Josep Anglada

List of Publications by Year
in descending order

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128 papers	5,035 citations	61857 43 h-index	110170 64 g-index
135 all docs	135 docs citations	135 times ranked	3657 citing authors

#	Article	IF	Citations
1	Photosensitization mechanisms at the airâ€“water interface of aqueous aerosols. Chemical Science, 2022, 13, 2624-2631.	3.7	17
2	Reactivity of Undissociated Molecular Nitric Acid at the Airâ€“Water Interface. Journal of the American Chemical Society, 2021, 143, 453-462.	6.6	14
3	Tight electrostatic regulation of the OH production rate from the photolysis of hydrogen peroxide adsorbed on surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	9
4	Molecular reactions at aqueous interfaces. Nature Reviews Chemistry, 2020, 4, 459-475.	13.8	149
5	Two-step reaction mechanism reveals new antioxidant capability of cysteine disulfides against hydroxyl radical attack. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 18216-18223.	3.3	17
6	The Aqueous Surface as an Efficient Transient Stop for the Reactivity of Gaseous NO₂ in Liquid Water. Journal of the American Chemical Society, 2020, 142, 20937-20941.	6.6	17
7	Photoinduced Oxidation Reactions at the Airâ€“Water Interface. Journal of the American Chemical Society, 2020, 142, 16140-16155.	6.6	38
8	Formation of a stable biradical triplet state cation versus a closed shell singlet state cation by oxidation of adducts of 3,6-dimethoxycarbazole and polychlorotriphenylmethyl radicals. Physical Chemistry Chemical Physics, 2019, 21, 20225-20231.	1.3	3
9	A New Mechanism of Acid Rain Generation from HOSO at the Airâ€“Water Interface. Journal of the American Chemical Society, 2019, 141, 16564-16568.	6.6	39
10	Photochemistry of HOSO radical in the gas phase. Journal of Chemical Physics, 2019, 151, 111103.	1.2	13
11	Theoretical Investigation of the Photoexcited NO₂+H₂O reaction at the Airâ€“Water Interface and Its Atmospheric Implications. Chemistry - A European Journal, 2019, 25, 13899-13904.	1.7	14
12	Atmospheric Spectroscopy and Photochemistry at Environmental Water Interfaces. Annual Review of Physical Chemistry, 2019, 70, 45-69.	4.8	38
13	Triplet state promoted reaction of SO₂ with H₂O by competition between proton coupled electron transfer (pcet) and hydrogen atom transfer (hat) processes. Physical Chemistry Chemical Physics, 2019, 21, 9779-9784.	1.3	27
14	The gas phase oxidation of HCOOH by Cl and NH2 radicals. Proton coupled electron transfer versus hydrogen atom transfer. Molecular Physics, 2019, 117, 1430-1441.	0.8	6
15	Reactivity of hydropersulfides toward the hydroxyl radical unraveled: disulfide bond cleavage, hydrogen atom transfer, and proton-coupled electron transfer. Physical Chemistry Chemical Physics, 2018, 20, 4793-4804.	1.3	9
16	Tropospheric oxidation of methyl hydrotrioxide (CH₃OOOH) by hydroxyl radical. Physical Chemistry Chemical Physics, 2018, 20, 27406-27417.	1.3	7
17	Photochemistry of SO₂ at the Airâ€“Water Interface: A Source of OH and HOSO Radicals. Journal of the American Chemical Society, 2018, 140, 12341-12344.	6.6	42
18	The atmospheric oxidation of CH₃OOH by the OH radical: the effect of water vapor. Physical Chemistry Chemical Physics, 2017, 19, 12331-12342.	1.3	28

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19	Role of Proton Tunneling and Metal-Free Organocatalysis in the Decomposition of Methanediol: A Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 4318-4325.	1.1	13
20	Relevance of the DFT method to study expanded porphyrins with different topologies. Journal of Computational Chemistry, 2017, 38, 2819-2828.	1.5	64
