

# Antonio Largo

## List of Publications by Year in descending order

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148  
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docs citations

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times ranked

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citing authors

| #  | ARTICLE   | IF   | CITATIONS |
|----|---|------|-----------|
| 1  | Theoretical methods that help understanding the structure and reactivity of gas phase ions. <i>International Journal of Mass Spectrometry</i> , 2005, 240, 37-99.   | 1.5  | 104       |
| 2  | Theoretical Study of $AlC_n$ , $AlC_n^+$ , and $AlC_n^-(n=1-7)$ Clusters. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4217-4225.  | 2.5  | 52        |
| 3  | <i>Planck</i> 2013 results. <i>Astronomy and Astrophysics</i> , 2014, 571, E1.  | 5.1  | 51        |
| 4  | Cyanides and Isocyanides of First-Row Transition Metals: Molecular Structure, Bonding, and Isomerization Barriers. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6334-6344.   | 2.5  | 50        |
| 5  | Gaussian functions in <i>hylleraas</i> CI calculations. I. Ground state energies for $H_2$ , $HeH^+$ , and $H_3$ . <i>Journal of Chemical Physics</i> , 1988, 88, 2091-2093.  | 3.0  | 46        |
| 6  | Theoretical study of $C_nCl$ , $C_nCl^+$ , $C_nCl^-(n=1-7)$ clusters. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 127-135.  | 2.0  | 46        |
| 7  | Structure and Bonding in First-Row Transition-Metal Dicarbides: Are They Related to the Stability of Met-cars?. <i>Chemistry - A European Journal</i> , 2006, 12, 6963-6975.  | 3.3  | 44        |
| 8  | On the Competition between Linear and Cyclic Isomers in Second-Row Dicarbides. <i>Journal of the American Chemical Society</i> , 2004, 126, 14611-14619.  | 13.7 | 42        |
| 9  | Theoretical Study of the $C_2P$ Radical and $(C_2P)^+$ Species. <i>The Journal of Physical Chemistry</i> , 1994, 98, 3985-3988.   | 2.9  | 40        |
| 10 | GAS-PHASE SYNTHESIS OF PRECURSORS OF INTERSTELLAR GLYCINE: A COMPUTATIONAL STUDY OF THE REACTIONS OF ACETIC ACID WITH HYDROXYLAMINE AND ITS IONIZED AND PROTONATED DERIVATIVES. <i>Astrophysical Journal</i> , 2012, 748, 99. | 4.5  | 37        |
| 11 | PEPTIDE BOND FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM: FORMAMIDE AND ACETAMIDE AS PROTOTYPES. <i>Astrophysical Journal</i> , 2014, 793, 32.   | 4.5  | 37        |
| 12 | A theoretical study of the $C_2H$ , $C_2F$ and $C_2Cl$ radicals and their positive ions. <i>Chemical Physics</i> , 1989, 138, 291-301.  | 1.9  | 36        |
| 13 | Theoretical Study of $MgC_n$ , $MgC_n^+$ , $MgC_n^-(n=1-7)$ Open-Chain Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4676-4682.   | 2.5  | 35        |
| 14 | Small Carbon Clusters Doped with Early Transition Metals: A Theoretical Study of $ScC_n$ , $ScC_n^+$ , and $ScC_n^-(n=1-8)$ Open-Chain Clusters. <i>Journal of Physical Chemistry A</i> , 2005, 109, 8594-8603.               | 2.5  | 35        |
| 15 | Theoretical Study of the $C_3P$ Radical and Its Cation. <i>The Journal of Physical Chemistry</i> , 1996, 100, 585-593.  | 2.9  | 34        |
| 16 | Theoretical Study of Small $MgC_n$ , $MgC_n^+$ , and $MgC_n^-$ Cyclic Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6317-6325.  | 2.5  | 34        |
| 17 | Theoretical study of possible ion-molecule reactions leading to precursors of glycine in the interstellar medium. <i>International Journal of Quantum Chemistry</i> , 2004, 98, 355-360.                                      | 2.0  | 34        |
| 18 | Small Carbon Clusters Doped with Vanadium Metal: A Density Functional Study of $VC_n(n=1-8)$ . <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 885-893.  | 5.3  | 33        |

