Silmar A Do Monte

List of Publications by Year
in descending order

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		759233	752698
51	500	12	20
papers	citations	h-index	g-index

52	52	52	536
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Solvent effects in electronically excited states using the continuum solvation model COSMO in combination with multireference configuration interaction with singles and doubles (MR-CISD). Theoretical Chemistry Accounts, 2004, 111, 78-89.	1.4	46
2	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
3	Synthesis and conformational study of a new class of highly bioactive compounds. Chemical Physics Letters, 2007, 449, 336-340.	2.6	31
4	Theoretical study of cooperative effects in the homo- and heteromeric hydrogen bond chains (HCN)nï£¿HF withn = 1, 2, and 3. International Journal of Quantum Chemistry, 2006, 106, 2714-2722.	2.0	29
5	Cope Rearrangement of 1,5-Hexadiene:â€‰ Full Geometry Optimizations Using Analytic MR-CISD and MR-AQCC Gradient Methods. Journal of Physical Chemistry A, 2003, 107, 1175-1180.	2.5	27
6	Photochemistry of CH₃Cl: Dissociation and CHÂ·Â·Â·Cl Hydrogen Bond Formation. Journal of the American Chemical Society, 2016, 138, 272-280.	13.7	27
7	An ab initio study of the C2H2HF, C2H(CH3) HF and C2(CH3)2HF hydrogen-bonded complexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 383-390.	3.9	23
8	Challenges encountered during development of Mn porphyrin-based, potent redox-active drug and superoxide dismutase mimic, MnTnBuOE-2-PyP5+, and its alkoxyalkyl analogues. Journal of Inorganic Biochemistry, 2017, 169, 50-60.	3.5	18
9	Dissociation of ground and nï*f* states of CF3Cl using multireference configuration interaction with singles and doubles and with multireference average quadratic coupled cluster extensivity corrections. Journal of Chemical Physics, 2007, 127, 164320.	3.0	17
10	Electronic factor for photoinduced electron transfer in porphyrinâ€“bridgeâ€“quinone systems. Chemical Physics Letters, 1998, 290, 136-142.	2.6	16
11	Revisiting the concept of the (a)synchronicity of dielsâ€alder reactions based on the dynamics of quasiclassical trajectories. Journal of Computational Chemistry, 2016, 37, 701-711.	3.3	16
12	Photochemical Deactivation Process of HCFC-133a (C₂H₂F₃Cl): A Nonadiabatic Dynamics Study. Journal of Physical Chemistry A, 2014, 118, 12041-12049.	2.5	15
13	CASSCF and MRâ€“CISD study of the nâˆ’4s and nâˆ’4pe Rydberg states of the CF3Cl. Chemical Physics Letters, 2012, 546, 30-33.	2.6	12
14	Dynamic Effects Dictate the Mechanism and Selectivity of Dehydrationâ€“Rearrangement Reactions of Protonated Alcohols [Me 2 (R)CCH(OH 2)Me] + (R=Me, Et, i Pr) in the Gas Phase. Chemistry - A European Journal, 2014, 20, 13742-13754.	3.3	12
15	A theoretical prediction of stability in hydrogen-bonded complexes formed between oxirane and oxetane rings with HX (X=F and Cl). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 156-160.	3.9	11
16	Assessment of density-functionals for describing the Xâˆ’ + CH3ONO2 gas-phase reactions with X = F, OH, CH2CN. Physical Chemistry Chemical Physics, 2014, 16, 26769-26778.	2.8	11
17	Ab initio and DFT conformational study on nitrosamine (H2Nâ€“N=O) and N-Nitrosodimethylamine [(CH3)2Nâ€“N=O]. Structural Chemistry, 2011, 22, 497-507.	2.0	10
18	Matrix isolation infrared spectroscopic and theoretical study of 1,1,1-trifluoro-2-chloroethane (HCFC-133a). Journal of Chemical Physics, 2013, 139, 204302.	3.0	10

