# Aristides Mavridis

List of Publications by Year
in descending order

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| 129 | 2,528 | 201674 | 289244 |
|---|---|---|---|
| papers | citations | 27 h-index | 40 g-index |

| 137 | 137 | 137 | 1562 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | An accurate description of the ground and excited states of CH. Journal of Chemical Physics, 1999, 111, 9536-9548. | 3.0 | 99 |
| 2 | Theoretical investigation of iron carbide, FeC. Journal of Chemical Physics, 2002, 116, 4901. | 3.0 | 75 |
| 3 | Electronic Structure and Bonding of the Early 3d-Transition Metal Diatomic Oxides and Their Ions: ScO<sup>0,Â±</sup>, TiO<sup>0,Â±</sup>, CrO<sup>0,Â±</sup>, and MnO<sup>0,Â±</sup><sup>â€</sup>. Journal of Physical Chemistry A, 2010, 114, 8536-8572. | 2.5 | 72 |
| 4 | Carbonyl Boron and Related Systems:â€‰ An ab Initio Study of Bâ^'X and YBâ‹®BY (1Î£g+), Where X = He, Ne, Ar, Kr, CO, CS, N2 and Y = Ar, Kr, CO, CS, N2. Journal of Physical Chemistry A, 2004, 108, 4335-4340. | 2.5 | 66 |
| 5 | Electronic Structure of Vanadium Oxide. Neutral and Charged Species, VO0,Â±. Journal of Physical Chemistry A, 2007, 111, 1953-1965. | 2.5 | 65 |
| 6 | On the dipole moment of the ground state Xâ€Š3Î" of iron carbide, FeC. Journal of Chemical Physics, 2003, 118, 4984-4986. | 3.0 | 63 |
| 7 | First principles study of the ground and excited states of FeO, FeO+, and FeOâ^'. Journal of Chemical Physics, 2011, 134, 234308. | 3.0 | 63 |
| 8 | Electronic structure and bonding of ozone. Journal of Chemical Physics, 2008, 129, 054312. | 3.0 | 56 |
| 9 | First principles study of the electronic structure and bonding of Mn2. Journal of Chemical Physics, 2008, 129, 154310. | 3.0 | 51 |
| 10 | First Principles Examination of the Acetyleneâ^'Water Clusters, HCCHâ^'(H2O)x,x= 2, 3, and 4. Journal of Physical Chemistry A, 2002, 106, 11327-11337. | 2.5 | 49 |
| 11 | CH2 revisited. Canadian Journal of Chemistry, 2004, 82, 684-693. | 1.1 | 49 |
| 12 | Asymmetrical changes in the tertiary structure of Î±-chymotrypsin with change in pH. Biochemistry, 1974, 13, 3661-3666. | 2.5 | 47 |
| 13 | Theoretical Investigation of Scandium Carbide, ScC. Journal of Physical Chemistry A, 2001, 105, 755-759. | 2.5 | 45 |
| 14 | On the electrostatic bonding of carbonyl to the monocations of the first-row transition elements. Journal of the American Chemical Society, 1989, 111, 2482-2487. | 13.7 | 44 |
| 15 | Electronic structure and bonding of the 3d transition metal borides, MB, M=Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu through all electron ab initio calculations. Journal of Chemical Physics, 2008, 128, 034309. | 3.0 | 41 |
| 16 | Interaction of Dioxygen with Al Clusters and Al(111):â€‰ A Comparative Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 6924-6932. | 3.1 | 41 |
| 17 | On the ground states of CaC and ZnC: A multireference Brillouinâ€"Wigner coupled cluster study. Journal of Chemical Physics, 2002, 117, 9733-9739. | 3.0 | 40 |
| 18 | First-Principles Investigation of the Boron and Aluminum Carbides BC and AlC and Their Anions BC-and AlC-. 1. Journal of Physical Chemistry A, 2001, 105, 1175-1184. | 2.5 | 39 |

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| 19 | The dissociation energies of NF(Xâ€‰3Î£â^) and NCl(Xâ€‰3Î£â^). Journal of Chemical Physics, 1997, 106, 3280-3286. | 3.0 | 36 |
| 20 | A Multireference Coupled-Cluster Potential Energy Surface of Diazomethane, CH2N2. Journal of Physical Chemistry A, 2005, 109, 10148-10152. | 2.5 | 35 |