21	Design of HÃ¼ckelâ€“MÃ¶bius Topological Switches with High Nonlinear Optical Properties. Journal of Physical Chemistry C, 2017, 121, 19348-19357.	1.5	34
22	The Atmospheric Oxidation of HONO by OH, Cl, and ClO Radicals. Journal of Physical Chemistry A, 2017, 121, 9698-9707.	1.1	15
23	Impacts of cloud water droplets on the OH production rate from peroxide photolysis. Physical Chemistry Chemical Physics, 2017, 19, 31621-31627.	1.3	11
24	Twisted intramolecular charge transfer in a carbazole-based chromophore: the stable [(4-N-carbazolyl)-2,3,5,6-tetrachlorophenyl]bis(2,3,5,6-tetrachlorophenyl)methyl radical. New Journal of Chemistry, 2017, 41, 8422-8430.	1.4	10
25	Computational Insights into the CH₃Cl+OH Chemical Reaction Dynamics at the Airâ€“Water Interface. ChemPhysChem, 2017, 18, 2747-2755.	1.0	4
26	The Stability of Î±â€Hydroperoxyalkyl Radicals. Chemistry - A European Journal, 2016, 22, 18092-18100.	1.7	24
27	Spectroscopic characterization of the ethyl radical-water complex. Journal of Chemical Physics, 2016, 145, 144301.	1.2	0
28	Impact of the water dimer on the atmospheric reactivity of carbonyl oxides. Physical Chemistry Chemical Physics, 2016, 18, 17698-17712.	1.3	78
29	Structure of hydrogen tetroxide in gas phase and in aqueous environments: relationship to the hydroperoxyl radical self-reaction. Structural Chemistry, 2016, 27, 231-242.	1.0	8
30	Interconnection of Reactive Oxygen Species Chemistry across the Interfaces of Atmospheric, Environmental, and Biological Processes. Accounts of Chemical Research, 2015, 48, 575-583.	7.6	90
31	Mechanistic Studies on the Intramolecular Cyclization of O-Tosyl Phytosphingosines to Jaspines. Natural Product Communications, 2014, 9, 1934578X1400900.	0.2	0
32	Unexpected Reactivity of Amidogen Radical in the Gas Phase Degradation of Nitric Acid. Journal of the American Chemical Society, 2014, 136, 6834-6837.	6.6	15
33	Spectroscopic signatures of ozone at the airâ€“water interface and photochemistry implications. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11618-11623.	3.3	58
34	Atmospheric formation of the NO₃ radical from gas-phase reaction of HNO₃ acid with the NH₂ radical: proton-coupled electron-transfer versus hydrogen atom transfer mechanisms. Physical Chemistry Chemical Physics, 2014, 16, 19437-19445.	1.3	17
35	Effect of the Meso-Substituent in the HÃ¼ckel-to-MÃ¶bius Topological Switches. Journal of Organic Chemistry, 2014, 79, 5036-5046.	1.7	27
36	Atmospheric Significance of Water Clusters and Ozoneâ€“Water Complexes. Journal of Physical Chemistry A, 2013, 117, 10381-10396.	1.1	101

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37	The gas-phase reaction of methane sulfonic acid with the hydroxyl radical without and with water vapor. Physical Chemistry Chemical Physics, 2013, 15, 5140.	1.3	26
38	The reaction of formaldehyde carbonyl oxide with the methyl peroxy radical and its relevance in the chemistry of the atmosphere. Physical Chemistry Chemical Physics, 2013, 15, 18921.	1.3	26
39	Sulfuric Acid as Autocatalyst in the Formation of Sulfuric Acid. Journal of the American Chemical Society, 2012, 134, 20632-20644.	6.6	126
40	Evaluation of the nonlinear optical properties for an expanded porphyrin HÃ¼ckel-MÃ¶bius aromaticity switch. Journal of Chemical Physics, 2012, 137, 184306.	1.2	35
41	Theoretical Study of the Switching between HÃ¼ckel and MÃ¶bius Topologies for Expanded Porphyrins. Journal of Physical Chemistry C, 2012, 116, 24358-24366.	1.5	28
42	Effects of a Single Water Molecule on the OH + H₂O₂ Reaction. Journal of Physical Chemistry A, 2012, 116, 5821-5829.	1.1	91
