

# Antonio Largo

## List of Publications by Year in descending order

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148  
papers

2,298  
citations

201385

27  
h-index

344852

36  
g-index

148  
all docs

148  
docs citations

148  
times ranked

1197  
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	0.7	104
2	Theoretical Study of $AlC_n$ , $AlC_n^+$ , and $AlC_n^-(n=1-7)$ Clusters. Journal of Physical Chemistry A, 2002, 106, 4217-4225.	1.1	52
3	<i>Planck</i> 2013 results. Astronomy and Astrophysics, 2014, 571, E1.	2.1	51
4	Cyanides and Isocyanides of First-Row Transition Metals: Molecular Structure, Bonding, and Isomerization Barriers. Journal of Physical Chemistry A, 2007, 111, 6334-6344.	1.1	50
5	Gaussian functions in hylleraas-Cl calculations. I. Ground state energies for $H_2$ , $HeH^+$ , and $H_3$ . Journal of Chemical Physics, 1988, 88, 2091-2093.	1.2	46
6	Theoretical study of $C_nCl$ , $C_nCl^+$ , $C_nCl^-(n=1-7)$ clusters. International Journal of Quantum Chemistry, 2001, 84, 127-135.	1.0	46
7	Structure and Bonding in First-Row Transition-Metal Dicarbides: Are They Related to the Stability of Met-cars?. Chemistry - A European Journal, 2006, 12, 6963-6975.	1.7	44
8	On the Competition between Linear and Cyclic Isomers in Second-Row Dicarbides. Journal of the American Chemical Society, 2004, 126, 14611-14619.	6.6	42
9	Theoretical Study of the $C_2P$ Radical and $(C_2P)^+$ Species. The Journal of Physical Chemistry, 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. Astrophysical Journal, 2012, 748, 99.	1.6	37
11	PEPTIDE BOND FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM: FORMAMIDE AND ACETAMIDE AS PROTOTYPES. Astrophysical Journal, 2014, 793, 32.	1.6	37
12	A theoretical study of the $C_2H$ , $C_2F$ and $C_2Cl$ radicals and their positive ions. Chemical Physics, 1989, 138, 291-301.	0.9	36
13	Theoretical Study of $MgC_n$ , $MgC_n^+$ , $MgC_n^-(n=1-7)$ Open-Chain Clusters. Journal of Physical Chemistry A, 2003, 107, 4676-4682.	1.1	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. Journal of Physical Chemistry A, 2005, 109, 8594-8603.	1.1	35
15	Theoretical Study of the $C_3P$ Radical and Its Cation. The Journal of Physical Chemistry, 1996, 100, 585-593.	2.9	34
16	Theoretical Study of Small $MgC_n$ , $MgC_n^+$ , and $MgC_n^-$ Cyclic Clusters. Journal of Physical Chemistry A, 2003, 107, 6317-6325.	1.1	34
17	Theoretical study of possible ion-molecule reactions leading to precursors of glycine in the interstellar medium. International Journal of Quantum Chemistry, 2004, 98, 355-360.	1.0	34
18	Small Carbon Clusters Doped with Vanadium Metal: A Density Functional Study of $VC_n(n=1-8)$ . Journal of Chemical Theory and Computation, 2006, 2, 885-893.	2.3	33

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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.	1.1	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.	0.9	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.	1.2	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.	1.2	29
24	SOME INSIGHTS INTO FORMAMIDE FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM. <i>Astrophysical Journal</i> , 2014, 780, 181.	1.6	29
25	A Theoretical study of the SiCN radical. <i>Chemical Physics Letters</i> , 1988, 147, 95-98.	1.2	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.	1.1	27
27	Structure and Stability of Small ZnCn Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 657-664.	2.3	27
28	Theoretical study of AlC <sub>3</sub> : linear or cyclic ground state?. <i>Chemical Physics Letters</i> , 2000, 320, 481-486.	1.2	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.	2.1	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.	1.1	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.	1.1	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.	1.6	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.	1.2	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.	1.1	23

