

# 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  
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148  
all docs

148  
docs citations

148  
times ranked

1197  
citing authors

#	ARTICLE	IF	CITATIONS
1	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
2	Amino acetaldehyde conformers: structure and spectroscopic properties. <i>Monthly Notices of the Royal Astronomical Society</i> , 2020, 492, 1827-1833.	1.6	2
3	Infrared-Assisted Synthesis of Prebiotic Glycine. <i>ChemPhysChem</i> , 2020, 21, 503-509.	1.0	3
4	Formation of interstellar cyanoacetamide: a rotational and computational study. <i>Astronomy and Astrophysics</i> , 2020, 644, A3.	2.1	4
5	Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules. <i>Astrophysical Journal</i> , 2020, 899, 135.	1.6	4
6	Alkaline and alkaline-earth cyanoacetylides: A combined theoretical and rotational spectroscopic investigation. <i>Journal of Chemical Physics</i> , 2019, 151, 054312.	1.2	6
7	Formation of Protonated Glycine Isomers in the Interstellar Medium. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 1170-1181.	1.2	7
8	Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest. <i>Astrophysical Journal</i> , 2019, 871, 180.	1.6	4
9	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.	1.1	3
10	Gas Phase Synthesis of Protonated Glycine by Chemical Dynamics Simulations. <i>Journal of Physical Chemistry A</i> , 2018, 122, 869-877.	1.1	19
11	Intrinsic Antioxidant Potential of the Aminoindole Structure: A Computational Kinetics Study of Tryptamine. <i>Journal of Physical Chemistry B</i> , 2018, 122, 6386-6395.	1.2	11
12	Structure and spectroscopic properties of imine acetaldehyde: a possible interstellar molecule. <i>Monthly Notices of the Royal Astronomical Society</i> , 2018, 478, 3042-3048.	1.6	5
13	The formation of urea in space. <i>Astronomy and Astrophysics</i> , 2018, 610, A26.	2.1	16
14	Complex Organic Molecules Formation in Space Through Gas Phase Reactions: A Theoretical Approach. <i>Astrophysical Journal</i> , 2017, 836, 240.	1.6	7
15	Metallic monoboronyl compounds: Prediction of their structure and comparison with the cyanide analogues. <i>Journal of Computational Chemistry</i> , 2017, 38, 807-815.	1.5	3
16	Structure and Spectroscopic Properties of [Mg,C,N,O] Isomers: Plausible Astronomical Molecules. <i>ACS Earth and Space Chemistry</i> , 2017, 1, 158-167.	1.2	15
17	Prebiotic molecules formation through the gas-phase reaction between HNO and CH <sub>2</sub> CHOH <sub>2</sub> <sup>+</sup> . <i>Astronomy and Astrophysics</i> , 2017, 603, A139.	2.1	8
18	Molecular Structure and Bonding in Plutonium Carbides: A Theoretical Study of PuC <sub>3</sub> . <i>Journal of Physical Chemistry A</i> , 2016, 120, 2232-2239.	1.1	9

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19	PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF NEW IRON COMPOUNDS: HYDRIDE OF IRON CYANIDE/ISOCYANIDE, HFeCN/HFeNC. <i>Astrophysical Journal</i> , 2016, 828, 45.	1.6	9
20	Metallic cyanoacetylides of copper, silver and gold: generation and structural characterization. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 28538-28547.	1.3	3
21	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
22	Is the reaction between formic acid and protonated aminomethanol a possible source of glycine precursors in the interstellar medium?. <i>Astronomy and Astrophysics</i> , 2015, 579, A125.	2.1	15
23	Structure and spectroscopic properties of neutral and cationic tetratomic [C,H,N,Zn] isomers: A theoretical study. <i>Journal of Chemical Physics</i> , 2015, 142, 184301.	1.2	8
24	<i>Planck</i>2013 results. <i>Astronomy and Astrophysics</i> , 2014, 571, E1.	2.1	51
25	SOME INSIGHTS INTO FORMAMIDE FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM. <i>Astrophysical Journal</i> , 2014, 780, 181.	1.6	29
26	Generation and structural characterization of aluminum cyanoacetylide. <i>Journal of Chemical Physics</i> , 2014, 141, 104305.	1.2	13
27	COMPUTATIONAL PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF METHANEDIOL, AN ELUSIVE MOLECULE FOR INTERSTELLAR DETECTION. <i>Astrophysical Journal</i> , 2014, 784, 132.	1.6	16
28	PEPTIDE BOND FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM: FORMAMIDE AND ACETAMIDE AS PROTOTYPES. <i>Astrophysical Journal</i> , 2014, 793, 32.	1.6	37
29	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
30	Computational study of peptide bond formation in the gas phase through ion-molecule reactions. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 13005.	1.3	14
31	Reactivity of First-Row Transition Metal Monocations (Sc <sup>+</sup> , Ti <sup>+</sup> ) <i>Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50</i> <i>Chemistry A</i> , 2013, 117, 2932-2943.	1.1	8
32	Kinetics Studies of the Reactions of Main Fourth-Period Monocations (Ga <sup>+</sup> ) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 227 Td (</i> <i>Chemistry A</i> , 2013, 117, 7742-7753.	1.1	2
33	Molecular structure of uranium carbides: Isomers of UC <sub>3</sub> . <i>Journal of Chemical Physics</i> , 2013, 138, 114307.	1.2	13
34	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
35	On the Molecular Structure of Uranium Dicarbid: T-Shape versus Linear Isomers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2972-2977.	1.1	23
36	Small carbides of third-row main group elements: structure and bonding in C <sub>3</sub> X compounds (X =) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50</i>	1.3	4