| 21 | A first principles study of the acetyleneâ€“water interaction. Journal of Chemical Physics, 2000, 112, 6178-6189. | 3.0 | 34 |
| 22 | Ab initio investigation of the ground and low-lying states of the diatomic fluorides TiF, VF, CrF, and MnF. Journal of Chemical Physics, 2004, 120, 11500-11521. | 3.0 | 34 |
| 23 | Theoretical Investigation of Titanium Carbide, TiC:â€‰ X3Î£+, aÎ£+, A3Î”, and b1Î” States. Journal of Physical Chemistry A, 2002, 106, 3905-3908. | 2.5 | 30 |
| 24 | On the Bonding Nature of the N5+(=N(N2)2+) Cation and Related Species N(CO)x+, N(NH3)x+, and NRx+, x = 1, 2 and R = He, Ne, Ar, Kr. Do We Really Need the Resonance Concept?. Journal of Physical Chemistry A, 2002, 106, 4435-4442. | 2.5 | 30 |
| 25 | The electronic structure of vanadium carbide, VC. Journal of Chemical Physics, 2005, 123, 014301. | 3.0 | 28 |
| 26 | Ab initio investigation of the electronic structure and bonding of BH, BHâ^', and HBBH molecules. Journal of Chemical Physics, 2008, 128, 144308. | 3.0 | 28 |
| 27 | The Sc2 dimer revisited. Journal of Chemical Physics, 2010, 132, 024309. | 3.0 | 28 |
| 28 | Theoretical Study of the Electronic and Geometrical Structure of the Ground and Low-Lying States of NCl2, PCl2, NCl, and PCl Radicals. The Journal of Physical Chemistry, 1995, 99, 10759-10765. | 2.9 | 27 |
| 29 | An accurate description of the ground and excited states of SiH. Journal of Chemical Physics, 2002, 116, 6529-6540. | 3.0 | 27 |
| 30 | On symmetry breaking in BNB: Real or artifactual?. Journal of Chemical Physics, 2004, 120, 1813-1819. | 3.0 | 27 |
| 31 | Electronic Structure of Cobalt Carbide, CoC. Journal of Physical Chemistry A, 2006, 110, 8952-8962. | 2.5 | 26 |
| 32 | Accurate ab initio calculations of the ground states of FeC, FeC+, and FeCâ^'. Journal of Chemical Physics, 2010, 132, 194312. | 3.0 | 26 |
| 33 | Ab Initio Investigation of the LiHe X2Î£+, A2Î, and B2Î£+States:Â A Basis Set Study. Journal of Physical Chemistry A, 2000, 104, 408-412. | 2.5 | 25 |
| 34 | Electronic structure of carbon-lithium, silicon-hydrogen, and silicon-lithium in the lowest 4.SIGMA.- and 2.pi. states. The Journal of Physical Chemistry, 1982, 86, 1979-1985. | 2.9 | 24 |
| 35 | The gas phase chemistry of bare and ligated transition metal ions: Correlations of reactivity with electronic structureâ€”I. M+ and MCO+. Polyhedron, 1988, 7, 1559-1572. | 2.2 | 24 |
| 36 | Theoretical investigation of theX2Î£+,A2Î, andB2Î£+ states of LiAr and LiKr. Journal of Chemical Physics, 2002, 116, 9305-9314. | 3.0 | 24 |

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| 37 | Electronic Structure of Scandium and Titanium Carbide Cations, ScC+and TiC+. Ground and Low-Lying States. Journal of Physical Chemistry A, 2000, 104, 11777-11785. | 2.5 | 23 |
| 38 | Electronic structure of the carbyne C-Li and the carbene Li2C. Journal of the American Chemical Society, 1982, 104, 3827-3833. | 13.7 | 22 |
| 39 | A Theoretical Investigation of the Structure and Bonding of Diazomethane, CH2N2. Journal of Physical Chemistry A, 1999, 103, 1255-1259. | 2.5 | 22 |
| 40 | Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. 2. Journal of Physical Chemistry A, 2001, 105, 7672-7685. | 2.5 | 22 |
| 41 | Ab Initio Study of the Ground and Excited States of Zinc Carbide, ZnC. Journal of Physical Chemistry A, 2003, 107, 6062-6072. | 2.5 | 22 |
| 42 | Multireference configuration interaction and coupled-cluster calculations on the X3Î£â^', a1Î”, and b1Î£+ states of the NF molecule. International Journal of Quantum Chemistry, 2005, 104, 458-467. | 2.0 | 22 |
