Silmar A Do Monte

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5209199/publications.pdf

Version: 2024-02-01

		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	Modeling the heating and cooling of a chromophore after photoexcitation. Physical Chemistry Chemical Physics, 2022, 24, 9403-9410.	2.8	3
2	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
3	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
4	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
5	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
6	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
7	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
8	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
9	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
10	Photoinduced Formation of H-Bonded Ion Pair in HCFC-133a. Journal of Physical Chemistry A, 2019, 123, 1953-1961.	2.5	10
11	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
12	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
13	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
14	Spinâ€Forbidden Branching in the Mechanism of the Intrinsic Haberâ€“Weiss Reaction. ChemistryOpen, 2017, 6, 360-363.	1.9	10
15	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
16	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
17	<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
18	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

#	Article	IF	Citations
19	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
20	Photochemical Deactivation Process of HCFC-133a (C₂H₂F₃Cl): A Nonadiabatic Dynamics Study. Journal of Physical Chemistry A, 2014, 118, 12041-12049.	2.5	15
21	Assessment of density-functionals for describing the Xâ¯ + CH3ONO2 gas-phase reactions with X = F, OH, CH2CN. Physical Chemistry Chemical Physics, 2014, 16, 26769-26778.	2.8	11
22	Valence and Rydberg states of CH₃Cl: a MR-CISD study. RSC Advances, 2014, 4, 64085-64092.	3.6	10
23	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
24	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
25	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
26	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
27	CASSCF and MRâ€“CISD study of the nâ¯4s and nâ¯4pe Rydberg states of the CF3Cl. Chemical Physics Letters, 2012, 546, 30-33.	2.6	12
28	Control of ionic properties of N-nitrosodimethylamine through hydrogen substitution by fluorine atoms. Structural Chemistry, 2012, 23, 1193-1201.	2.0	2
29	Ab initio and DFT conformational study on N-nitrosodiethylamine, (C2H5)2N-N=O. Journal of Molecular Modeling, 2012, 18, 339-350.	1.8	3
30	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
31	A importÃ¢ncia do mÃ©todo de Hartree no ensino de quÃmica quÃ¢ntica. Quimica Nova, 2011, 34, 527-534.	0.3	0
32	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
33	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
34	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
35	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
36	Dissociation of ground and nÏ* 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

#	Article	IF	Citations
37	Synthesis and conformational study of a new class of highly bioactive compounds. Chemical Physics Letters, 2007, 449, 336-340.	2.6	31
38	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	6
39	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
40	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
41	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
42	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
43	Effects of wave function modifications on calculated carbonâ€“carbontriple bond lengths. Computational and Theoretical Chemistry, 2006, 758, 253-258.	1.5	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	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
46	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
47	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
48	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
49	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
50	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
51	Electronic factor for photoinduced electron transfer in porphyrinâ€“bridgeâ€“quinone systems. Chemical Physics Letters, 1998, 290, 136-142.	2.6	16