Carmen Barrientos

List of Publications by Year in descending order

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133	1,983	236612	395343
papers	citations	25 h-index	33 g-index

133	133	133	922
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hydroaluminum Isocyanide Isomers: Prediction of Spectroscopic Properties. Astrophysical Journal, 2022, 928, 69.	1.6	4
2	Computational study on the affinity of potential drugs to SARS-CoV-2 main protease. Journal of Physics Condensed Matter, 2022, 34, 294005.	0.7	2
3	Amino acetaldehyde conformers: structure and spectroscopic properties. Monthly Notices of the Royal Astronomical Society, 2020, 492, 1827-1833.	1.6	2
4	Structure and Spectroscopic Properties of Hydrocalcium Isocyanide Isomers: Plausible Astronomical Ca-bearing Molecules. Astrophysical Journal, 2020, 899, 135.	1.6	4
5	Alkaline and alkaline-earth cyanoacetylides: A combined theoretical and rotational spectroscopic investigation. Journal of Chemical Physics, 2019, 151, 054312.	1.2	6
6	Formation of Protonated Glycine Isomers in the Interstellar Medium. ACS Earth and Space Chemistry, 2019, 3, 1170-1181.	1.2	7
7	Spectroscopic Parameters of HTiCN/HTiNC: New Titanium Compounds of Astrochemical Interest. Astrophysical Journal, 2019, 871, 180.	1.6	4
8	Structural Trends in Monoboronyl Compounds: Analysis of the Interaction of Second-Row Elements with BO. Journal of Physical Chemistry A, 2018, 122, 398-409.	1.1	3
9	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
10	Complex Organic Molecules Formation in Space Through Gas Phase Reactions: A Theoretical Approach. Astrophysical Journal, 2017, 836, 240.	1.6	7
11	Metallic monoboronyl compounds: Prediction of their structure and comparison with the cyanide analogues. Journal of Computational Chemistry, 2017, 38, 807-815.	1.5	3
12	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
13	Prebiotic molecules formation through the gas-phase reaction between HNO and CH2CHOH2+. Astronomy and Astrophysics, 2017, 603, A139.	2.1	8
14	Molecular Structure and Bonding in Plutonium Carbides: A Theoretical Study of PuC₃. Journal of Physical Chemistry A, 2016, 120, 2232-2239.	1.1	9
15	PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF NEW IRON COMPOUNDS: HYDRIDE OF IRON CYANIDE/ISOCYANIDE, HFeCN/HFeNC. Astrophysical Journal, 2016, 828, 45.	1.6	9
16	Metallic cyanoacetylides of copper, silver and gold: generation and structural characterization. Physical Chemistry Chemical Physics, 2016, 18, 28538-28547.	1.3	3
17	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
18	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