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19	Valence and Rydberg states of CH₃Cl: a MR-CISD study. RSC Advances, 2014, 4, 64085-64092.	3.6	10
20	Spinâ€Forbidden Branching in the Mechanism of the Intrinsic Haberâ€“Weiss Reaction. ChemistryOpen, 2017, 6, 360-363.	1.9	10
21	Photochemistry of CF₃Cl: Quenching of Charged Fragments Is Caused by Nonadiabatic Effects. Journal of Chemical Theory and Computation, 2018, 14, 4844-4855.	5.3	10
22	Photoinduced Formation of H-Bonded Ion Pair in HCFC-133a. Journal of Physical Chemistry A, 2019, 123, 1953-1961.	2.5	10
23	MR-CISD and MR-AQCC Calculation of Excited States of Malonaldehyde: Geometry Optimizations Using Analytical Energy Gradient Methods and a Systematic Investigation of Reference Configuration Sets. Collection of Czechoslovak Chemical Communications, 2003, 68, 447-462.	1.0	10
24	A theoretical study of hydrogen complexes of the XH-Ï€ type between propyne and HF, HCL or HCN. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 412-417.	3.9	6
25	<scp>UV</scp>â€photoexcitation and ultrafast dynamics of <scp>HCFC</scp>â€132b (<scp>CF</scp>₂<scp>C</scp>l<scp>CH</scp>₂<scp>C</scp>l). Journal of Computational Chemistry, 2016, 37, 675-683.	3.3	6
26	Effects of Ï€ bond type, backbone size, and halogen on structural and spectroscopic properties of hydrogen-bonded complexes of the Xï£¿H â€¦ Ï€ type between alkenes or alkynes and haloacids (HF and) Tj ETQq0 0 0 rgBT /Overlock 1	2.0	5
27	Matrix Isolation FTIR Spectroscopic and Theoretical Study of 3,3-Dichloro-1,1,1-Trifluoropropane (HCFC-243). Journal of Physical Chemistry A, 2008, 112, 11641-11648.	2.5	5
28	CASSCF and multireference CI with singles and doubles study of lowâ€lying valence and Rydberg states of 2Hâ€tetrazole. Journal of Computational Chemistry, 2009, 30, 1075-1081.	3.3	5
29	Hydrogen-bonded contact ion pair in gaseous chloroethane: a multi-reference configuration interaction with singles and doubles (MR-CISD) study including extensivity corrections. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	5
30	The reduction of 2-bromomethyl-3-methyl- and 2,3-bis-bromomethyl-1,4-naphthoquinones, potential bioreductive alkylating agents. Electrochemical and computational studies. Journal of Electroanalytical Chemistry, 2003, 560, 79-86.	3.8	4
31	Accurate calculation of the ionization energies of the chlorine lone pairs in 1,1,1-trifluoro-2-chloroethane (HCFC-133a). Journal of Molecular Modeling, 2014, 20, 2393.	1.8	4
32	Can a gas phase contact ion pair containing a hydrocarbon carbocation be formed in the ground state?. RSC Advances, 2021, 11, 4221-4230.	3.6	4
33	Ab-initio study of the electronic factor (Î”) conformational dependence in [CH2â€“(phenylene)nâ€“CH2]â^' electron transfer model systems. Chemical Physics, 2005, 313, 311-323.	1.9	3
34	Theoretical calculations of the substituent effect on molecular properties of the RCNâ‹¯HF hydrogen-bonded complexes with R=NH2, CH3O, CH3, OH, SH, H, Cl, F, CF3, CN and NO2. Vibrational Spectroscopy, 2009, 49, 133-141.	2.2	3
35	Ab initio and DFT conformational study on N-nitrosodiethylamine, (C2H5)2N-N=O. Journal of Molecular Modeling, 2012, 18, 339-350.	1.8	3
36	Photochemistry of Monohydrated Chloromethane: Formation of Free and Hydrated Cl^{â€“} and CH₃⁺ Ions from a Solvent-Shared Semi-Ion-Pair. Journal of Physical Chemistry A, 2021, 125, 8603-8614.	2.5	3

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37	Modeling the heating and cooling of a chromophore after photoexcitation. Physical Chemistry Chemical Physics, 2022, 24, 9403-9410.	2.8	3
38	Effects of Zn and substituents(methyl and p-tolyl) on the decay of electron transfer rates in porphyrinâ€“benzeneâ€“(bicyclo[2.2.2]octane) â€“quinone (n=0,1,2) systems. Chemical Physics Letters, 2001, 336, 462-466.	2.6	2
39	Effects of wave function modifications on calculated carbonâ€“carbontriple bond lengths. Computational and Theoretical Chemistry, 2006, 758, 253-258.	1.5	2
40	Control of ionic properties of N-nitrosodimethylamine through hydrogen substitution by fluorine atoms. Structural Chemistry, 2012, 23, 1193-1201.	2.0	2
41	Electronic properties of the low-lying spin states of dimethylnitrosamine coordinated to Fe(III) heme models: An ab initio study. International Journal of Quantum Chemistry, 2014, 114, 508-520.	2.0	2
42	A multi-reference CI study of the low-lying valence and Rydberg states of CF₃ radical. Molecular Physics, 2018, 116, 2187-2195.	1.7	2
43	Increasing the kinetic stability of a gasâ€phase contact ionâ€pair through enhancement of the carbocation stability. International Journal of Quantum Chemistry, 2022, 122, .	2.0	2
44	Effects of wave function modifications on calculated carbonâ€“hydrogen bond lengths. Computational and Theoretical Chemistry, 2006, 760, 21-27.	1.5	1
45	O ensino de reaÃ§Ãµes orgÃ¢nicas usando quÃmica computacional: I. reaÃ§Ãµes de adiÃ§Ã£o eletrofÃlica a alquenos. Quimica Nova, 2008, 31, 1243-1249.	0.3	1
46	Effect of methylation on relative energies of tautomers and on the intramolecular proton transfer barriers of protonated nitrosamine: A <scp>MR</scp>â€<scp>CISD</scp> study. Journal of Computational Chemistry, 2015, 36, 2027-2036.	3.3	1
47	Solvent effect on the tautomers' stabilities of protonated N,Nâ€dimethylnitrosamine: The role of hydrogen bonds network. International Journal of Quantum Chemistry, 2017, 117, e25311.	2.0	1
48	Competition between electron transfer and base-induced elimination mechanisms in the gas-phase reactions of superoxide with alkyl hydroperoxides. Physical Chemistry Chemical Physics, 2021, 23, 5583-5595.	2.8	1
49	A multireference configuration interaction study with singles and doubles of some mesoionic rings: reaction and activation free energies for the ringâ€opening reaction. International Journal of Quantum Chemistry, 2020, 120, e26391.	2.0	0
50	A comparative multiâ€reference configuration interaction study of the lowâ€lying states of two thione isomers of thiophenol. International Journal of Quantum Chemistry, 2020, 120, e26263.	2.0	0
51	A importÃ¢ncia do mÃ©todo de Hartree no ensino de quÃmica quÃ¢ntica. Quimica Nova, 2011, 34, 527-534.	0.3	0