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37	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.	1.6	37
38	On the electric dipole moments of small sodium clusters from different theoretical approaches. <i>Chemical Physics</i> , 2012, 399, 252-257.	0.9	9
39	Theoretical study of the C-F bond activation in methyl fluoride by alkaline-earth metal monocations. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 609-618.	0.5	6
40	Structure and stability of neutral cyanide complexes of copper and zinc. <i>Chemical Physics Letters</i> , 2011, 504, 125-129.	1.2	8
41	The reaction between $\text{NH}_3^+ + \text{CH}_3\text{COOH}$ : a possible process for the formation of glycine precursors in the interstellar medium. <i>Astronomy and Astrophysics</i> , 2010, 516, A79.	2.1	26
42	Could the reactions of formic acid with $\text{CH}_3\text{NH}_2^+/\text{CH}_3\text{NH}_3^+$ produce protonated glycine?. <i>International Journal of Mass Spectrometry</i> , 2010, 295, 21-25.	0.7	6
43	A computational study of arsenic dicarbide (C2As). <i>Chemical Physics Letters</i> , 2010, 485, 286-289.	1.2	8
44	Neutral cyanide complexes of iron: Structure and stability. <i>Chemical Physics Letters</i> , 2010, 500, 9-13.	1.2	7
45	Structure and bonding in third-row main group dicarbides $\text{C}_2\text{X}$ (X=K-Br). <i>Journal of Chemical Physics</i> , 2010, 133, 124306.	1.2	20
46	Cyanide complexes of Ti(IV): A computational study. <i>Journal of Chemical Physics</i> , 2009, 131, 094507.	1.2	4
47	Stability of protonated and ionized hydroxylamine in the interstellar medium. <i>Chemical Physics Letters</i> , 2009, 476, 174-177.	1.2	12
48	Polyisocyanides of Titanium. <i>Journal of Physical Chemistry A</i> , 2009, 113, 1574-1577.	1.1	5
49	A density functional study of $\text{CoC}_n$ ( $n = 1-8$ ) clusters: Structures and stabilities. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1684-1695.	1.0	15
50	Structures and stabilities of charged cobalt-doped carbon clusters. <i>International Journal of Mass Spectrometry</i> , 2008, 272, 187-198.	0.7	14
51	Structural and electronic properties of $\text{ZnC}_n^+/\tilde{\text{a}}$ clusters. <i>International Journal of Mass Spectrometry</i> , 2008, 273, 87-94.	0.7	16
52	Gas-Phase Reaction of $\text{NH}_2^+ + \text{CH}_3\text{COOH}$ with Acetic Acid: Implications in Astrochemistry. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 2085-2093.	2.3	9
53	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.	1.1	50
54	Structure and Stability of Small $\text{ZnC}_n$ Clusters. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 657-664.	2.3	27