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19	SOME INSIGHTS INTO FORMAMIDE FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM. Astrophysical Journal, 2014, 780, 181.	1.6	29
20	Generation and structural characterization of aluminum cyanoacetylide. Journal of Chemical Physics, 2014, 141, 104305.	1.2	13
21	COMPUTATIONAL PREDICTION OF THE SPECTROSCOPIC PARAMETERS OF METHANEDIOL, AN ELUSIVE MOLECULE FOR INTERSTELLAR DETECTION. Astrophysical Journal, 2014, 784, 132.	1.6	16
22	PEPTIDE BOND FORMATION THROUGH GAS-PHASE REACTIONS IN THE INTERSTELLAR MEDIUM: FORMAMIDE AND ACETAMIDE AS PROTOTYPES. Astrophysical Journal, 2014, 793, 32.	1.6	37
23	Halogen-abstraction reactions from chloromethane and bromomethane molecules by alkaline-earth monocations. Physical Chemistry Chemical Physics, 2014, 16, 16121-16136.	1.3	2
24	Computational study of peptide bond formation in the gas phase through ionâ€“molecule reactions. Physical Chemistry Chemical Physics, 2013, 15, 13005.	1.3	14
25	Reactivity of First-Row Transition Metal Monocations (Sc⁺, Ti⁺,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Chemistry A, 2013, 117, 2932-2943.	1.1	8
26	Kinetics Studies of the Reactions of Main Fourth-Period Monocations (Ga⁺,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 Td (Chemistry A, 2013, 117, 7742-7753.	1.1	2
27	Small carbides of third-row main group elements: structure and bonding in C3X compounds (X =) Tj ETQq1 1 0.784314 rgBT /Overloc	1.3	4
28	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
29	Theoretical study of the Câ€“F bond activation in methyl fluoride by alkaline-earth metal monocations. Theoretical Chemistry Accounts, 2011, 128, 609-618.	0.5	6
30	Structure and stability of neutral cyanide complexes of copper and zinc. Chemical Physics Letters, 2011, 504, 125-129.	1.2	8
31	The reaction between NH₃⁺and CH₃COOH: a possible process for the formation of glycine precursors in the interstellar medium. Astronomy and Astrophysics, 2010, 516, A79.	2.1	26
32	Could the reactions of formic acid with CH3NH2+/CH3NH3+ produce protonated glycine?. International Journal of Mass Spectrometry, 2010, 295, 21-25.	0.7	6
33	A computational study of arsenic dicarbide (C2As). Chemical Physics Letters, 2010, 485, 286-289.	1.2	8
34	Neutral cyanide complexes of iron: Structure and stability. Chemical Physics Letters, 2010, 500, 9-13.	1.2	7
35	Structure and bonding in third-row main group dicarbides C2X (X=Kâ€“Br). Journal of Chemical Physics, 2010, 133, 124306.	1.2	20
36	Cyanide complexes of Ti(IV): A computational study. Journal of Chemical Physics, 2009, 131, 094507.	1.2	4

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37	Small iron doped carbon clusters: A comparison with early and late first-row transition metal doped clusters. Journal of Chemical Physics, 2009, 130, 134304.	1.2	15
38	Charged FeCn clusters: A comparison with (TM=Sc, Ti, V, Co and Zn, n=1â€“8) systems. Chemical Physics, 2009, 364, 1-13.	0.9	15
39	Stability of protonated and ionized hydroxylamine in the interstellar medium. Chemical Physics Letters, 2009, 476, 174-177.	1.2	12
40	Polyisocyanides of Titanium. Journal of Physical Chemistry A, 2009, 113, 1574-1577.	1.1	5
41	Gas-phase reaction between calcium monocation and fluoromethane: Analysis of the potential energy hypersurface and kinetics calculations. Journal of Chemical Physics, 2009, 131, 144309.	1.2	8
42	A density functional study of CoC_n (n = 1â€“8) clusters: Structures and stabilities. International Journal of Quantum Chemistry, 2008, 108, 1684-1695.	1.0	15
43	Structures and stabilities of charged cobalt-doped carbon clusters. International Journal of Mass Spectrometry, 2008, 272, 187-198.	0.7	14
44	Structural and electronic properties of ZnCn+/â^' clusters. International Journal of Mass Spectrometry, 2008, 273, 87-94.	0.7	16
45	Gas-Phase Reaction of NH₂⁺ with Acetic Acid: Implications in Astrochemistry. Journal of Chemical Theory and Computation, 2008, 4, 2085-2093.	2.3	9
46	Cyanides and Isocyanides of First-Row Transition Metals:â€‰ Molecular Structure, Bonding, and Isomerization Barriers. Journal of Physical Chemistry A, 2007, 111, 6334-6344.	1.1	50
47	Structure and Stability of Small ZnCn Clusters. Journal of Chemical Theory and Computation, 2007, 3, 657-664.	2.3	27
48	Structure and Bonding in First-Row Transition Metal Dicarbide Cations MC2+. Journal of Physical Chemistry A, 2007, 111, 6345-6353.	1.1	25
49	A theoretical study of the [FeCN]+ system: Cyanideâ€“isocyanide competition and isomerization barrier. Chemical Physics Letters, 2007, 445, 22-27.	1.2	4
50	Structures and stabilities of non-linear VCn+/â^' (n=1â€“8) clusters. International Journal of Mass Spectrometry, 2007, 263, 101-112.	0.7	19
51	Charged titanium-doped carbon clusters: Structures and energetics. International Journal of Mass Spectrometry, 2007, 266, 50-61.	0.7	25
52	On the application of the counterpoise correction for the basis set superposition error in geometry optimization calculations of molecular systems: some inconsistent results. Theoretical Chemistry Accounts, 2007, 118, 733-738.	0.5	13
53	Small Carbon Clusters Doped with Vanadium Metal:Â A Density Functional Study of VCn(n= 1â^'8). Journal of Chemical Theory and Computation, 2006, 2, 885-893.	2.3	33
54	Small ScCn Cyclic Clusters:â€‰ A Density Functional Study of Their Structure and Stability. Journal of Physical Chemistry A, 2006, 110, 4057-4064.	1.1	32