| #  | ARTICLE   | IF  | CITATIONS |
|----|---|-----|-----------|
| 19 | Theoretical study of acetyleneboron and acetylenealuminum isomers: the interactions of boron and aluminum atoms with acetylene. <i>The Journal of Physical Chemistry</i> , 1992, 96, 3015-3021.                                       | 2.9 | 32        |
| 20 | Small ScCn Cyclic Clusters: A Density Functional Study of Their Structure and Stability. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4057-4064.   | 2.5 | 32        |
| 21 | Low-lying states of AlC <sub>2</sub> and SiC <sub>2</sub> <sup>+</sup> : Competition between linear and cyclic configurations. <i>Chemical Physics</i> , 1990, 140, 19-26.  | 1.9 | 30        |
| 22 | Computational study on the kinetics of the reaction of N(4S) with CH <sub>2</sub> F. <i>Chemical Physics Letters</i> , 2003, 374, 594-600.  | 2.6 | 30        |
| 23 | Computational study of the reaction of N(D <sub>2</sub> ) atoms with CH <sub>2</sub> F radicals: An example of a barrier-free reaction involving very high internal energies. <i>Journal of Chemical Physics</i> , 2005, 123, 114312. | 3.0 | 29        |
| 24 | SOME INSIGHTS INTO FORMAMIDE FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM. <i>Astrophysical Journal</i> , 2014, 780, 181.   | 4.5 | 29        |
| 25 | A Theoretical study of the SiCN radical. <i>Chemical Physics Letters</i> , 1988, 147, 95-98.  | 2.6 | 28        |
| 26 | Structure and Stability of Small NaCn, NaCn <sup>+</sup> , and NaCn <sup>-</sup> Clusters: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 212-224.  | 2.5 | 27        |
| 27 | Structure and Stability of Small ZnCn Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 657-664.   | 5.3 | 27        |
| 28 | Theoretical study of AlC <sub>3</sub> : linear or cyclic ground state?. <i>Chemical Physics Letters</i> , 2000, 320, 481-486.   | 2.6 | 26        |
| 29 | The reaction between NH <sub>3</sub> <sup>+</sup> and CH <sub>3</sub> COOH: a possible process for the formation of glycine precursors in the interstellar medium. <i>Astronomy and Astrophysics</i> , 2010, 516, A79.                | 5.1 | 26        |
| 30 | Structure and Properties of the Open-Chain Calcium-Doped Carbon Clusters CaCn, CaCn <sup>+</sup> , and CaCn <sup>-</sup> (n = 1-8). <i>Journal of Physical Chemistry A</i> , 2004, 108, 6421-6429.                                    | 2.5 | 25        |
| 31 | Structure and Bonding in First-Row Transition Metal Dicarbide Cations MC <sub>2</sub> <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , 2007, 111, 6345-6353.   | 2.5 | 25        |
| 32 | Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with ammonia. <i>The Journal of Physical Chemistry</i> , 1991, 95, 170-175.                             | 2.9 | 24        |
| 33 | SYNTHESIS OF FORMAMIDE AND RELATED ORGANIC SPECIES IN THE INTERSTELLAR MEDIUM VIA CHEMICAL DYNAMICS SIMULATIONS. <i>Astrophysical Journal</i> , 2016, 826, 107.   | 4.5 | 24        |
| 34 | A preliminary theoretical study of the SiC <sub>2</sub> H radical: Implications in astrophysics. <i>Chemical Physics Letters</i> , 1988, 147, 90-94.  | 2.6 | 23        |
| 35 | Structures and energies of the chlorine-substituted analogues of C <sub>3</sub> H <sub>2</sub> : an ab initio and density functional theory comparative study. <i>Computational and Theoretical Chemistry</i> , 2000, 505, 221-232.   | 1.5 | 23        |
| 36 | On the Molecular Structure of Uranium Dicarbide: T-Shape versus Linear Isomers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2972-2977.  | 2.5 | 23        |