43	Is the HO₄^{â”} Anion a Key Species in the Aqueousâ€Phase Decomposition of Ozone?. Chemistry - A European Journal, 2012, 18, 13435-13445.	1.7	11
44	Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet. Journal of the American Chemical Society, 2012, 134, 11821-11827.	6.6	65
45	Correlation between Photophysical Parameters and Goldâ€“Gold Distances in Gold(I) (4-Pyridyl)ethynyl Complexes. Inorganic Chemistry, 2012, 51, 7636-7641.	1.9	69
46	Reactivity of Atmospherically Relevant Small Radicals at the Airâ€“Water Interface. Angewandte Chemie - International Edition, 2012, 51, 5413-5417.	7.2	69
47	Anharmonicity and the Eigen-Zundel Dilemma in the IR Spectrum of the Protonated 21 Water Cluster. Journal of Chemical Theory and Computation, 2011, 7, 467-472.	2.3	29
48	Impact of Water on the OH + HOCl Reaction. Journal of the American Chemical Society, 2011, 133, 3345-3353.	6.6	92
49	Effects of the substituents on the reactivity of carbonyl oxides. A theoretical study on the reaction of substituted carbonyl oxides with water. Physical Chemistry Chemical Physics, 2011, 13, 13034.	1.3	173
50	Evaluation of the Nonlinear Optical Properties for Annulenes with HÃ¼ckel and MÃ¶bius Topologies. Journal of Chemical Theory and Computation, 2011, 7, 3935-3943.	2.3	86
51	Water effects on atmospheric reactions. International Reviews in Physical Chemistry, 2011, 30, 335-369.	0.9	119
52	The reaction between HO and (H2O) n (nÂ=Â1, 3) clusters: reaction mechanisms and tunneling effects. Theoretical Chemistry Accounts, 2011, 128, 579-592.	0.5	37
53	Structure, stability, and dynamics of hydrogen polyoxides. International Journal of Quantum Chemistry, 2011, 111, 1543-1554.	1.0	19
54	Protonation of Water Clusters Induced by Hydroperoxyl Radical Surface Adsorption. Chemistry - A European Journal, 2011, 17, 5076-5085.	1.7	14

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55	The gas phase reaction of carbonyl oxide with hydroxyl radical in presence of water vapor. A theoretical study on the reaction mechanism. Computational and Theoretical Chemistry, 2011, 965, 313-320.	1.1	15
56	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	1.7	20
57	On the Dissociation of Ground State trans-HOOO Radical: A Theoretical Study. Journal of Chemical Theory and Computation, 2010, 6, 2743-2750.	2.3	42
58	The reactions of SO3 with HO2 radical and H2Oâ‹¯HO2 radical complex. Theoretical study on the atmospheric formation of HSO5 and H2SO4. Physical Chemistry Chemical Physics, 2010, 12, 2116.	1.3	106
59	Gas Phase Reaction of Nitric Acid with Hydroxyl Radical without and with Water. A Theoretical Investigation. Journal of Physical Chemistry A, 2010, 114, 9151-9162.	1.1	74
60	Different Catalytic Effects of a Single Water Molecule: The Gasâ€Phase Reaction of Formic Acid with Hydroxyl Radical in Water Vapor. ChemPhysChem, 2009, 10, 3034-3045.	1.0	69
61	Hyperconjugation in adjacent OO bonds: Remarkable odd/even effects. Chemical Physics Letters, 2009, 481, 180-182.	1.2	20
62	The 65th birthday of Professor Santiago Olivella Nello. Theoretical Chemistry Accounts, 2009, 123, 1-2.	0.5	0
63	A Bohmian total potential view to quantum effects. II: decay of temporarily trapped states. Theoretical Chemistry Accounts, 2009, 123, 51-58.	0.5	3
64	Role of vibrational anharmonicity in atmospheric radical hydrogen-bonded complexes. Physical Chemistry Chemical Physics, 2009, 11, 6377.	1.3	12
65	Description of pentacoordinated phosphorus under an external electric field: which basis sets and semi-empirical methods are needed?. Physical Chemistry Chemical Physics, 2008, 10, 2442.	1.3	15
