journal of Chemical Physics, 1989, 90, 366-370. | 3.0 | 58 |
| 28 | Relating polarizability to volume, ionization energy, electronegativity, hardness, moments of momentum, and other molecular properties. Journal of Chemical Physics, 2014, 141, 074306. | 3.0 | 57 |
| 29 | How important is electron correlation for the hyperpolarizability of ethyne?. Journal of Chemical Physics, 1990, 93, 652-656. | 3.0 | 56 |
| 30 | Polarizabilities of aromatic six-membered rings: azines and â€˜inorganic benzenesâ€™. Molecular Physics, 1994, 81, 557-567. | 1.7 | 56 |
| 31 | Extracules, Intracules, Correlation Holes, Potentials, Coefficients and All That. , 1987, , 553-581. | | 56 |
| 32 | Polarizabilities of Aromatic Five-Membered Rings: Azoles. The Journal of Physical Chemistry, 1995, 99, 12790-12796. | 2.9 | 55 |
| 33 | First Born differential cross-sections for electronic excitation in the helium atom. Journal of Electron Spectroscopy and Related Phenomena, 2002, 123, 143-159. | 1.7 | 55 |
| 34 | Basis set quality. II. Information theoretic appraisal of variouss- orbitals. International Journal of Quantum Chemistry, 1983, 24, 527-550. | 2.0 | 54 |
| 35 | Molecular x-ray- and electron-scattering intensities. Physical Review A, 1984, 29, 1108-1113. | 2.5 | 54 |
| 36 | Polarizabilities and hyperpolarizabilities for the atoms Al, Si, P, S, Cl, and Ar: Coupled cluster calculations. Journal of Chemical Physics, 2005, 122, 044301. | 3.0 | 54 |

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| 37 | Numerical Hartreeâ€“Fock energies of lowâ€lying excited states of neutral atoms with Zâ‰18. Journal of Chemical Physics, 1994, 101, 4945-4948. | 3.0 | 53 |
| 38 | Moments and expansion coefficients of atomic electron momentum densities: numerical Hartree - Fock calculations for hydrogen to lawrencium. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, 2973-2983. | 1.5 | 53 |
| 39 | Momentum space properties of various orbital basis sets used in quantum chemical calculations. International Journal of Quantum Chemistry, 1982, 21, 419-429. | 2.0 | 51 |
| 40 | Accurate algebraic densities and intracules for heliumlike ions. International Journal of Quantum Chemistry, 1993, 46, 689-699. | 2.0 | 51 |
| 41 | Accurate multipole moments for H2 and D2 including the effects of electron correlation and molecular vibration and rotation. Molecular Physics, 1993, 78, 1039-1046. | 1.7 | 51 |
| 42 | Form factors and total scattering intensities for the helium-like ions from explicitly correlated wavefunctions. Journal of Physics B: Atomic and Molecular Physics, 1978, 11, 3803-3820. | 1.6 | 50 |
| 43 | Approximate relationships between density power integrals, moments of the momentum density, and interelectronic repulsions in diatomic molecules. Journal of Chemical Physics, 1986, 85, 958-962. | 3.0 | 50 |
| 44 | Dipole and quadrupole moments of small molecules. An ab initio study using perturbatively corrected, multi-reference, configuration interaction wave functions. Computational and Theoretical Chemistry, 1995, 334, 7-13. | 1.5 | 50 |
| 45 | Static response properties of second-period atoms: coupled cluster calculations. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 2215-2223. | 1.5 | 50 |
| 46 | Quadrupole polarizabilities and hyperpolarizabilities of Kr and Xe from fourthâ€order manyâ€body perturbation theory calculations. Journal of Chemical Physics, 1988, 89, 7320-7323. | 3.0 | 49 |
| 47 | Reliable anisotropic dipole properties, and dispersion energy coefficients, for O2evaluated using constrained dipole oscillator strength techniques. Journal of Chemical Physics, 1996, 105, 4927-4937. | 3.0 | 48 |
| 48 | Chain length dependence of static longitudinal polarizabilities and hyperpolarizabilities in linear polyynes. Journal of Chemical Physics, 1993, 98, 8324-8329. | 3.0 | 47 |