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 37 | Theoretical studies of potential astrophysical molecules. The ClCC and SC2H radicals. <i>Chemical Physics Letters</i> , 1989, 155, 550-556.  | 2.6 | 21        |
| 38 | Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with hydrogen cyanide and protonation of cyanogen phosphide compounds. <i>The Journal of Physical Chemistry</i> , 1991, 95, 9864-9868. | 2.9 | 21        |
| 39 | Theoretical Study of SiC3+. <i>Journal of Physical Chemistry A</i> , 1998, 102, 3953-3958.   | 2.5 | 21        |
| 40 | Theoretical study of the structures and stabilities of AlC <sub>n</sub> , AlC <sub>n</sub> <sup>+</sup> , and AlC <sub>n</sub> <sup>-</sup> (n = 1-7) monocyclic clusters. <i>International Journal of Quantum Chemistry</i> , 2004, 96, 615-626.                    | 2.0 | 21        |
| 41 | The Hylleraas-Cl method in molecular calculations: Two-electron integrals. <i>Journal of Computational Chemistry</i> , 1987, 8, 1191-1198.   | 3.3 | 20        |
| 42 | Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with water. <i>The Journal of Physical Chemistry</i> , 1991, 95, 5443-5445.  | 2.9 | 20        |
| 43 | Structures and stabilities of MgC3 isomers: a theoretical study. <i>Chemical Physics Letters</i> , 2001, 335, 64-70.   | 2.6 | 20        |
| 44 | Structure and bonding in third-row main group dicarbides C2X (X=KBr). <i>Journal of Chemical Physics</i> , 2010, 133, 124306.  | 3.0 | 20        |
| 45 | Structures and stabilities of non-linear VC <sub>n</sub> <sup>+</sup> (n=1-8) clusters. <i>International Journal of Mass Spectrometry</i> , 2007, 263, 101-112.  | 1.5 | 19        |
| 46 | Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 869-877.   | 2.5 | 19        |
| 47 | A theoretical study of the structures and stabilities of (H2PO) <sup>+</sup> species and the proton affinities of HPO and POH. <i>The Journal of Physical Chemistry</i> , 1991, 95, 4318-4323.   | 2.9 | 18        |
| 48 | Theoretical study of the C3Cl radical and its cation. <i>Chemical Physics Letters</i> , 1999, 315, 224-232.  | 2.6 | 18        |
| 49 | Reaction of C3H2 <sup>+</sup> with Atomic Nitrogen: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11541-11548.  | 2.5 | 18        |
| 50 | Structure and Stability of AlC2N Isomers: A Comparative ab Initio and DFT Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6724-6728.  | 2.5 | 18        |
| 51 | Ionization potential and electron affinity of VC <sub>n</sub> (n=1-8) open-chain clusters: A theoretical study. <i>Computational and Theoretical Chemistry</i> , 2006, 769, 225-236.   | 1.5 | 18        |
| 52 | Theoretical studies of possible processes for interstellar production of phosphorus compounds: reaction of phosphorus(1+) with methane. <i>The Journal of Physical Chemistry</i> , 1991, 95, 6553-6557.  | 2.9 | 17        |
| 53 | Theoretical study of possible interstellar processes for the production of C2Cl precursors. <i>Computational and Theoretical Chemistry</i> , 1998, 432, 75-88.   | 1.5 | 17        |
| 54 | Theoretical study of the structures and stabilities of NaC3 isomers. <i>Chemical Physics Letters</i> , 2001, 343, 563-570.   | 2.6 | 17        |