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55	Structure and Bonding in First-Row Transition Metal Dicarbide Cations MC <sub>2</sub> <sup>+</sup> . Journal of Physical Chemistry A, 2007, 111, 6345-6353.	1.1	25
56	A theoretical study of the [FeCN] <sup>+</sup> system: Cyanide vs isocyanide competition and isomerization barrier. Chemical Physics Letters, 2007, 445, 22-27.	1.2	4
57	Structures and stabilities of non-linear VC <sub>n</sub> <sup>+</sup> (n=1-8) clusters. International Journal of Mass Spectrometry, 2007, 263, 101-112.	0.7	19
58	Small Carbon Clusters Doped with Vanadium Metal: A Density Functional Study of VC <sub>n</sub> (n=1-8). Journal of Chemical Theory and Computation, 2006, 2, 885-893.	2.3	33
59	Small ScC <sub>n</sub> Cyclic Clusters: A Density Functional Study of Their Structure and Stability. Journal of Physical Chemistry A, 2006, 110, 4057-4064.	1.1	32
60	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
61	Reaction of N(2D) atoms with bromomethyl radicals: A theoretical study. Chemical Physics, 2006, 328, 45-52.	0.9	14
62	Structure of binary titaniumcarbon ions: A theoretical study of $\text{TiC}^+$ . Journal of Physical Chemistry A, 2006, 110, 10912-10920.	1.2	4
63	A computational study on the reaction of N(2D) atoms with CH <sub>2</sub> Cl radicals. Chemical Physics Letters, 2006, 422, 276-281.	1.2	2
64	Ionization potential and electron affinity of VC <sub>n</sub> (n=1-8) open-chain clusters: A theoretical study. Computational and Theoretical Chemistry, 2006, 769, 225-236.	1.5	18
65	On the reaction of ground-state nitrogen atoms with bromomethyl radicals: A computational study. International Journal of Mass Spectrometry, 2006, 249-250, 451-461.	0.7	3
66	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
67	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
68	On the Competition Between Linear and Cyclic Isomers in Second-Row Dicarbides. ChemInform, 2005, 36, no.	0.1	0
69	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. Journal of Chemical Physics, 2005, 123, 114312.	1.2	29
70	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
71	Small Carbon Clusters Doped with Early Transition Metals: A Theoretical Study of ScC <sub>n</sub> , ScC <sub>n</sub> <sup>+</sup> , and ScC <sub>n</sub> <sup>-</sup> (n=1-8) Open-Chain Clusters. Journal of Physical Chemistry A, 2005, 109, 8594-8603.	1.1	35
72	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. International Journal of Quantum Chemistry, 2004, 96, 615-626.	1.0	21

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73	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.	1.0	34
74	Structures and stabilities of $\text{CaC}_3^+$ and $\text{CaC}_3\text{H}^+$ isomers. <i>Computational and Theoretical Chemistry</i> , 2004, 709, 143-155.	1.5	0
75	On the Competition between Linear and Cyclic Isomers in Second-Row Dicarbides. <i>Journal of the American Chemical Society</i> , 2004, 126, 14611-14619.	6.6	42
76	Structure and Stability of Small $\text{NaC}_n$ , $\text{NaC}_n^+$ , and $\text{NaC}_n^-$ Clusters: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 212-224.	1.1	27
77	Theoretical Study of the Structures and Stabilities of Small $\text{CaC}_n$ , $\text{CaC}_n^+$ , and $\text{CaC}_n$ ( $n = 1 \sim 8$ ) Cyclic Clusters. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11132-11140.	1.1	16
78	Structure and Properties of the Open-Chain Calcium-Doped Carbon Clusters $\text{CaC}_n$ , $\text{CaC}_n^+$ , and $\text{CaC}_n^-$ ( $n = 1 \sim 8$ ). <i>Journal of Physical Chemistry A</i> , 2004, 108, 6421-6429.	1.1	25
79	Structure and stability of binary calcium-carbon compounds: a comparative ab initio and DFT study of $\text{CaC}_2$ . <i>Chemical Physics Letters</i> , 2003, 382, 150-159.	1.2	13
80	Computational study on the kinetics of the reaction of $\text{N}(4\text{S})$ with $\text{CH}_2\text{F}$ . <i>Chemical Physics Letters</i> , 2003, 374, 594-600.	1.2	30
81	Structures and stabilities of $\text{C}_3\text{Cl}_2$ and $\text{C}_3\text{Cl}_2^+$ isomers: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2003, 621, 59-73.	1.5	7
82	Ionization and protonation of $\text{NaC}_3$ : a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2003, 630, 59-73.	1.5	1
83	Structure and stability of $\text{BC}_2\text{P}$ isomers: a theoretical study. <i>Computational and Theoretical Chemistry</i> , 2003, 633, 57-65.	1.5	1
84	Reactivity of gaseous protonated ozone: a computational investigation on the carbon monoxide oxidation reaction. <i>International Journal of Mass Spectrometry</i> , 2003, 228, 613-627.	0.7	5
85	Theoretical Study of $\text{MgC}_n$ , $\text{MgC}_n^+$ , $\text{MgC}_n^-$ ( $n = 1 \sim 7$ ) Open-Chain Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 4676-4682.	1.1	35
86	Theoretical Study of Small $\text{MgC}_n$ , $\text{MgC}_n^+$ , and $\text{MgC}_n^-$ Cyclic Clusters. <i>Journal of Physical Chemistry A</i> , 2003, 107, 6317-6325.	1.1	34
87	Theoretical Study of the Reaction of $\text{HCl}$ with $\text{C}_3\text{H}_2^+$ : A Possible Source of Carbon-Chlorine Compounds in Space. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5844-5853.	1.1	2
88	Reaction of $\text{C}_3\text{H}_2^+$ with Atomic Chlorine: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6346-6351.	1.1	2
89	Theoretical Study of $\text{AlC}_n$ , $\text{AlC}_n^+$ , and $\text{AlC}_n$ ( $n = 1 \sim 7$ ) Clusters. <i>Journal of Physical Chemistry A</i> , 2002, 106, 4217-4225.	1.1	52
90	Ionization and protonation of $\text{MgC}_3$ : A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 114-121.	1.0	4