| 49 | On a representation of the long-range interatomic interaction potential. Journal of Physics B: Atomic and Molecular Physics, 1974, 7, L321-L325. | 1.6 | 46 |
| 50 | Charge densities and two-electron intracules for the low-lying excited states of the helium-like ions. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 3391-3403. | 1.6 | 46 |
| 51 | Toward improved density functionals for the correlation energy. Journal of Chemical Physics, 2009, 131, 134109. | 3.0 | 46 |
| 52 | Coupled-cluster calculation of hyperpolarizabilities and polarizabilities for Be. Physical Review A, 1989, 40, 1130-1132. | 2.5 | 45 |
| 53 | Static hyperpolarizabilities and polarizabilities of linear polyynes. Journal of Chemical Physics, 1991, 95, 9060-9064. | 3.0 | 45 |
| 54 | How often is the minimum polarizability principle violated?. Chemical Physics Letters, 2013, 556, 346-349. | 2.6 | 45 |

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| 55 | Water nanodroplets: Predictions of five model potentials. Journal of Chemical Physics, 2013, 138, 194302. | 3.0 | 45 |
| 56 | Static hyperpolarisabilities and polarisabilities for Be: a fourth-order Moller-Plesset perturbation theory calculation. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 3819-3831. | 1.5 | 44 |
| 57 | Static hyperpolarisabilities and polarisabilities of Li. Journal of Physics B: Atomic, Molecular and Optical Physics, 1989, 22, 2439-2446. | 1.5 | 44 |
| 58 | Finite-field many-body-perturbation-theory calculation of the static hyperpolarizabilities and polarizabilities of Mg,Al+, and Ca. Physical Review A, 1991, 44, 5478-5484. | 2.5 | 44 |
| 59 | Numerical Hartreeâ€“Fock energies of singly charged cations and anions with Nâ‰54. Journal of Chemical Physics, 1994, 100, 8140-8144. | 3.0 | 44 |
| 60 | Extraction of momentum expectation values from Compton profiles. Molecular Physics, 1980, 41, 1153-1162. | 1.7 | 42 |
| 61 | Approximate solutions of the momentum-space integral SchrÃ¶dinger equation for two-electron atoms. Physical Review A, 1984, 30, 30-34. | 2.5 | 42 |
| 62 | Methanol clusters (CH3OH)n: Putative global minimum-energy structures from model potentials and dispersion-corrected density functional theory. Journal of Chemical Physics, 2013, 138, 224303. | 3.0 | 42 |
| 63 | Structures of the formic acid trimer. Chemical Physics Letters, 2004, 386, 162-168. | 2.6 | 40 |
| 64 | An analysis of energy differences in atomic multiplets in connection with the inequality formulation of Hund's rules. Molecular Physics, 1975, 29, 1861-1875. | 1.7 | 39 |
| 65 | Pump-probe studies of the effects of permanent dipoles in one- and two-colour molecular excitations. Chemical Physics, 1994, 186, 375-394. | 1.9 | 39 |
| 66 | Choosing a density functional for static molecular polarizabilities. Chemical Physics Letters, 2015, 635, 257-261. | 2.6 | 39 |
| 67 | Asymptotic behavior of atomic momentals. Journal of Chemical Physics, 1987, 86, 5060-5062. | 3.0 | 38 |
| 68 | Polarizabilities of Oxazoles:Â Ab Initio Calculations and Simple Models. The Journal of Physical Chemistry, 1996, 100, 8752-8757. | 2.9 | 38 |
| 69 | Momentum space properties of two-electron atoms. Journal of Physics B: Atomic and Molecular Physics, 1985, 18, 3061-3071. | 1.6 | 37 |
| 70 | Static polarizabilities and hyperpolarizabilities, and multipole moments for Cl2 and Br2. Electron correlation and molecular vibration effects. Chemical Physics Letters, 1993, 201, 485-492. | 2.6 | 36 |
| 71 | Asymptotic expansions of the electron momentum densities of the atoms from hydrogen through lawrencium. Journal of Chemical Physics, 1987, 87, 1212-1215. | 3.0 | 35 |