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|----|--|-----|-----------|
| 55 | The Reaction of Nitrogen Atoms with Methyl Radicals: Are Spin-Forbidden Channels Important?. Journal of Physical Chemistry A, 2006, 110, 10912-10920.  | 2.5 | 17        |
| 56 | Theoretical Study of the Structures and Stabilities of Small CaC <sub>n</sub> , CaC <sub>n</sub> <sup>+</sup> , and CaC <sub>n</sub> -(n= 1-8) Cyclic Clusters. Journal of Physical Chemistry A, 2004, 108, 11132-11140. | 2.5 | 16        |
| 57 | Structural and electronic properties of ZnC <sub>n</sub> <sup>+/0</sup> clusters. International Journal of Mass Spectrometry, 2008, 273, 87-94.  | 1.5 | 16        |
| 58 | COMPUTATIONAL PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF METHANEDIOL, AN ELUSIVE MOLECULE FOR INTERSTELLAR DETECTION. Astrophysical Journal, 2014, 784, 132.  | 4.5 | 16        |
| 59 | The formation of urea in space. Astronomy and Astrophysics, 2018, 610, A26.  | 5.1 | 16        |
| 60 | Theoretical study of possible processes for the interstellar production of phosphorus compounds. Reaction of phosphorus(1+) with hydrogen sulfide. The Journal of Physical Chemistry, 1993, 97, 1521-1525.               | 2.9 | 15        |
| 61 | A density functional study of CoC <sub>n</sub> (n = 1-8) clusters: Structures and stabilities. International Journal of Quantum Chemistry, 2008, 108, 1684-1695.   | 2.0 | 15        |
| 62 | Is the reaction between formic acid and protonated aminomethanol a possible source of glycine precursors in the interstellar medium?. Astronomy and Astrophysics, 2015, 579, A125.                                       | 5.1 | 15        |
| 63 | Structure and Spectroscopic Properties of [Mg,C,N,O] Isomers: Plausible Astronomical Molecules. ACS Earth and Space Chemistry, 2017, 1, 158-167.   | 2.7 | 15        |
| 64 | Reaction of N(2D) atoms with bromomethyl radicals: A theoretical study. Chemical Physics, 2006, 328, 45-52.  | 1.9 | 14        |
| 65 | Structures and stabilities of charged cobalt-doped carbon clusters. International Journal of Mass Spectrometry, 2008, 272, 187-198.  | 1.5 | 14        |
| 66 | Computational study of peptide bond formation in the gas phase through ion-molecule reactions. Physical Chemistry Chemical Physics, 2013, 15, 13005.   | 2.8 | 14        |
| 67 | An ab initio study of Si2C protonation. Chemical Physics Letters, 1988, 145, 128-133.  | 2.6 | 13        |
| 68 | Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. The Reaction of P <sup>+</sup> with Acetylene. The Journal of Physical Chemistry, 1995, 99, 6432-6440.                | 2.9 | 13        |
| 69 | Reaction of carbon atoms with H <sub>2</sub> Cl <sup>+</sup> : an ab initio study of a possible interstellar process. Computational and Theoretical Chemistry, 1996, 363, 319-331.                                       | 1.5 | 13        |
| 70 | Structure and stability of binary calcium-carbon compounds: a comparative ab initio and DFT study of CaC <sub>2</sub> . Chemical Physics Letters, 2003, 382, 150-159.  | 2.6 | 13        |
| 71 | Molecular structure of uranium carbides: Isomers of UC <sub>3</sub> . Journal of Chemical Physics, 2013, 138, 114307.  | 3.0 | 13        |
| 72 | Generation and structural characterization of aluminum cyanoacetylide. Journal of Chemical Physics, 2014, 141, 104305.   | 3.0 | 13        |