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55	Reaction of N(2D) atoms with bromomethyl radicals: A theoretical study. Chemical Physics, 2006, 328, 45-52.	0.9	14
56	Structure of small TiCn clusters: A theoretical study. Chemical Physics, 2006, 330, 431-440.	0.9	33
57	Structure of binary titaniumcarbon ions: A theoretical study of <mml:math altimg="si5.gif" display="inline" overflow="scroll" xmlns:xocs="http://www.elsevier.com/xml/xocs/dtd" xmlns:xs="http://www.w3.org/2001/XMLSchema" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xmlns="http://www.elsevier.com/xml/ja/dtd" xmlns:ja="http://www.elsevier.com/xml/ja/dtd" xmlns:mml="http://www.w3.org/1998/Math/MathML" xmlns:tb="http://www.elsevier.com/xml/common/table/dtd" xmlns:sb="http://www.elsevier.com/xml/c	1.2	4
58	A computational study on the reaction of N(2D) atoms with CH2Cl radicals. Chemical Physics Letters, 2006, 422, 276-281.	1.2	2
59	Ionization potential and electron affinity of VCn (n=1â€“8) open-chain clusters: A theoretical study. Computational and Theoretical Chemistry, 2006, 769, 225-236.	1.5	18
60	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
61	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
62	On the Competition Between Linear and Cyclic Isomers in Second-Row Dicarbides. ChemInform, 2005, 36, no.	0.1	0
63	Computational study of the reaction of N(D2) atoms with CH2F radicals: An example of a barrier-free reaction involving very high internal energies. Journal of Chemical Physics, 2005, 123, 114312.	1.2	29
64	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
65	Small Carbon Clusters Doped with Early Transition Metals:Â A Theoretical Study of ScCn, ScCn+, and ScCn-(n= 1â^8) Open-Chain Clusters. Journal of Physical Chemistry A, 2005, 109, 8594-8603.	1.1	35
66	Theoretical study of the structures and stabilities of AlCn, AlC+n, and AlC?n (n = 1-7) monocyclic clusters. International Journal of Quantum Chemistry, 2004, 96, 615-626.	1.0	21
67	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
68	Structures and stabilities of CaC3+ and CaC3H+ isomers. Computational and Theoretical Chemistry, 2004, 709, 143-155.	1.5	0
69	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
70	Structure and Stability of Small NaCn, NaCn+, and NaCn- Clusters:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 212-224.	1.1	27
71	Theoretical Study of the Structures and Stabilities of Small CaCn, CaCn+, and CaCn-(n= 1â^8) Cyclic Clusters. Journal of Physical Chemistry A, 2004, 108, 11132-11140.	1.1	16
72	Structure and Properties of the Open-Chain Calcium-Doped Carbon Clusters CaCn, CaCn+, and CaCn- (n = 1â^8). Journal of Physical Chemistry A, 2004, 108, 6421-6429.	1.1	25

