Rene F K Spada

List of Publications by Year
in descending order

24 papers	200 citations	1163117 8 h-index	1125743 13 g-index
25 all docs	25 docs citations	25 times ranked	208 citing authors

#	Article	IF	Citations
1	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	1.7	3
2	The influence of the environment in chemical reactivity: the HCOOH formation from the H2O + CO reaction. Journal of Molecular Modeling, 2021, 27, 264.	1.8	5
3	Methanol and glycolaldehyde production from formaldehyde in massive star-forming regions. Monthly Notices of the Royal Astronomical Society, 2020, 497, 4486-4494.	4.4	2
4	Tunneling Enhancement of the Gas-Phase CH + CO₂ Reaction at Low Temperature. Journal of Physical Chemistry A, 2020, 124, 10717-10725.	2.5	1
5	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
6	A Proposal for the Mechanism of the CH + CO2 Reaction. ACS Omega, 2019, 4, 17843-17849.	3.5	5
7	Potential Energy Curves for Formation of the CH2O2 Criegee Intermediate on the 3CH2 + 3O2 Singlet and Triplet Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 8968-8975.	2.5	5
8	Could HCN Be Responsible for the Formamide Synthesis in Earthâ€™s Primitive Atmosphere?. Astrophysical Journal, Supplement Series, 2019, 245, 11.	7.7	3
9	Reply to â€œComment on â€˜Thermochemical and Kinetics of the CH3OH+(4S)N Reactional Systemâ€™â€•. Journal of Physical Chemistry A, 2019, 123, 967-969.	2.5	0
10	Implications of the (H2O)nÂ+ÂCO â†” trans-HCOOHÂ+Â(H2O)nâ€“1 (nÂ=Â1, 2, and 3) reactions for primordial atmospheres of Venus and Earth. Monthly Notices of the Royal Astronomical Society, 2018, 475, 3191-3200.	4.4	4
11	Thermochemical and Kinetics of the CH₃OH + (⁴S)N Reactional System. Journal of Physical Chemistry A, 2018, 122, 5905-5910.	2.5	2
12	Accurate rovibrational energies of ozone isotopologues up to J = 10 utilizing artificial neural networks. Journal of Chemical Physics, 2018, 149, 024307.	3.0	17
13	Thermochemical and Kinetics of CH₃SH + H Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. Journal of Physical Chemistry A, 2017, 121, 419-428.	2.5	10
14	Investigation of the ozone formation reaction pathway: Comparisons of full configuration interaction quantum Monte Carlo and fixed-node diffusion Monte Carlo with contracted and uncontracted MRCI. Journal of Chemical Physics, 2017, 147, 094306.	3.0	10
15	Accurate Calculations of Rate Constants for the Forward and Reverse H₂O + CO â†” HCOOH Reactions. ChemistrySelect, 2017, 2, 7267-7272.	1.5	8
16	THE H₂Â+ÂCOÂ ÂH₂CO REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. Astrophysical Journal, Supplement Series, 2016, 225, 2.	7.7	10
17	Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. Journal of Physical Chemistry A, 2015, 119, 1628-1635.	2.5	12
18	Thermochemical and Kinetics of Hydrazine Dehydrogenation by an Oxygen Atom in Hydrazine-Rich Systems: A Dimer Model. Journal of Physical Chemistry A, 2015, 119, 12607-12614.	2.5	7

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19	Thermochemical and kinetics studies of the CH3SH+S (3P) hydrogen abstraction and insertion reactions. Journal of Molecular Modeling, 2014, 20, 2449.	1.8	3
20	Thermochemistry and kinetics of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si24.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="italic">trans</mml:mi><mml:mtext>-</mml:mtext><mml:msub><mml:mrow><mml:mi>N</mml:mi></mml:mrow><mml:m reaction. Chemical Physics Letters, 2013, 557, 37-42.	2.6	13
21	A multireference configuration interaction study of CuB and CuAl molecular constants and photoionization spectra. Journal of Chemical Physics, 2013, 139, 124316.	3.0	3
22	Dehydrogenation of N2H X (X = 2 â^' 4) by nitrogen atoms: Thermochemical and kinetics. Journal of Chemical Physics, 2013, 139, 194301.	3.0	8
23	O (³P) + CH₃SH reactions: Structures, energetics, and kinetics. International Journal of Quantum Chemistry, 2012, 112, 3269-3275.	2.0	18
24	Valence Band Structure of Coupled Diluted Magnetic Quantum Dots. Journal of Superconductivity and Novel Magnetism, 2010, 23, 121-125.	1.8	3