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|----|---|-----|-----------|
| 73 | Theoretical study of a basic process in interstellar chlorine chemistry: reaction of carbon(1+) with hydrogen chloride. The Journal of Physical Chemistry, 1993, 97, 173-176.   | 2.9 | 12        |
| 74 | Theoretical Study of the Structures and Stabilities of (SiC <sub>2</sub> H <sub>2</sub> ) <sup>+</sup> Species. The Reaction of Si <sup>+</sup> with Acetylene. The Journal of Physical Chemistry, 1994, 98, 3978-3984.           | 2.9 | 12        |
| 75 | Computational study of the thermal reaction rate between S <sup>+</sup> (4S) and acetylene. Chemical Physics, 2001, 265, 251-261.   | 1.9 | 12        |
| 76 | Stability of protonated and ionized hydroxylamine in the interstellar medium. Chemical Physics Letters, 2009, 476, 174-177.   | 2.6 | 12        |
| 77 | Theoretical study of the interactions of beryllium and magnesium atoms with acetylene. The Journal of Physical Chemistry, 1991, 95, 9278-9288.  | 2.9 | 11        |
| 78 | Ab initio characterization of gaseous phosphorus oxide (P <sub>2</sub> O <sub>2</sub> ). The Journal of Physical Chemistry, 1993, 97, 4078-4079.  | 2.9 | 11        |
| 79 | The Reaction of N(4S) with CH <sub>2</sub> F: A Comparative ab Initio and DFT Study. Journal of Physical Chemistry A, 2001, 105, 9917-9925.   | 2.5 | 11        |
| 80 | Intrinsic Antioxidant Potential of the Aminoindole Structure: A Computational Kinetics Study of Tryptamine. Journal of Physical Chemistry B, 2018, 122, 6386-6395.  | 2.6 | 11        |
| 81 | Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds: The Reaction of P <sup>+</sup> with C <sub>3</sub> H <sub>2</sub> . The Journal of Physical Chemistry, 1996, 100, 14643-14650. | 2.9 | 10        |
| 82 | Theoretical Study of the Reaction of Si <sup>+</sup> with C <sub>3</sub> H <sub>2</sub> . Journal of Physical Chemistry A, 1999, 103, 3310-3320.  | 2.5 | 10        |
| 83 | A theoretical study of the structures and stabilities of SC <sub>2</sub> H <sub>2</sub> <sup>+</sup> species: the reaction of sulfur(1+) with acetylene. The Journal of Physical Chemistry, 1992, 96, 5808-5814.                  | 2.9 | 9         |
| 84 | Reactions of methylium ion with second-row atoms: an ab initio study. The Journal of Physical Chemistry, 1994, 98, 1090-1099.   | 2.9 | 9         |
| 85 | Structures and stabilities of CaC <sub>3</sub> isomers. Chemical Physics Letters, 2002, 355, 509-516.   | 2.6 | 9         |
| 86 | Gas-Phase Reaction of NH <sub>2</sub> <sup>+</sup> with Acetic Acid: Implications in Astrochemistry. Journal of Chemical Theory and Computation, 2008, 4, 2085-2093.  | 5.3 | 9         |
| 87 | On the electric dipole moments of small sodium clusters from different theoretical approaches. Chemical Physics, 2012, 399, 252-257.  | 1.9 | 9         |
| 88 | Molecular Structure and Bonding in Plutonium Carbides: A Theoretical Study of PuC <sub>3</sub> . Journal of Physical Chemistry A, 2016, 120, 2232-2239.   | 2.5 | 9         |
| 89 | PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF NEW IRON COMPOUNDS: HYDRIDE OF IRON CYANIDE/ISOCYANIDE, HFeCN/HFeNC. Astrophysical Journal, 2016, 828, 45.  | 4.5 | 9         |
| 90 | Theoretical Study of the Reaction of S <sup>+</sup> with C <sub>3</sub> H <sub>2</sub> . Journal of Physical Chemistry A, 1999, 103, 9125-9131.   | 2.5 | 8         |