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73	Structure and stability of binary calciumâ€“carbon compounds: a comparative ab initio and DFT study of CaC2. Chemical Physics Letters, 2003, 382, 150-159.	1.2	13
74	Computational study on the kinetics of the reaction of N(4S) with CH2F. Chemical Physics Letters, 2003, 374, 594-600.	1.2	30
75	Ionization and protonation of NaC3: a theoretical study. Computational and Theoretical Chemistry, 2003, 630, 59-73.	1.5	1
76	Structure and stability of BC2P isomers: a theoretical study. Computational and Theoretical Chemistry, 2003, 633, 57-65.	1.5	1
77	Theoretical Study of MgCn, MgCn+, MgCn- (n = 1â^'7) Open-Chain Clusters. Journal of Physical Chemistry A, 2003, 107, 4676-4682.	1.1	35
78	Theoretical Study of Small MgCn, MgCn+, and MgCn- Cyclic Clusters. Journal of Physical Chemistry A, 2003, 107, 6317-6325.	1.1	34
79	Theoretical Study of AlCn, AlCn+, and AlCn-(n= 1â^'7) Clusters. Journal of Physical Chemistry A, 2002, 106, 4217-4225.	1.1	52
80	Ionization and protonation of MgC3: A theoretical study. International Journal of Quantum Chemistry, 2002, 86, 114-121.	1.0	4
81	Structures and stabilities of CaC3 isomers. Chemical Physics Letters, 2002, 355, 509-516.	1.2	9
82	The Reaction of N(4S) with CH2F:Â A Comparative ab Initio and DFT Study. Journal of Physical Chemistry A, 2001, 105, 9917-9925.	1.1	11
83	Structure and Stability of AlC2N Isomers:Â A Comparative ab Initio and DFT Study. Journal of Physical Chemistry A, 2001, 105, 6724-6728.	1.1	18
84	Theoretical study of CnCl, CnCl+, CnClâ^'(n=1-7) clusters. International Journal of Quantum Chemistry, 2001, 84, 127-135.	1.0	46
85	Theoretical study of AlC3+. International Journal of Quantum Chemistry, 2001, 84, 660-669.	1.0	7
86	Structures and stabilities of MgC3 isomers: a theoretical study. Chemical Physics Letters, 2001, 335, 64-70.	1.2	20
87	Theoretical study of the structures and stabilities of NaC3 isomers. Chemical Physics Letters, 2001, 343, 563-570.	1.2	17
88	Theoretical study of AlC3: linear or cyclic ground state?. Chemical Physics Letters, 2000, 320, 481-486.	1.2	26
89	Theoretical study of the reaction of CN with C 2 H 2 +. Theoretical Chemistry Accounts, 2000, 104, 199-202.	0.5	5
90	Reaction of C3H2+ with Atomic Nitrogen:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2000, 104, 11541-11548.	1.1	18