66	Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. Journal of Chemical Theory and Computation, 2008, 4, 49-63.	2.3	21
67	Unconventional Biradical Character of Titanium Enolates. Journal of the American Chemical Society, 2008, 130, 3242-3243.	6.6	46
68	The Gas Phase HO-Initiated Oxidation of Furan: A Theoretical Investigation on the Reaction Mechanism. The Open Chemical Physics Journal, 2008, 1, 80-93.	0.7	12
69	The Gas-Phase Hydrogen-Bonded Complex between Ozone and Hydroperoxyl Radical. A Theoretical Study. Journal of Physical Chemistry A, 2007, 111, 976-981.	1.1	25
70	New Insight into the Gas-Phase Bimolecular Self-Reaction of the HOO Radical. Journal of Physical Chemistry A, 2007, 111, 1695-1704.	1.1	46
71	On the nature of the unusually long OO bond in HO3 and HO4 radicals. Physical Chemistry Chemical Physics, 2007, 9, 5865.	1.3	51
72	The Gas-Phase Reaction between O3 and HO Radical: A Theoretical Study. ChemPhysChem, 2007, 8, 1534-1539.	1.0	29

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73	Reaction Mechanism between Carbonyl Oxide and Hydroxyl Radical:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 4001-4011.	1.1	29
74	Hydrogen Transfer between Sulfuric Acid and Hydroxyl Radical in the Gas Phase:â€‰ Competition among Hydrogen Atom Transfer, Proton-Coupled Electron-Transfer, and Double Proton Transfer. Journal of Physical Chemistry A, 2006, 110, 1982-1990.	1.1	33
75	Mechanistic Study of the CH3O2â€¢+ HO2â€¢â†’ CH3O2H + O2Reaction in the Gas Phase. Computational Evidence for the Formation of a Hydrogen-Bonded Diradical Complex. Journal of Physical Chemistry A, 2006, 110, 6073-6082.	1.1	58
76	On the Gas Phase Hydrogen Bond Complexes between Formic Acid and Hydroperoxyl Radical. A Theoretical Study. Journal of Physical Chemistry A, 2006, 110, 9718-9726.	1.1	23
77	On the Regio- and Stereoselective Synthesis of Aminocyclitols from Cyclitol Epoxides: The Effect of Li as a Chelating Agent. Chemistry - A European Journal, 2006, 12, 349-349.	1.7	0
78	Theoretical Characterization of the Gas-Phase O3â‹…â‹…â‹…HO Hydrogen-Bonded Complex. ChemPhysChem, 2006, 7, 1488-1493.	1.0	12
79	On the Regio- and Stereoselective Synthesis of Aminocyclitols from Cyclitol Epoxides: The Effect of Li as a Chelating Agent. Chemistry - A European Journal, 2005, 11, 4465-4472.	1.7	13
80	Mechanism for the Gas-Phase Reaction between Formaldehyde and Hydroperoxyl Radical. A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 10786-10794.	1.1	60
81	The Gas-Phase Hydrogen Bond Complexes between Formic Acid with Hydroxyl Radical: A Theoretical Study. ChemPhysChem, 2004, 5, 183-191.	1.0	37
82	Mechanism of the Hydrogen Transfer from the OH Group to Oxygen-Centered Radicals: Proton-Coupled Electron-Transfer versus Radical Hydrogen Abstraction. Chemistry - A European Journal, 2004, 10, 3404-3410.	1.7	63
83	Complex Mechanism of the Gas Phase Reaction between Formic Acid and Hydroxyl Radical. Proton Coupled Electron Transfer versus Radical Hydrogen Abstraction Mechanisms. Journal of the American Chemical Society, 2004, 126, 9809-9820.	6.6	86
84	Studies on the Intramolecular Cî”HÂ·Â·Â·X (X = O, S) Interactions in (S)-N-Acyl-4-isopropyl-1,3-thiazolidine-2-thiones and Related 1,3-Oxazolidin-2-ones. Organic Letters, 2003, 5, 2809-2812.	2.4	14
85	Theoretical Studies of the Isoprene Ozonolysis under Tropospheric Conditions. 2. Unimolecular and Water-Assisted Decomposition of the Î±-Hydroxy Hydroperoxides. Journal of Physical Chemistry A, 2003, 107, 5812-5820.	1.1	58
86	Theoretical Studies on Isoprene Ozonolysis under Tropospheric Conditions. 1. Reaction of Substituted Carbonyl Oxides with Water. Journal of Physical Chemistry A, 2003, 107, 5798-5811.	1.1	43