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|-----|---|-----|-----------|
| 91  | A computational study of arsenic dicarbide (C2As). Chemical Physics Letters, 2010, 485, 286-289.  | 2.6 | 8         |
| 92  | Structure and stability of neutral cyanide complexes of copper and zinc. Chemical Physics Letters, 2011, 504, 125-129.  | 2.6 | 8         |
| 93  | Reactivity of First-Row Transition Metal Monocations (Sc <sup>+</sup> , Ti <sup>+</sup> ,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf<br>Chemistry A, 2013, 117, 2932-2943.   | 2.5 | 8         |
| 94  | Structure and spectroscopic properties of neutral and cationic tetratomic [C,H,N,Zn] isomers: A theoretical study. Journal of Chemical Physics, 2015, 142, 184301.  | 3.0 | 8         |
| 95  | Prebiotic molecules formation through the gas-phase reaction between HNO and CH <sub>2</sub> CHOH <sub>2</sub> <sup>+</sup> . Astronomy and Astrophysics, 2017, 603, A139.  | 5.1 | 8         |
| 96  | Theoretical study of AlC <sub>3</sub> <sup>+</sup> . International Journal of Quantum Chemistry, 2001, 84, 660-669.   | 2.0 | 7         |
| 97  | Structures and stabilities of C <sub>3</sub> Cl <sub>2</sub> and C <sub>3</sub> Cl <sub>2</sub> <sup>+</sup> isomers: a theoretical study. Computational and Theoretical Chemistry, 2003, 621, 59-73.                         | 1.5 | 7         |
| 98  | Neutral cyanide complexes of iron: Structure and stability. Chemical Physics Letters, 2010, 500, 9-13.  | 2.6 | 7         |
| 99  | Complex Organic Molecules Formation in Space Through Gas Phase Reactions: A Theoretical Approach. Astrophysical Journal, 2017, 836, 240.  | 4.5 | 7         |
| 100 | Formation of Protonated Glycine Isomers in the Interstellar Medium. ACS Earth and Space Chemistry, 2019, 3, 1170-1181.  | 2.7 | 7         |
| 101 | Theoretical study of the reaction of S <sup>+</sup> with acetylene. Chemical Physics Letters, 1999, 306, 168-178.   | 2.6 | 6         |
| 102 | Could the reactions of formic acid with CH <sub>3</sub> NH <sub>2</sub> <sup>+</sup> /CH <sub>3</sub> NH <sub>3</sub> <sup>+</sup> produce protonated glycine?. International Journal of Mass Spectrometry, 2010, 295, 21-25. | 1.5 | 6         |
| 103 | Theoretical study of the C-F bond activation in methyl fluoride by alkaline-earth metal monocations. Theoretical Chemistry Accounts, 2011, 128, 609-618.  | 1.4 | 6         |
| 104 | Alkaline and alkaline-earth cyanoacetylides: A combined theoretical and rotational spectroscopic investigation. Journal of Chemical Physics, 2019, 151, 054312.   | 3.0 | 6         |
| 105 | A theoretical study of SiC <sub>2</sub> <sup>+</sup> . Chemical Physics Letters, 1987, 140, 26-30.  | 2.6 | 5         |
| 106 | A theoretical study of protonation of triatomic silicon-carbon compounds. International Journal of Quantum Chemistry, 1989, 36, 241-253.  | 2.0 | 5         |
| 107 | An ab initio study of C <sub>2</sub> S protonation. Chemical Physics Letters, 1991, 184, 168-174.   | 2.6 | 5         |
| 108 | Ab-initio study of phosphorus ion complexes of ammonia and water. The Journal of Physical Chemistry, 1993, 97, 9337-9340.   | 2.9 | 5         |