| 72 | Noninteger principal quantum numbers increase the efficiency of Slater-type basis sets. International Journal of Quantum Chemistry, 1997, 62, 1-11. | 2.0 | 35 |

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| 73 | Anisotropy of the Coulomb hole in H2. Journal of Physics B: Atomic and Molecular Physics, 1984, 17, 3405-3416. | 1.6 | 34 |
| 74 | Accurate Compton profiles for H2 and D2 including the effects of electron correlation and molecular vibration and rotation. Journal of Chemical Physics, 1977, 67, 3676-3682. | 3.0 | 33 |
| 75 | Bounding and estimation of van der Waals coefficients. Journal of Chemical Physics, 1984, 81, 1919-1928. | 3.0 | 33 |
| 76 | Structures, Vibrational Frequencies and Polarizabilities of Diazaborinines, Triazadiborinines, Azaboroles, and Oxazaboroles. Journal of Physical Chemistry A, 1999, 103, 2141-2151. | 2.5 | 33 |
| 77 | The Momentum Density Perspective of the Electronic Structure of Atoms and Molecules. Advances in Chemical Physics, 2004, , 303-352. | 0.3 | 33 |
| 78 | Moments of the electron momentum density: Requirements for ab initio and density functional theory calculations. International Journal of Quantum Chemistry, 2005, 102, 673-683. | 2.0 | 33 |
| 79 | Intramolecular bond length dependence of the anisotropic dispersion coefficients for H2â€“rare gas interactions. Journal of Chemical Physics, 1993, 98, 7140-7144. | 3.0 | 32 |
| 80 | Dipole oscillator strength distributions with improved high-energy behavior: Dipole sum rules and dispersion coefficients for Ne, Ar, Kr, and Xe revisited. Journal of Chemical Physics, 2010, 132, 074301. | 3.0 | 32 |
| 81 | Accurate all-electron correlation energies for the closed-shell atoms from Ar to Rn and their relationship to the corresponding MP2 correlation energies. Journal of Chemical Physics, 2011, 134, 044102. | 3.0 | 32 |
| 82 | Static hyperpolarizability of atomic lithium. Physical Review A, 1994, 50, 2948-2952. | 2.5 | 31 |
| 83 | A comparison of the predictions of various model N2â€“He potential energy surfaces with experiment. Journal of Chemical Physics, 1984, 80, 5561-5567. | 3.0 | 30 |
| 84 | Medium-size Gaussian basis sets for hydrogen through argon. Theoretica Chimica Acta, 1993, 85, 391-394. | 0.8 | 30 |
| 85 | New Relationships Connecting the Dipole Polarizability, Radius, and Second Ionization Potential for Atoms. Journal of Physical Chemistry A, 2012, 116, 697-703. | 2.5 | 30 |
| 86 | Examination of a new intermolecular potential function. Chemical Physics Letters, 1972, 17, 274-276. | 2.6 | 29 |
| 87 | Angular-correlation coefficients for first-row atoms. Physical Review A, 1982, 25, 1820-1825. | 2.5 | 29 |
| 88 | Gaussian vs. Slater representations ofd orbitals: An information theoretic appraisal based on both position and momentum space properties. International Journal of Quantum Chemistry, 1985, 28, 429-449. | 2.0 | 29 |
| 89 | Hyperpolarizabilities and polarizabilities of Liâ^'1 and B+: finite-field coupled-cluster calculations. Chemical Physics Letters, 1990, 173, 579-584. | 2.6 | 29 |
| 90 | Charge and intracule densities in singly excited heliumlike ions. Journal of Chemical Physics, 1993, 98, 7132-7139. | 3.0 | 29 |

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| 91 | Numerical Hartree-Fock results for atoms Cs through Lr. International Journal of Quantum Chemistry, 1995, 54, 261-263. | 2.0 | 29 |
| 92 | Improved Roothaan-Hartree-Fock wavefunctions for isoelectronic series of the atoms He to Ne. Journal of Physics B: Atomic, Molecular and Optical Physics, 1995, 28, 3113-3121. | 1.5 | 29 |
| 93 | Potential energy surface for interactions between N2 and He: Ab initio calculations, analytic fits, and second virial coefficients. Journal of Chemical Physics, 1996, 104, 2541-2547. | 3.0 | 29 |