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91	Structures and stabilities of CaC <sub>3</sub> isomers. Chemical Physics Letters, 2002, 355, 509-516.	1.2	9
92	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
93	Structure and Stability of AlC <sub>2</sub> N Isomers: A Comparative ab Initio and DFT Study. Journal of Physical Chemistry A, 2001, 105, 6724-6728.	1.1	18
94	Computational study of the thermal reaction rate between S+(4S) and acetylene. Chemical Physics, 2001, 265, 251-261.	0.9	12
95	Theoretical study of C <sub>n</sub> Cl, C <sub>n</sub> Cl <sup>+</sup> , C <sub>n</sub> Cl <sup>-</sup> (n=1-7) clusters. International Journal of Quantum Chemistry, 2001, 84, 127-135.	1.0	46
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 MgC <sub>3</sub> isomers: a theoretical study. Chemical Physics Letters, 2001, 335, 64-70.	1.2	20
98	Theoretical study of the structures and stabilities of NaC <sub>3</sub> isomers. Chemical Physics Letters, 2001, 343, 563-570.	1.2	17
99	Theoretical study of AlC <sub>3</sub> : linear or cyclic ground state?. Chemical Physics Letters, 2000, 320, 481-486.	1.2	26
100	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. Computational and Theoretical Chemistry, 2000, 505, 221-232.	1.5	23
101	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
102	Reaction of C <sub>3</sub> H <sub>2</sub> <sup>+</sup> with Atomic Nitrogen: A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 11541-11548.	1.1	18
103	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
104	Theoretical study of the reaction of S <sup>+</sup> with acetylene. Chemical Physics Letters, 1999, 306, 168-178.	1.2	6
105	Theoretical study of the C <sub>3</sub> Cl radical and its cation. Chemical Physics Letters, 1999, 315, 224-232.	1.2	18
106	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
107	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
108	Theoretical study of possible interstellar processes for the production of C <sub>2</sub> Cl precursors. Computational and Theoretical Chemistry, 1998, 432, 75-88.	1.5	17