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|-----|---|-----|-----------|
| 109 | Theoretical Studies of Simple Organoboron Compounds: Structures and Stabilities of BC <sub>2</sub> H <sub>4</sub> Isomers. Applied Organometallic Chemistry, 1996, 10, 283-295.                         | 3.5 | 5         |
| 110 | Theoretical study of the reaction of CN with C <sub>2</sub> H <sub>2</sub> <sup>+</sup> . Theoretical Chemistry Accounts, 2000, 104, 199-202.   | 1.4 | 5         |
| 111 | Theoretical Study of the Reaction of Cl <sup>+</sup> with C <sub>3</sub> H <sub>2</sub> . Journal of Physical Chemistry A, 2000, 104, 9733-9739.  | 2.5 | 5         |
| 112 | Reactivity of gaseous protonated ozone: a computational investigation on the carbon monoxide oxidation reaction. International Journal of Mass Spectrometry, 2003, 228, 613-627.                        | 1.5 | 5         |
| 113 | Polyisocyanides of Titanium. Journal of Physical Chemistry A, 2009, 113, 1574-1577.   | 2.5 | 5         |
| 114 | Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. Monthly Notices of the Royal Astronomical Society, 2018, 478, 3042-3048.                                | 4.4 | 5         |
| 115 | A comparative theoretical study of the C <sub>2</sub> N <sup>+</sup> and SiCN <sup>+</sup> ions and their formation processes. Chemical Physics Letters, 1988, 148, 79-85.                              | 2.6 | 4         |
| 116 | Ab initio characterization of novel gaseous phosphorus oxide ((PO) <sub>2</sub> <sup>+</sup> ) species. The Journal of Physical Chemistry, 1993, 97, 5860-5863.   | 2.9 | 4         |
| 117 | Ionization and protonation of MgC <sub>3</sub> : A theoretical study. International Journal of Quantum Chemistry, 2002, 86, 114-121.  | 2.0 | 4         |
| 118 | A Computational Study of the Reaction of Ground-State Nitrogen Atoms with Chloromethyl Radicals. Journal of Physical Chemistry A, 2005, 109, 6540-6548.   | 2.5 | 4         |
| 119 | Structure of binary titanium-carbon ions: A theoretical study of $\text{TiC}^+$ . Chemical Physics Letters, 2007, 445, 22-27.   | 2.6 | 4         |
| 120 | A theoretical study of the [FeCN] <sup>+</sup> system: Cyanide-isocyanide competition and isomerization barrier. Chemical Physics Letters, 2007, 445, 22-27.  | 2.6 | 4         |
| 121 | Cyanide complexes of Ti(IV): A computational study. Journal of Chemical Physics, 2009, 131, 094507.   | 3.0 | 4         |
| 122 | Small carbides of third-row main group elements: structure and bonding in C <sub>3</sub> X compounds (X = Tl, Pb, Bi, Po, At, Rn). Journal of Physical Chemistry A, 2009, 113, 10743-10750.             | 2.8 | 4         |
| 123 | Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest. Astrophysical Journal, 2019, 871, 180.   | 4.5 | 4         |
| 124 | Formation of interstellar cyanoacetamide: a rotational and computational study. Astronomy and Astrophysics, 2020, 644, A3.  | 5.1 | 4         |
| 125 | Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules. Astrophysical Journal, 2020, 899, 135.  | 4.5 | 4         |
| 126 | Interelectronic repulsion distribution functions in the ground state of helium: slow convergence of CI wavefunctions. Journal of Physics B: Atomic, Molecular and Optical Physics, 1988, 21, 2377-2387. | 1.5 | 3         |



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|-----|---|-----|-----------|
| 127 | On the reaction of ground-state nitrogen atoms with bromomethyl radicals: A computational study. <i>International Journal of Mass Spectrometry</i> , 2006, 249-250, 451-461.  | 1.5 | 3         |
| 128 | Metallic cyanoacetylides of copper, silver and gold: generation and structural characterization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28538-28547.  | 2.8 | 3         |
| 129 | Metallic monoboronyl compounds: Prediction of their structure and comparison with the cyanide analogues. <i>Journal of Computational Chemistry</i> , 2017, 38, 807-815.   | 3.3 | 3         |
| 130 | Structural Trends in Monoboronyl Compounds: Analysis of the Interaction of Second-Row Elements with BO. <i>Journal of Physical Chemistry A</i> , 2018, 122, 398-409.  | 2.5 | 3         |
| 131 | Infrared-Assisted Synthesis of Prebiotic Glycine. <i>ChemPhysChem</i> , 2020, 21, 503-509.  | 2.1 | 3         |
| 132 | The correlation effects at a local level. CI partitions. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 845-852.   | 2.0 | 2         |
| 133 | An ab initio study of Si <sub>3</sub> protonation. <i>Chemical Physics Letters</i> , 1988, 147, 79-83.  | 2.6 | 2         |
| 134 | Ab Initio Characterization of Gaseous (CO <sub>2</sub> P) <sup>+</sup> Species. <i>The Journal of Physical Chemistry</i> , 1994, 98, 2294-2297.   | 2.9 | 2         |
| 135 | Topological Analysis of the Charge Density for Phosphorus Ion Molecule Complexes Bound to Water and Ammonia Molecules. <i>The Journal of Physical Chemistry</i> , 1994, 98, 3148-3153.  | 2.9 | 2         |
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