87	Reaction Modes of Carbonyl Oxide, Dioxirane, and Methylenebis(oxy) with Ethylene:â€‰ A New Reaction Mechanism. Journal of Physical Chemistry A, 2002, 106, 3917-3929.	1.1	57
88	The Reaction of CH2(X3B1) with O2(X3):Â A Theoretical CASSCF/CASPT2 Investigation. Journal of Physical Chemistry A, 2002, 106, 1877-1884.	1.1	46
89	Atmospheric Formation of OH Radicals and H2O2 from Alkene Ozonolysis under Humid Conditions. ChemPhysChem, 2002, 3, 215-221.	1.0	100
90	A new look at the reduced-gradient-following path. Theoretical Chemistry Accounts, 2002, 107, 130-139.	0.5	63

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91	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	0.5	16
92	Cysteinyl-flavan-3-ol Conjugates from Grape Procyanidins. Antioxidant and Antiproliferative Properties. Bioorganic and Medicinal Chemistry, 2002, 10, 2497-2509.	1.4	72
93	The Ozonolysis of AcetyleneA Quantum Chemical Investigation. Journal of the American Chemical Society, 2001, 123, 6127-6141.	6.6	51
94	Finding transition states using reduced potential-energy surfaces. Theoretical Chemistry Accounts, 2001, 105, 463-472.	0.5	81
95	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. Journal of Computational Chemistry, 2001, 22, 387-406.	1.5	52
96	Tropospheric Formation of Hydroxymethyl Hydroperoxide, Formic Acid, H2O2, and OH from Carbonyl Oxide in the Presence of Water Vapor: A Theoretical Study of the Reaction Mechanism. Chemistry - A European Journal, 2001, 7, 2227-2235.	1.7	92
97	The ozoneâ€“acetylene reaction: concerted or non-concerted reaction mechanism? A quantum chemical investigation. Chemical Physics Letters, 2001, 347, 268-276.	1.2	25
98	m-Benzyne and bicyclo[3.1.0]hexatriene â€“ which isomer is more stable? â€“ a quantum chemical investigation. Chemical Physics Letters, 2001, 348, 115-125.	1.2	64
99	Ab initio1Aâ€² ground potential energy surface and transition state theory kinetics study of the O(1D)+N2Oâ†’2NO, N2+O2(aâ€‰1Î”g) reactions. Journal of Chemical Physics, 2001, 115, 7015-7031.	1.2	21
100	Quantum Chemical Reactivity: Beyond the Study of Small Molecules. Mathematical and Computational Chemistry, 2001, , 125-141.	0.3	1
101	Accurate and efficient determination of higher roots in diagonalization of large matrices based in function restricted optimization algorithms. Journal of Computational Chemistry, 2000, 21, 1375-1386.	1.5	9
102	Large-scale matrix diagonalization methods by direct optimization of Taylor expansion of Rayleighâ€“Ritz quotient up to third order. Chemical Physics Letters, 2000, 329, 160-167.	1.2	2
103	Theoretical investigation of the eight low-lying electronic states of thecis- andtrans-nitric oxide dimers and its isomerization using multiconfigurational second-order perturbation theory (CASPT2). Journal of Chemical Physics, 2000, 112, 6608-6624.	1.2	67
104	Inductive Effects in Neutral Pentacoordinated Silicon Compounds Containing a Si â†•N Dative Bond. A Theoretical Study. Organometallics, 1999, 18, 5584-5593.	1.1	69
105	Title is missing!. Journal of Mathematical Chemistry, 1999, 25, 85-92.	0.7	15
106	Remarks on large-scale matrix diagonalization using a Lagrange-Newton-Raphson minimization in a subspace. Theoretical Chemistry Accounts, 1999, 103, 163-166.	0.5	12
107	Prediction of approximate transition states by Bell-Evans-Polanyi principle: I. Journal of Computational Chemistry, 1999, 20, 1112-1129.	1.5	28
108	Prediction of approximate transition states by Bell-Evans-Polanyi principle: II. Gas phase unimolecular decomposition of methyldioxirane. Journal of Computational Chemistry, 1999, 20, 1130-1137.	1.5	5