| 94 | Local density functional approximations and conjectured bounds for momentum moments. International Journal of Quantum Chemistry, 1990, 38, 327-338. | 2.0 | 28 |
| 95 | A coupled cluster calculation of the quadrupole polarizability of CO. Journal of Chemical Physics, 1990, 92, 812-813. | 3.0 | 28 |
| 96 | Partial wave analysis of the momentum density. Journal of Chemical Physics, 1984, 81, 2953-2961. | 3.0 | 27 |
| 97 | Electron momentum densities of atoms. Journal of Chemical Physics, 1998, 109, 1601-1606. | 3.0 | 27 |
| 98 | Formic acid tetramers: a structural study. Chemical Physics Letters, 2004, 393, 347-354. | 2.6 | 27 |
| 99 | Isotropic and directional Compton profiles for N2, CO and BF. Molecular Physics, 1980, 41, 1143-1151. | 1.7 | 26 |
| 100 | Comments on inequalities among atomic expectation values. Journal of Chemical Physics, 1982, 76, 747-748. | 3.0 | 26 |
| 101 | Very shortâ€range interatomic potentials. Journal of Chemical Physics, 1987, 87, 2186-2190. | 3.0 | 26 |
| 102 | Pentamers of formic acid. Chemical Physics, 2005, 312, 119-126. | 1.9 | 26 |
| 103 | How well do static electronic dipole polarizabilities from gas-phase experiments compare with density functional and MP2 computations?. Journal of Chemical Physics, 2015, 143, 144302. | 3.0 | 26 |
| 104 | Contracted gaussian basis sets for sodium through to argon. Computational and Theoretical Chemistry, 1994, 306, 249-260. | 1.5 | 25 |
| 105 | Bond orders in heteroaromatic rings. International Journal of Quantum Chemistry, 2002, 90, 534-540. | 2.0 | 25 |
| 106 | Weakly bound ground states in three-body Coulomb systems with unit charges. Physical Review A, 1992, 46, 4418-4420. | 2.5 | 24 |
| 107 | Azaborinines:Â Structures, Vibrational Frequencies, and Polarizabilities. Journal of Physical Chemistry A, 1998, 102, 4679-4686. | 2.5 | 23 |
| 108 | Electron-pair densities of group 14, 15, and 16 atoms in their low-lying multiplet states. Journal of Chemical Physics, 1999, 110, 5763-5771. | 3.0 | 23 |

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| 109 | Quadrupole oscillator strengths for the helium isoelectronic sequence:n1S-m1D,n3S-m3D,n1P-m1P, andn3P-m3P transitions withn<7 andm<7. Journal of Physics B: Atomic, Molecular and Optical Physics, 2002, 35, 421-435. | 1.5 | 23 |
| 110 | The polarizability of sodium: theory and experiment reconciled. Chemical Physics Letters, 2005, 402, 270-273. | 2.6 | 23 |
| 111 | A hierarchy for additive models of polarizability. AIP Conference Proceedings, 2012, , . | 0.4 | 23 |
| 112 | Atomic interactions in neon and helium. Molecular Physics, 1974, 27, 593-604. | 1.7 | 22 |
| 113 | Statistical electron correlation coefficients for 29 states of the heliumlike ions. International Journal of Quantum Chemistry, 1993, 48, 33-42. | 2.0 | 22 |
| 114 | An improved potential energy curve for the C1Îu state of H2. Chemical Physics Letters, 1994, 222, 65-68. | 2.6 | 22 |
| 115 | Polarizabilities of purine, allopurinol, hypoxanthine, xanthine and alloxanthine. Computational and Theoretical Chemistry, 1996, 366, 185-193. | 1.5 | 22 |
| 116 | Polarizabilities of heteroaromatic molecules: Azines revisited. International Journal of Quantum Chemistry, 1996, 60, 1633-1642. | 2.0 | 21 |
| 117 | TABS: A database of molecular structures. Computational and Theoretical Chemistry, 2014, 1043, 13-16. | 2.5 | 21 |
| 118 | N-electron zero-momentum energy expression: A criterion for assessing the accuracy of approximate wave functions. Physical Review A, 1978, 18, 841-844. | 2.5 | 20 |
| 119 | The higher order electronâ€“electron coalescence condition for the intracule function for states of maximum spin multiplicity. Journal of Chemical Physics, 1986, 84, 6830-6832. | 3.0 | 20 |