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109	Theoretical Study of SiC <sub>3</sub> <sup>+</sup> . Journal of Physical Chemistry A, 1998, 102, 3953-3958.	1.1	21
110	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
111	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
112	Theoretical Study of the C <sub>3</sub> P Radical and Its Cation. The Journal of Physical Chemistry, 1996, 100, 585-593.	2.9	34
113	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
114	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
115	Reactions of methylium ion with second-row atoms: an ab initio study. The Journal of Physical Chemistry, 1994, 98, 1090-1099.	2.9	9
116	Ab Initio Characterization of Gaseous (CO <sub>2</sub> P) <sup>+</sup> Species. The Journal of Physical Chemistry, 1994, 98, 2294-2297.	2.9	2
117	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
118	Theoretical Study of the C <sub>2</sub> P Radical and (C <sub>2</sub> P) <sup>+</sup> Species. The Journal of Physical Chemistry, 1994, 98, 3985-3988.	2.9	40
119	Topological Analysis of the Charge Density for Phosphorus Ion Molecule Complexes Bound to Water and Ammonia Molecules. The Journal of Physical Chemistry, 1994, 98, 3148-3153.	2.9	2
120	Ab-initio study of phosphorus ion complexes of ammonia and water. The Journal of Physical Chemistry, 1993, 97, 9337-9340.	2.9	5
121	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
122	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
123	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
124	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
125	Theoretical study of acetyleneboron and acetylenealuminum isomers: the interactions of boron and aluminum atoms with acetylene. The Journal of Physical Chemistry, 1992, 96, 3015-3021.	2.9	32
126	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



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127	Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with ammonia. The Journal of Physical Chemistry, 1991, 95, 170-175.	2.9	24
128	Theoretical studies of possible processes for the interstellar production of phosphorus compounds: reaction of phosphorus(1+) with water. The Journal of Physical Chemistry, 1991, 95, 5443-5445.	2.9	20
129	Theoretical studies of possible processes for interstellar production of phosphorus compounds: reaction of phosphorus(1+) with methane. The Journal of Physical Chemistry, 1991, 95, 6553-6557.	2.9	17
130	Theoretical study of the interactions of beryllium and magnesium atoms with acetylene. The Journal of Physical Chemistry, 1991, 95, 9278-9288.	2.9	11
131	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. The Journal of Physical Chemistry, 1991, 95, 9864-9868.	2.9	21
132	An ab initio study of C2S protonation. Chemical Physics Letters, 1991, 184, 168-174.	1.2	5
133	A theoretical study of the structures and stabilities of (H2PO)+ species and the proton affinities of HPO and POH. The Journal of Physical Chemistry, 1991, 95, 4318-4323.	2.9	18
134	Low-lying states of AlC2 and SiC2+: Competition between linear and cyclic configurations. Chemical Physics, 1990, 140, 19-26.	0.9	30
135	Theoretical studies of potential astrophysical molecules. The ClCC and SC2H radicals. Chemical Physics Letters, 1989, 155, 550-556.	1.2	21
136	A theoretical study of the C2H, C2F and C2Cl radicals and their positive ions. Chemical Physics, 1989, 138, 291-301.	0.9	36
137	A theoretical study of protonation of triatomic silicon-carbon compounds. International Journal of Quantum Chemistry, 1989, 36, 241-253.	1.0	5
138	An ab initio study of Si2C protonation. Chemical Physics Letters, 1988, 145, 128-133.	1.2	13
139	An ab initio study of Si3 protonation. Chemical Physics Letters, 1988, 147, 79-83.	1.2	2
140	A preliminary theoretical study of the SiC2H radical: Implications in astrophysics. Chemical Physics Letters, 1988, 147, 90-94.	1.2	23
141	A comparative theoretical study of the C2N+ and SiCN+ ions and their formation processes. Chemical Physics Letters, 1988, 148, 79-85.	1.2	4
142	A Theoretical study of the SiCN radical. Chemical Physics Letters, 1988, 147, 95-98.	1.2	28
143	Correlation effects at a local level and CI partitions: 23S State of helium. International Journal of Quantum Chemistry, 1988, 33, 323-326.	1.0	1
144	Gaussian functions in hylleraasâ€”CI calculations. I. Ground state energies for H2, HeH+, and H+3. Journal of Chemical Physics, 1988, 88, 2091-2093.	1.2	46

#	ARTICLE	IF	CITATIONS
145	Interelectronic repulsion distribution functions in the ground state of helium: slow convergence of CI wavefunctions. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 1988, 21, 2377-2387.	0.6	3
146	A theoretical study of SiC <sub>2</sub> <sup>+</sup> . <i>Chemical Physics Letters</i> , 1987, 140, 26-30.	1.2	5
147	The Hylleraas-CI method in molecular calculations: Two-electron integrals. <i>Journal of Computational Chemistry</i> , 1987, 8, 1191-1198.	1.5	20
148	The correlation effects at a local level. CI partitions. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 845-852.	1.0	2