| 43 | Ab initio Study of the Diatomic Fluorides FeF, CoF, NiF, and CuF. Journal of Physical Chemistry A, 2008, 112, 11235-11250. | 2.5 | 22 |
| 44 | Ab initioinvestigation of the ground state properties of PO, PO+, and POâ^'. Journal of Chemical Physics, 2003, 119, 5981-5987. | 3.0 | 21 |
| 45 | Electronic and geometric structure of the 3d-transition metal monocarbonyls MCO, M=Sc, Ti, V, and Cr. Journal of Chemical Physics, 2005, 123, 074327. | 3.0 | 21 |
| 46 | First principles study of the diatomic charged fluorides MFÂ±, M=Sc, Ti, V, Cr, and Mn. Journal of Chemical Physics, 2005, 122, 054312. | 3.0 | 21 |
| 47 | Crystal and molecular structure of dimethoxyporphinato-germanium(IV). Inorganic Chemistry, 1976, 15, 2723-2727. | 4.0 | 20 |
| 48 | An ab initio study of the electronic structure of the ground triplet and low-lying singlet states of formylnitrene, HCON and formylphosphinidene, HCOP. Journal of the American Chemical Society, 1980, 102, 7651-7655. | 13.7 | 20 |
| 49 | Ground states of BeC and MgC: A comparative multireference Brillouin-Wigner coupled cluster and configuration interaction study. International Journal of Quantum Chemistry, 2005, 102, 762-774. | 2.0 | 20 |
| 50 | Theoretical investigation of the ground and low-lying excited states of nickel carbide, NiC. Journal of Chemical Physics, 2007, 126, 194304. | 3.0 | 20 |
| 51 | Electronic Structure and Bonding of Cobalt Monoxide, CoO, and Its Ions CoO+ and CoOâ€“: An Ab Initio Study. Journal of Physical Chemistry A, 2012, 116, 6935-6949. | 2.5 | 20 |
| 52 | First principles exploration of NiO and its ions NiO+ and NiOâ^'. Journal of Chemical Physics, 2013, 138, 054308. | 3.0 | 20 |
| 53 | First principles investigation of chromium carbide, CrC. Journal of Chemical Physics, 2005, 123, 014302. | 3.0 | 19 |
| 54 | Electronic spectroscopy and electronic structure of diatomic CrC. Journal of Chemical Physics, 2010, 133, 034303. | 3.0 | 19 |

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| 55 | An Accurate Description of the LiNe X 2Î£+, A 2Î, and B 2Î£+ States. Journal of Physical Chemistry A, 2001, 105, 1983-1987. | 2.5 | 18 |
| 56 | A molecular level study of the aqueous microsolvation of acetylene. Chemical Physics Letters, 2001, 340, 538-546. | 2.6 | 18 |
| 57 | The dipole moments of the excited states of FeC. Journal of Chemical Physics, 2005, 122, 056101. | 3.0 | 18 |
| 58 | On the electron affinity of SiN and spectroscopic constants of SiNâ¯. Journal of Chemical Physics, 2005, 123, 124301. | 3.0 | 18 |
| 59 | An ab initio study of the electronic structure of BF and BF+. Journal of Chemical Physics, 2013, 138, 104312. | 3.0 | 18 |
| 60 | Ab initio structural study of the B4H4 molecule. Asymmetric structure for a â€˜symmetricâ€™ system. Chemical Physics Letters, 1994, 226, 469-474. | 2.6 | 17 |
| 61 | Electronic structure of vanadium and chromium carbide cations, VC+and CrC+. Ground and low-lying states. Molecular Physics, 2004, 102, 2451-2466. | 1.7 | 17 |
| 62 | First Principles Investigation of the Electronic Structure of the Iron Carbide Cation, FeC+. Journal of Physical Chemistry A, 2005, 109, 9249-9258. | 2.5 | 17 |
| 63 | Bonding Elucidation of the Three Common Acids H2SO4, HNO3, and HClO4. Journal of Physical Chemistry A, 2009, 113, 13972-13975. | 2.5 | 16 |
| 64 | An accurate first principles study of the geometric and electronic structure of B2, B2â¯, B3, B3â¯, and B3H: Ground and excited states. Journal of Chemical Physics, 2010, 132, 164307. | 3.0 | 16 |
| 65 | The electronic structure of Ti2 and Ti2+. Journal of Chemical Physics, 2011, 135, 134302. | 3.0 | 16 |