| 120 | Roothaan-Hartree-Fock wavefunctions for ions with N<or=54. Journal of Physics B: Atomic, Molecular and Optical Physics, 1993, 26, 2529-2532. | 1.5 | 20 |
| 121 | Improved Double-Zeta Description for the Atoms Li through Xe. Bulletin of the Chemical Society of Japan, 1993, 66, 3135-3141. | 3.2 | 20 |
| 122 | Does the most stable formic acid tetramer have Ï€ stacking or Câ€“Hâ‹¯O interactions?. Journal of Chemical Physics, 2006, 124, 224313. | 3.0 | 20 |
| 123 | A simple additive model for polarizabilities: Application to amino acids. Chemical Physics Letters, 2009, 472, 232-236. | 2.6 | 20 |
| 124 | Additive models for the molecular polarizability and volume. Chemical Physics Letters, 2014, 610-611, 163-166. | 2.6 | 20 |
| 125 | Atomic interactions in the heavy Noble gases. Molecular Physics, 1974, 27, 191-208. | 1.7 | 19 |
| 126 | Model studies of the Tamm-like and field-sustained surface states of germanium. Surface Science, 1978, 74, 168-180. | 1.9 | 19 |

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| 127 | Angle and bond-length dependent C6 coefficients for H2 interacting with H, Li, Be and rare gas atoms. Theoretica Chimica Acta, 1992, 82, 57-73. | 0.8 | 19 |
| 128 | Vibrational deactivation of N2(v=1) by inelastic collisions with He3 and He4: An experimental and a theoretical study. Journal of Chemical Physics, 1997, 107, 2329-2339. | 3.0 | 19 |
| 129 | Hydrogen-bonded complexes of glycolic acid with one and two water molecules. Chemical Physics Letters, 2004, 387, 142-148. | 2.6 | 19 |
| 130 | Clusters of glycolic acid and 16 water molecules. Chemical Physics Letters, 2007, 434, 176-181. | 2.6 | 19 |
| 131 | Comments on explicitly correlated wave functions for the ground state of the helium atom. Physical Review A, 1977, 16, 1740-1742. | 2.5 | 18 |
| 132 | Compton profiles and other momentum-space properties ofN2. Physical Review A, 1986, 34, 4695-4703. | 2.5 | 18 |
| 133 | Static hyperpolarizability of N2. Journal of Chemical Physics, 1994, 100, 7471-7475. | 3.0 | 18 |
| 134 | ATOMIC POLARIZABILITIES AND HYPERPOLARIZABILITIES: A CRITICAL COMPILATION. , 2006, , 505-529. | | 18 |
| 135 | Dipole polarizability, sum rules, mean excitation energies, and long-range dispersion coefficients for buckminsterfullerene C60. Chemical Physics Letters, 2011, 516, 208-211. | 2.6 | 18 |
| 136 | A technique for increasing the utility of the Wigner-Kirkwood expansion for the second virial coefficient. Molecular Physics, 1978, 36, 887-892. | 1.7 | 17 |
| 137 | What do kinetic energy anisotropies tell us about chemical bonding? II. Firstâ€row A2, AO, and AF diatomics. Journal of Chemical Physics, 1986, 85, 2845-2849. | 3.0 | 17 |
| 138 | Momentum-space properties of the neutral atoms from H through U. Atomic Data and Nuclear Data Tables, 1991, 48, 213-229. | 2.4 | 17 |
| 139 | Incoherent scattering factors. Journal of Chemical Physics, 1984, 81, 1943-1946. | 3.0 | 16 |
| 140 | What do kinetic-energy anisotropies tell us about chemical bonding? I. Diatomic hydrides. International Journal of Quantum Chemistry, 1986, 29, 323-332. | 2.0 | 16 |
| 141 | Momentum-space properties ofN2: Improved configuration-interaction calculations. Physical Review A, 1990, 42, 1336-1345. | 2.5 | 16 |
| 142 | Ab initiostatic polarizabilities and multipole moments of I2. Molecular Physics, 1991, 73, 1235-1240. | 1.7 | 16 |
| 143 | Accurate Heitler-London interaction energy for He2. Computational and Theoretical Chemistry, 1995, 343, 43-48. | 1.5 | 16 |
| 144 | Discrete and continuum contributions to multipole polarizabilities and shielding factors of hydrogen. International Journal of Quantum Chemistry, 1983, 24, 345-352. | 2.0 | 15 |

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| 145 | Partial-wave analysis of the momentum densities of 14 electron diatomics. International Journal of Quantum Chemistry, 1984, 26, 385-392. | 2.0 | 15 |