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109	The Ozonolysis of Ethylene: A Theoretical Study of the Gas-Phase Reaction Mechanism. Chemistry - A European Journal, 1999, 5, 1809-1822.	1.7	134
110	The Mechanism of Methoxy Radical Oxidation by O2in the Gas Phase. Computational Evidence for Direct H Atom Transfer Assisted by an Intermolecular Noncovalent OÂ·Â·Â·O Bonding Interaction. Journal of the American Chemical Society, 1999, 121, 1337-1347.	6.6	77
111	How good is a Broyden-Fletcher-Goldfarb-Shanno-like update Hessian formula to locate transition structures? Specific reformulation of Broyden-Fletcher-Goldfarb-Shanno for optimizing saddle points. Journal of Computational Chemistry, 1998, 19, 349-362.	1.5	43
112	Theoretical Investigation of the Low-Lying Electronic States of Dioxirane:â€‰ Ring Opening to Dioxymethane and Dissociation into CO2 and H2. Journal of Physical Chemistry A, 1998, 102, 3398-3406.	1.1	36
113	Electronic Structure and Unimolecular Reactions of Cyclopropenone Carbonyl Oxide. A Theoretical Studyâ€. Journal of Organic Chemistry, 1997, 62, 2720-2726.	1.7	21
114	A reduced-restricted-quasi-Newton-Raphson method for locating and optimizing energy crossing points between two potential energy surfaces. Journal of Computational Chemistry, 1997, 18, 992-1003.	1.5	91
115	On the restricted step method coupled with the augmented Hessian for the search of stationary points of any continuous function. International Journal of Quantum Chemistry, 1997, 62, 153-165.	1.0	21
116	A symmetric orthogonal transformation applied to molecular geometry optimizations constrained on a hypersphere. Chemical Physics Letters, 1997, 269, 469-474.	1.2	1
117	Unimolecular Isomerizations and Oxygen Atom Loss in Formaldehyde and Acetaldehyde Carbonyl Oxides. A Theoretical Investigation. Journal of the American Chemical Society, 1996, 118, 4636-4647.	6.6	137
118	N,Nâ€²â€Cyclization of carbodiimides with 2â€(bromomethyl)acrylic acid. A direct entry to the system 5â€methyleneâ€6Hâ€pyrimidineâ€2,4â€dione, a new class of thymine analogues. Journal of Heterocyclic Chemistry, 1996, 33, 1259-1270.	1.4	11
119	Practical remarks on the selection of the active space in the CAS-SCF wavefunction. Chemical Physics Letters, 1995, 243, 151-157.	1.2	44
120	Theoretical Study of the Low-Lying Electronic States of 4-Oxo-2,5-cyclohexadienylidene and Their Formation from 1H-Bicyclo[3.1.0]hexa-3,5-dien-2-one. The Journal of Physical Chemistry, 1995, 99, 5934-5944.	2.9	19
121	A geometry optimization benchmark using highly correlated wavefunctions (FCI and MRD-CI). Theoretica Chimica Acta, 1995, 92, 369-381.	0.9	23
122	Ab initio CI calculations on ScC2H4+ ions. Chemical Physics Letters, 1990, 167, 421-428.	1.2	4
123	Theoretical study of lowâ€lying electronic states of CoH+. Journal of Chemical Physics, 1990, 92, 6732-6741.	1.2	13
124	Theoretical investigation of the low-lying electronic states of TiH. Molecular Physics, 1990, 69, 281-303.	0.8	30
125	The electronic spectrum of ScH. Molecular Physics, 1989, 66, 541-563.	0.8	23
126	Comparison between isoelectronic transition metal hydrides. MRD-CI results for ScH+ and TiH+. Computational and Theoretical Chemistry, 1984, 107, 163-168.	1.5	9

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127	MRD-CI calculations for the low-lying electronic states of scandiumhydride and titaniumhydride. Computational and Theoretical Chemistry, 1983, 93, 299-308.	1.5	9
128	Low-lying electronic states of CSi-and electron affinity of CSi according to ab initio MRD-CI calculations. Journal of Physics B: Atomic and Molecular Physics, 1983, 16, 2469-2484.	1.6	26