| 66 | Ab initio Study of the Electronic Structure of Zinc Oxide and its Ions, ZnO0,Â±. Ground and Excited States. Journal of Physical Chemistry A, 2010, 114, 9333-9341. | 2.5 | 15 |
| 67 | First-Principles Investigation of the Early 3d Transition Metal Diatomic Chlorides and Their Ions, ScCl0,Â±, TiCl0,Â±, VCl0,Â±, and CrCl0,Â±. Journal of Physical Chemistry A, 2009, 113, 6818-6840. | 2.5 | 14 |
| 68 | Myths and Reality of Hypervalent Molecules. The Electronic Structure of FClO<sub>x</sub>, x = 1â¯3, Cl<sub>3</sub>PO, Cl<sub>3</sub>PCH<sub>2</sub>, Cl<sub>3</sub>CClO, and C(ClO)<sub>4</sub>. Journal of Physical Chemistry A, 2011, 115, 2378-2384. | 2.5 | 14 |
| 69 | Electronic Structure of the Ground and Low-Lying Excited States of TiP. The Journal of Physical Chemistry, 1996, 100, 13971-13975. | 2.9 | 13 |
| 70 | A Theoretical Study of Calcium Monohydride, CaH:â€‰ Low-Lying States and Their Permanent Electric Dipole Moments. Journal of Physical Chemistry A, 2007, 111, 371-374. | 2.5 | 13 |
| 71 | Electronic and geometric structure of amidoscandium(1+) and amminescandium(1+). The Journal of Physical Chemistry, 1991, 95, 6854-6859. | 2.9 | 12 |
| 72 | Elucidation of the structural characteristics of the isovalent species Li[CO] and Li[CS] by ab anitio calculations. Chemical Physics Letters, 1996, 259, 185-192. | 2.6 | 12 |

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| 73 | On the Electronic Structure of ScB+: Ground and Low-Lying Excited States. Advances in Quantum Chemistry, 1998, , 69-91. | 0.8 | 12 |
| 74 | SiH2, a critical study. Molecular Physics, 2004, 102, 2597-2606. | 1.7 | 12 |
| 75 | Ab initio study of the electronic structure of manganese carbide. Journal of Chemical Physics, 2006, 124, 154308. | 3.0 | 12 |
| 76 | First principles study of cobalt hydride, CoH, and its ions CoH+ and CoHâ^'. Journal of Chemical Physics, 2012, 137, 034309. | 3.0 | 12 |
| 77 | Electronic and geometric structure of the titanium hydrides, TiH+ and TiH + 2. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1391. | 1.1 | 11 |
| 78 | Electronic and geometrical structure of the NF2 radical. Chemical Physics Letters, 1993, 216, 167-172. | 2.6 | 11 |
| 79 | Bonding Investigation of the Ground and Low-Lying States of the Titanium Boride Cation, TiB+. Journal of Physical Chemistry A, 1998, 102, 5982-5992. | 2.5 | 11 |
| 80 | â€œHypervalencyâ€•and the chemical bond. Computational and Theoretical Chemistry, 2019, 1153, 65-74. | 2.5 | 11 |
| 81 | Ground and Low-Lying States of the Vanadium Boride Cation, VB+:â€‰ An ab Initio Investigation. Journal of Physical Chemistry A, 1999, 103, 3336-3345. | 2.5 | 10 |
| 82 | Structure and Bonding of the Polytopic Molecule Li[BO]. A Theoretical Investigation. Journal of Physical Chemistry A, 2001, 105, 7106-7110. | 2.5 | 10 |
| 83 | Electronic structure of linear TiCH. Journal of Chemical Physics, 2003, 119, 3745-3750. | 3.0 | 10 |
| 84 | Ab Initio Investigation of the Electronic and Geometric Structure of Magnesium Diboride, MgB2. Journal of Physical Chemistry A, 2005, 109, 10663-10674. | 2.5 | 10 |
| 85 | Structure and Energetics of Gaseous HZnCl. Journal of Physical Chemistry A, 2006, 110, 10899-10903. | 2.5 | 9 |
| 86 | The electronic structure of the two lowest states of CuC. Journal of Chemical Physics, 2008, 129, 174306. | 3.0 | 9 |
| 87 | Li atoms attached to helium nanodroplets. International Journal of Quantum Chemistry, 2011, 111, 400-405. | 2.0 | 9 |