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37	Theoretical studies of potential astrophysical molecules. The ClCC and SC2H radicals. <i>Chemical Physics Letters</i> , 1989, 155, 550-556.	1.2	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.	1.1	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.	1.0	21
41	The Hylleraas-CI method in molecular calculations: Two-electron integrals. <i>Journal of Computational Chemistry</i> , 1987, 8, 1191-1198.	1.5	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.	1.2	20
44	Structure and bonding in third-row main group dicarbides C2X (X=KBr). <i>Journal of Chemical Physics</i> , 2010, 133, 124306.	1.2	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.	0.7	19
46	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 869-877.	1.1	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.	1.2	18
49	Reaction of C3H2 <sup>+</sup> with Atomic Nitrogen: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11541-11548.	1.1	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.	1.1	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.	1.2	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.	1.1	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.	1.1	16
57	Structural and electronic properties of ZnC <sub>n</sub> <sup>+/0</sup> clusters. International Journal of Mass Spectrometry, 2008, 273, 87-94.	0.7	16
58	COMPUTATIONAL PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF METHANEDIOL, AN ELUSIVE MOLECULE FOR INTERSTELLAR DETECTION. Astrophysical Journal, 2014, 784, 132.	1.6	16
59	The formation of urea in space. Astronomy and Astrophysics, 2018, 610, A26.	2.1	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.	1.0	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.	2.1	15
63	Structure and Spectroscopic Properties of [Mg,C,N,O] Isomers: Plausible Astronomical Molecules. ACS Earth and Space Chemistry, 2017, 1, 158-167.	1.2	15
64	Reaction of N(2D) atoms with bromomethyl radicals: A theoretical study. Chemical Physics, 2006, 328, 45-52.	0.9	14
65	Structures and stabilities of charged cobalt-doped carbon clusters. International Journal of Mass Spectrometry, 2008, 272, 187-198.	0.7	14
66	Computational study of peptide bond formation in the gas phase through ion-molecule reactions. Physical Chemistry Chemical Physics, 2013, 15, 13005.	1.3	14
67	An ab initio study of Si2C protonation. Chemical Physics Letters, 1988, 145, 128-133.	1.2	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.	1.2	13
71	Molecular structure of uranium carbides: Isomers of UC <sub>3</sub> . Journal of Chemical Physics, 2013, 138, 114307.	1.2	13
72	Generation and structural characterization of aluminum cyanoacetylide. Journal of Chemical Physics, 2014, 141, 104305.	1.2	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.	0.9	12
76	Stability of protonated and ionized hydroxylamine in the interstellar medium. Chemical Physics Letters, 2009, 476, 174-177.	1.2	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.	1.1	11
80	Intrinsic Antioxidant Potential of the Aminoindole Structure: A Computational Kinetics Study of Tryptamine. Journal of Physical Chemistry B, 2018, 122, 6386-6395.	1.2	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.	1.1	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 methylum 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.	1.2	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.	2.3	9
87	On the electric dipole moments of small sodium clusters from different theoretical approaches. Chemical Physics, 2012, 399, 252-257.	0.9	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.	1.1	9
89	PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF NEW IRON COMPOUNDS: HYDRIDE OF IRON CYANIDE/ISOCYANIDE, HFeCN/HFeNC. Astrophysical Journal, 2016, 828, 45.	1.6	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.	1.1	8