| 146 | Sum rules for atomic form factors and total xâ€ray scattering intensities. Journal of Chemical Physics, 1985, 83, 747-749. | 3.0 | 15 |
| 147 | Double even tempering of orbital exponents: Application to Roothaan-Hartree-Fock calculations for He through Xe in Slater-type basis sets. Theoretica Chimica Acta, 1994, 88, 273-283. | 0.8 | 15 |
| 148 | Reliable anisotropic dipole properties and dispersion energy coefficients for NO, evaluated using constrained dipole oscillator strength techniques. Molecular Physics, 1997, 90, 721-728. | 1.7 | 15 |
| 149 | Cross sections for x-ray and high-energy electron scattering by small molecules. Journal of Physics B: Atomic, Molecular and Optical Physics, 1998, 31, 3675-3692. | 1.5 | 15 |
| 150 | Mist: A New Interatomic Potential Function. Chemical Physics Letters, 1974, 24, 157-161. | 2.6 | 14 |
| 151 | Mixed-pole terms in the anisotrophy of the long-range interaction coefficients for H2î—¸He and H2î—¸H2. Chemical Physics Letters, 1977, 46, 453-456. | 2.6 | 14 |
| 152 | Correlation energy generating potentials for molecular hydrogen. Journal of Chemical Physics, 1985, 83, 3577-3583. | 3.0 | 14 |
| 153 | Hydrogen bonding in the glycolic acid dimer. Computational and Theoretical Chemistry, 2002, 591, 189-197. | 1.5 | 14 |
| 154 | Compact Hylleraas-type wavefunctions for the lithium isoelectronic sequence. Chemical Physics Letters, 2002, 366, 95-99. | 2.6 | 14 |
| 155 | Clusters of glycolic acid with three to six water molecules. Journal of Chemical Physics, 2005, 122, 074313. | 3.0 | 14 |
| 156 | Structural characteristics of formic acid dodecamers, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si19.gif" display="inline" overflow="scroll"><mml:mrow><mml:mo stretchy="false">(</mml:mo><mml:mtext>HCOOH</mml:mtext><mml:msub><mml:mrow><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 T | 2.6 | 14 |
| 157 | Chemical Physics Letters, 2008, 450, 258-262. Interelectronic angles: Rounding out a geometric picture of the helium atom. Chemical Physics Letters, 2011, 512, 287-289. | 2.6 | 14 |
| 158 | Small clusters of formic acid: Tests and applications of density functional theory with dispersion-correcting potentials. Chemical Physics Letters, 2013, 560, 71-74. | 2.6 | 14 |
| 159 | Interatomic forces and Compton profiles. International Journal of Quantum Chemistry, 1983, 23, 227-234. | 2.0 | 13 |
| 160 | Momentum-space properties ofN2. Physical Review A, 1987, 36, 5111-5117. | 2.5 | 13 |
| 161 | Optimal single-zeta description for the atoms Al through Xe. Theoretica Chimica Acta, 1993, 85, 363-370. | 0.8 | 13 |
| 162 | Variational calculations for helium-like ions using generalized Kinoshita-type expansions. Theoretical Chemistry Accounts, 2003, 109, 36-39. | 1.4 | 13 |

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| 164 | Compact and accurate integral-transform wave functions. III. Radially correlated wave functions for the ground state of the lithium atom. Physical Review A, 1977, 15, 2143-2146. | 2.5 | 12 |
| 165 | Substituent effects in alkynes and cyanides: a momentum density perspective. Canadian Journal of Chemistry, 1985, 63, 1412-1417. | 1.1 | 12 |
| 166 | The quality ofs-orbitals determined by least-squares fitting and constrained variational methods. International Journal of Quantum Chemistry, 1986, 30, 717-735. | 2.0 | 12 |
| 167 | Electron-momentum densities of singly charged ions. Physical Review A, 1999, 59, 4805-4808. | 2.5 | 12 |
| 168 | Expansion coefficients and moments of electron momentum densities for singly charged ions. Theoretical Chemistry Accounts, 1999, 103, 70-76. | 1.4 | 12 |
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