| 88 | Electronic spectroscopy and electronic structure of diatomic TiFe. Journal of Chemical Physics, 2012, 137, 054302. | 3.0 | 9 |
| 89 | Accurate first principles calculations on chlorine fluoride ClF and its ions ClFÂ±. Theoretical Chemistry Accounts, 2014, 133, 1. | 1.4 | 9 |
| 90 | Electronic structure of CNa and CNa2 in their electronic ground states. The Journal of Physical Chemistry, 1984, 88, 4973-4978. | 2.9 | 8 |

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| 91 | On the electronic structure of the ground (X3Î£â¯) and some low-lying excited states (A3Î, a1Î”, b1â¯+, B3Î£â¯) of the isovalent species Pî—¸Li and Pî—¸Na. Computational and Theoretical Chemistry, 1997, 417, 277-287. | 1.5 | 8 |
| 92 | Electronic structure determination of chromium boride cation, CrB+. Journal of Chemical Physics, 2000, 113, 2270-2281. | 3.0 | 8 |
| 93 | A highly accurate first principles determination of the electron affinity of BO(X2Î£+) and binding energy of BOâ¯(X1Î£+). Chemical Physics Letters, 2001, 341, 382-386. | 2.6 | 8 |
| 94 | Theoretical Investigation of Organo-Noble Gas Compounds, HC(Ng)n+,n= 1, 2; Ng = He, Ne, Ar, Kr, and Xe. Evidence for Potentially Isolable HCArn+, HCKrn+, and HCXen+Species. Journal of Physical Chemistry A, 2004, 108, 11127-11131. | 2.5 | 8 |
| 95 | Ab Initio Study of the Electronic Structure and Bonding of Aluminum Nitride. Journal of Physical Chemistry A, 2007, 111, 11221-11231. | 2.5 | 8 |
| 96 | All-Electron First Principles Calculations of the Ground and Some Low-Lying Excited States of BaI. Journal of Physical Chemistry A, 2007, 111, 10002-10009. | 2.5 | 8 |
| 97 | Electronic Structure and Bonding of the Fastidious Species CN<sub>2</sub> and CP<sub>2</sub>: A First-Principles Study. Journal of Physical Chemistry A, 2019, 123, 10290-10302. | 2.5 | 8 |
| 98 | Near-Hartreeâ€“Fock calculations on the ground state of the fluoronium ion, FH+2. Journal of the Chemical Society, Faraday Transactions 2, 1982, 78, 447-455. | 1.1 | 7 |
| 99 | An ab initio structural study of cyanamide. Computational and Theoretical Chemistry, 1993, 279, 151-156. | 1.5 | 7 |
| 100 | Ab initio study of the ground and several excited states of the NLi system. Chemical Physics Letters, 1996, 250, 409-414. | 2.6 | 7 |
| 101 | Theoretical Investigation of the Ground X3Î£- State of Nitrogen Bromide. Journal of Physical Chemistry A, 1998, 102, 10536-10539. | 2.5 | 7 |
| 102 | Electronic Structure and Bonding Nature of the Ground State Monocarbide Cations, ScC+, TiC+, VC+, and CrC+. Collection of Czechoslovak Chemical Communications, 2003, 68, 387-404. | 1.0 | 7 |
| 103 | All-Electron ab Initio Calculations on Tetramethyltin. The Journal of Physical Chemistry, 1994, 98, 8906-8909. | 2.9 | 6 |
| 104 | Electronic and Geometrical Structure of the Sc[BO]+Cation. An Ab Initio Investigation. Journal of Physical Chemistry A, 1999, 103, 9359-9363. | 2.5 | 6 |
| 105 | Predissociation lifetimes of the E2Î and F2Î states of CH. Chemical Physics Letters, 2000, 331, 89-94. | 2.6 | 6 |
| 106 | Conditions conducive to the chemi-ionization reaction O(3P)+CH(Xâ€Š2Î,aâ€Š4Î£â¯)â†'HCO+(Xâ€Š1Î£+)+eâ¯. Journal of Chemical Physics, 2001, 115, 6946-6950. | 3.0 | 6 |
| 107 | On the ground state of titanium phosphide, TiP: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 2646. | 3.0 | 6 |
| 108 | Structural parameters of the ground states of the quasiâ€stable diatomic anions CO<sup>â¯</sup>, BF<sup>â¯</sup>, and BCl<sup>â¯</sup> as obtained by conventional Ab Initio methods. International Journal of Quantum Chemistry, 2015, 115, 771-778. | 2.0 | 6 |