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91	Theoretical Study of the Reaction of Cl+ with C3H2. Journal of Physical Chemistry A, 2000, 104, 9733-9739.	1.1	5
92	Theoretical study of the reaction of S+ with acetylene. Chemical Physics Letters, 1999, 306, 168-178.	1.2	6
93	Theoretical study of the C3Cl radical and its cation. Chemical Physics Letters, 1999, 315, 224-232.	1.2	18
94	Theoretical Study of the Reaction of Si+ with C3H2. Journal of Physical Chemistry A, 1999, 103, 3310-3320.	1.1	10
95	Theoretical Study of the Reaction of S+with C3H2. Journal of Physical Chemistry A, 1999, 103, 9125-9131.	1.1	8
96	Theoretical study of possible interstellar processes for the production of C2Cl precursors. Computational and Theoretical Chemistry, 1998, 432, 75-88.	1.5	17
97	Reaction of carbon atoms with H2Cl+: an ab initio study of a possible interstellar process. Computational and Theoretical Chemistry, 1996, 363, 319-331.	1.5	13
98	Theoretical Studies of Simple Organoboron Compounds: Structures and Stabilities of BC2H4 Isomers. Applied Organometallic Chemistry, 1996, 10, 283-295.	1.7	5
99	Theoretical Study of the C3P Radical and Its Cation. The Journal of Physical Chemistry, 1996, 100, 585-593.	2.9	34
100	Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds:Â The Reaction of P+with C3H2. The Journal of Physical Chemistry, 1996, 100, 14643-14650.	2.9	10
101	Theoretical Studies of Possible Processes for the Interstellar Production of Phosphorus Compounds. The Reaction of P+ with Acetylene. The Journal of Physical Chemistry, 1995, 99, 6432-6440.	2.9	13
102	Reactions of methylium ion with second-row atoms: an ab initio study. The Journal of Physical Chemistry, 1994, 98, 1090-1099.	2.9	9
103	Ab Initio Characterization of Gaseous (CO2P)+ Species. The Journal of Physical Chemistry, 1994, 98, 2294-2297.	2.9	2
104	Theoretical Study of the Structures and Stabilities of (SiC2H2)+ Species. The Reaction of Si+ with Acetylene. The Journal of Physical Chemistry, 1994, 98, 3978-3984.	2.9	12
105	Theoretical Study of the C2P Radical and (C2P)+ Species. The Journal of Physical Chemistry, 1994, 98, 3985-3988.	2.9	40
106	Relativistic quantum defect calculations on the copper isoelectronic sequence. International Journal of Quantum Chemistry, 1994, 50, 411-428.	1.0	8
107	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
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 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
110	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
111	Ab initio characterization of gaseous phosphorus oxide (P2O2). The Journal of Physical Chemistry, 1993, 97, 4078-4079.	2.9	11
112	Ab initio characterization of novel gaseous phosphorus oxide ((PO)2+) species. The Journal of Physical Chemistry, 1993, 97, 5860-5863.	2.9	4
113	A theoretical study of the structures and stabilities of SC2H2+ species: the reaction of sulfur(1+) with acetylene. The Journal of Physical Chemistry, 1992, 96, 5808-5814.	2.9	9
114	Quantum-defect studies of systematic trends of â¨•values. Transitions in subordinate spectral series. Journal of Quantitative Spectroscopy and Radiative Transfer, 1992, 48, 287-293.	1.1	6
115	Quantum-defect studies of transitions in the diffuse spectral series of the potassium isoelectronic sequence. Journal of Quantitative Spectroscopy and Radiative Transfer, 1992, 47, 411-419.	1.1	15
116	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
117	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
118	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
119	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
120	Systematic trends along the potassium sequence: Study of ns²Sâ€“mp²P⁰ transitions. Canadian Journal of Physics, 1991, 69, 1273-1283.	0.4	13
121	An ab initio study of C2S protonation. Chemical Physics Letters, 1991, 184, 168-174.	1.2	5
122	Comment on â€˜â€˜Analytical wave functions for atomic quantum-defect theoryâ€™â€™. Physical Review A, 1991, 43, 4061-4062.	1.0	4
123	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
124	Theoretical study of transitions involving three rydberg series in two-valence electron systems: MgI and its electronic sequence. International Journal of Quantum Chemistry, 1990, 37, 221-240.	1.0	14
125	Quantum-defect studies of systematic trends offvalues. Physical Review A, 1990, 42, 432-439.	1.0	19
126	Theoretical studies of potential astrophysical molecules. The ClCC and SC2H radicals. Chemical Physics Letters, 1989, 155, 550-556.	1.2	21

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127	A theoretical study of the C2H, C2F and C2Cl radicals and their positive ions. Chemical Physics, 1989, 138, 291-301.	0.9	36
128	Core-polarization effects in subordinate series of the alkali atoms. Canadian Journal of Physics, 1989, 67, 996-1001.	0.4	15
129	A comparative theoretical study of the C2N+ and SiCN+ ions and their formation processes. Chemical Physics Letters, 1988, 148, 79-85.	1.2	4
130	Oscillator strength distribution in the alkaline-earth elements. Canadian Journal of Physics, 1988, 66, 29-33.	0.4	18
131	Oscillator-strength distribution in the discrete and continuous spectra of the alkali elements. Canadian Journal of Physics, 1987, 65, 435-437.	0.4	21
132	Core-polarization effects in the alkali atoms: oscillator-strength calculations. Canadian Journal of Physics, 1986, 64, 867-871.	0.4	18
133	Quantum defect orbital calculations on the alkaline-earth elements: oscillator strengths and photoionization cross sections. Canadian Journal of Physics, 1985, 63, 1441-1445.	0.4	10