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91	A computational study of arsenic dicarbide (C2As). Chemical Physics Letters, 2010, 485, 286-289.	1.2	8
92	Structure and stability of neutral cyanide complexes of copper and zinc. Chemical Physics Letters, 2011, 504, 125-129.	1.2	8
93	Reactivity of First-Row Transition Metal Monocations (Sc <sup>+</sup> , Ti <sup>+</sup> ,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf Chemistry A, 2013, 117, 2932-2943.	1.1	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.	1.2	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.	2.1	8
96	Theoretical study of AlC <sub>3</sub> <sup>+</sup> . International Journal of Quantum Chemistry, 2001, 84, 660-669.	1.0	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.	1.2	7
99	Complex Organic Molecules Formation in Space Through Gas Phase Reactions: A Theoretical Approach. Astrophysical Journal, 2017, 836, 240.	1.6	7
100	Formation of Protonated Glycine Isomers in the Interstellar Medium. ACS Earth and Space Chemistry, 2019, 3, 1170-1181.	1.2	7
101	Theoretical study of the reaction of S <sup>+</sup> with acetylene. Chemical Physics Letters, 1999, 306, 168-178.	1.2	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.	0.7	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.	0.5	6
104	Alkaline and alkaline-earth cyanoacetylides: A combined theoretical and rotational spectroscopic investigation. Journal of Chemical Physics, 2019, 151, 054312.	1.2	6
105	A theoretical study of SiC <sub>2</sub> <sup>+</sup> . Chemical Physics Letters, 1987, 140, 26-30.	1.2	5
106	A theoretical study of protonation of triatomic silicon-carbon compounds. International Journal of Quantum Chemistry, 1989, 36, 241-253.	1.0	5
107	An ab initio study of C <sub>2</sub> S protonation. Chemical Physics Letters, 1991, 184, 168-174.	1.2	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.	1.7	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.	0.5	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.	1.1	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.	0.7	5
113	Polyisocyanides of Titanium. Journal of Physical Chemistry A, 2009, 113, 1574-1577.	1.1	5
114	Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. Monthly Notices of the Royal Astronomical Society, 2018, 478, 3042-3048.	1.6	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.	1.2	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.	1.0	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.	1.1	4
119	Structure of binary titanium carbide ions: A theoretical study of $\text{TiC}_2^+$ . Chemical Physics Letters, 2007, 445, 22-27.	1.2	4
120	A theoretical study of the [FeCN] <sup>+</sup> system: Cyanide-isocyanide competition and isomerization barrier. Chemical Physics Letters, 2007, 445, 22-27.	1.2	4
121	Cyanide complexes of Ti(IV): A computational study. Journal of Chemical Physics, 2009, 131, 094507.	1.2	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, 1574-1577.	1.3	4
123	Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest. Astrophysical Journal, 2019, 871, 180.	1.6	4
124	Formation of interstellar cyanoacetamide: a rotational and computational study. Astronomy and Astrophysics, 2020, 644, A3.	2.1	4
125	Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules. Astrophysical Journal, 2020, 899, 135.	1.6	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.	0.6	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.	0.7	3
128	Metallic cyanoacetylides of copper, silver and gold: generation and structural characterization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28538-28547.	1.3	3
129	Metallic monoboron compounds: Prediction of their structure and comparison with the cyanide analogues. <i>Journal of Computational Chemistry</i> , 2017, 38, 807-815.	1.5	3
130	Structural Trends in Monoboron Compounds: Analysis of the Interaction of Second-Row Elements with BO. <i>Journal of Physical Chemistry A</i> , 2018, 122, 398-409.	1.1	3
131	Infrared-Assisted Synthesis of Prebiotic Glycine. <i>ChemPhysChem</i> , 2020, 21, 503-509.	1.0	3
132	The correlation effects at a local level. CI partitions. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 845-852.	1.0	2
133	An ab initio study of Si <sub>3</sub> protonation. <i>Chemical Physics Letters</i> , 1988, 147, 79-83.	1.2	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
136	Reaction of C <sub>3</sub> H <sub>2</sub> <sup>+</sup> with Atomic Chlorine: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6346-6351.	1.1	2
137	Theoretical Study of the Reaction of HCl with C <sub>3</sub> H <sub>2</sub> <sup>+</sup> : A Possible Source of Carbon-Chlorine Compounds in Space. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5844-5853.	1.1	2
138	A computational study on the reaction of N(2D) atoms with CH <sub>2</sub> Cl radicals. <i>Chemical Physics Letters</i> , 2006, 422, 276-281.	1.2	2
139	Computational Study of the Reaction of P <sup>+</sup> with Acetylene: Does Spin-Crossing Play a Significant Role?. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3014-3022.	1.1	2
140	Kinetics Studies of the Reactions of Main Fourth-Period Monocations (Ga <sup>+</sup> , Tl <sup>+</sup> , Pb <sup>+</sup> , Bi <sup>+</sup> , Sn <sup>+</sup> , Sb <sup>+</sup> , Te <sup>+</sup> , I <sup>+</sup> , Xe <sup>+</sup> , Rn <sup>+</sup> ) with Ethylene. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7742-7753.	1.1	2
141	Halogen-abstraction reactions from chloromethane and bromomethane molecules by alkaline-earth monocations. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16121-16136.	1.3	2
142	Amino acetaldehyde conformers: structure and spectroscopic properties. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 492, 1827-1833.	1.6	2
143	Computational study on the affinity of potential drugs to SARS-CoV-2 main protease. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 294005.	0.7	2
144	Correlation effects at a local level and CI partitions: 23S State of helium. <i>International Journal of Quantum Chemistry</i> , 1988, 33, 323-326.	1.0	1

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145	Ionization and protonation of NaC <sub>3</sub> : a theoretical study. Computational and Theoretical Chemistry, 2003, 630, 59-73.	1.5	1
146	Structure and stability of BC <sub>2</sub> P isomers: a theoretical study. Computational and Theoretical Chemistry, 2003, 633, 57-65.	1.5	1
147	Structures and stabilities of CaC <sub>3</sub> <sup>+</sup> and CaC <sub>3</sub> H <sup>+</sup> isomers. Computational and Theoretical Chemistry, 2004, 709, 143-155.	1.5	0
148	On the Competition Between Linear and Cyclic Isomers in Second-Row Dicarbides. ChemInform, 2005, 36, no.	0.1	0