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| 109 | The story of the B 4 H 4 molecule told again. Computational and Theoretical Chemistry, 2017, 1115, 217-222. | 2.5 | 6 |
| 110 | Theoretical Investigation of the Electronic States of Calcium Carbide, CaC. Journal of Physical Chemistry A, 2003, 107, 7650-7655. | 2.5 | 5 |
| 111 | A theoretical study of the geometrical structure and energy inversion barriers of the cyanopnictogens Nî—¼C-XY2 (X = N or P; Y = H, F, Cl or Br). Computational and Theoretical Chemistry, 1994, 305, 225-239. | 1.5 | 4 |
| 112 | On the Electronic Structure of NLi2and PLi2, Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 1998, 102, 2223-2230. | 2.5 | 3 |
| 113 | The Electronic Structure of ScAl+. Ground and Low-Lying Excited States. Journal of Physical Chemistry A, 2000, 104, 6861-6870. | 2.5 | 3 |
| 114 | CH(X2â^¸a4â^ˆâ^') â€¦ OH2 and CH2(??3B1, Ã£1A1) â€¦ OH2 interactions. A first principles investigation. International Journal of Quantum Chemistry, 2005, 104, 497-511. | 2.0 | 3 |
| 115 | Interaction of the early 3d transition metals Sc, Ti, V, and Cr with N2: An ab initio study. Journal of Chemical Physics, 2006, 124, 104306. | 3.0 | 3 |
| 116 | Structural characterization of scandium monophosphide (1+). The Journal of Physical Chemistry, 1993, 97, 10955-10957. | 2.9 | 2 |
| 117 | Ab Initio Investigation of the Electronic Structure and Bonding of the HC(N2)x+ and HC(CO)x+ Cations, x = 1, 2. Journal of Physical Chemistry A, 2005, 109, 6549-6554. | 2.5 | 2 |
| 118 | Structure and bonding of ScCN and ScNC: Ground and low-lying states. Chemical Physics, 2012, 399, 46-49. | 1.9 | 2 |
| 119 | All electron ab initio calculations on the ScTi molecule: a really hard nut to crack. Theoretical Chemistry Accounts, 2013, 132, 1. | 1.4 | 2 |
| 120 | Accurate ab Initio Structural Parameters of the Diatomic and Triatomic van der Waals Molecules <sup>11</sup>BNg (X<sup>2</sup>Î, A<sup>2</sup>Î£<sup>+</sup>) and <sup>11</sup>BNg<sub>2</sub> (XÌƒ<sup>2</sup>B<sub>1</sub>), Ng = <sup>4</sup>He, <sup>20</sup>Ne, <sup>40</sup>Ar, <sup>84</sup>Kr, and <sup>132</sup>Xe. Journal of Physical Chemistry A, 2014, 118, 3990-3995. | 2.5 | 2 |
| 121 | An ab initio study of Li+ â€¦Cî—¼S, a purely electrostatic system. Computational and Theoretical Chemistry, 1995, 357, 97-101. | 1.5 | 1 |
| 122 | The electronic structure and bonding of AlNAl. Journal of Chemical Physics, 2009, 130, 154308. | 3.0 | 1 |
| 123 | Accurate structural parameters and binding energy of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mover accent="true"><mml:mrow><mml:msup><mml:mrow><mml:mi>X</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msup></mml:mrow><mml:mo stretchy="false">~</mml:mo></mml:mover></mml:mrow></mml:math> state of diazomethane through. Chemical Physics Letters, 2014, 600, 103-105. | 2.6 | 1 |
| 124 | A well known quantum theorem revisited. European Journal of Physics, 1990, 11, 152-154. | 0.6 | 0 |
| 125 | The ScPH+ Cation. The Journal of Physical Chemistry, 1994, 98, 12232-12235. | 2.9 | 0 |
| 126 | Ab initio Study of the Ground and Excited States of Zinc Carbide, ZnC.. ChemInform, 2003, 34, no. | 0.0 | 0 |

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| 127 | 1937 Nobel Prize. American Journal of Physics, 2006, 74, 373-373. | 0.7 | 0 |
| 128 | Electronic and Geometric Structure of the 3d-Transition Metal Monocarbonyls MCO, M = Sc, Ti, V and Cr. , 2006, , 1505-1505. | | 0 |
| 129 | The Interaction of the Early 3d-transition metals Sc, Ti, V and Cr with N2 . An ab initio Study. , 2006, , 1497-1497. | | 0 |