

# Rene F K Spada

## List of Publications by Year in descending order

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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	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
2	O ( <sup>3</sup> P) + CH <sub>3</sub> SH reactions: Structures, energetics, and kinetics. International Journal of Quantum Chemistry, 2012, 112, 3269-3275.	2.0	18
3	Accurate rovibrational energies of ozone isotopologues up to $J = 10$ utilizing artificial neural networks. Journal of Chemical Physics, 2018, 149, 024307.	3.0	17
4	Thermochemistry and kinetics of the $\text{O}(\text{^3P}) + \text{CH}_3\text{SH}$ reaction. Chemical Physics Letters, 2013, 557, 37-42.	2.6	13
5	Hydrogen Abstraction from the Hydrazine Molecule by an Oxygen Atom. Journal of Physical Chemistry A, 2015, 119, 1628-1635.	2.5	12
6	THE $\text{H}_2 + \text{CO}$ REACTION: RATE CONSTANTS AND RELEVANCE TO HOT AND DENSE ASTROPHYSICAL MEDIA. Astrophysical Journal, Supplement Series, 2016, 225, 2.	7.7	10
7	Thermochemical and Kinetics of $\text{CH}_3\text{SH} + \text{H}$ Reactions: The Sensitivity of Coupling the Low and High-Level Methodologies. Journal of Physical Chemistry A, 2017, 121, 419-428.	2.5	10
8	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
9	Dehydrogenation of $\text{N}_2\text{H}_2$ ( $X = 2 \text{ to } 4$ ) by nitrogen atoms: Thermochemical and kinetics. Journal of Chemical Physics, 2013, 139, 194301.	3.0	8
10	Accurate Calculations of Rate Constants for the Forward and Reverse $\text{H}_2\text{O} + \text{CO} \rightleftharpoons \text{HCOOH}$ Reactions. ChemistrySelect, 2017, 2, 7267-7272.	1.5	8
11	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
12	A Proposal for the Mechanism of the $\text{CH} + \text{CO}_2$ Reaction. ACS Omega, 2019, 4, 17843-17849.	3.5	5
13	Potential Energy Curves for Formation of the $\text{CH}_2\text{O}_2$ Criegee Intermediate on the $3\text{CH}_2 + 3\text{O}_2$ Singlet and Triplet Potential Energy Surfaces. Journal of Physical Chemistry A, 2019, 123, 8968-8975.	2.5	5
14	The influence of the environment in chemical reactivity: the $\text{HCOOH}$ formation from the $\text{H}_2\text{O} + \text{CO}$ reaction. Journal of Molecular Modeling, 2021, 27, 264.	1.8	5
15	Implications of the $(\text{H}_2\text{O})_n + \text{CO} \rightleftharpoons \text{trans-HCOOH} + (\text{H}_2\text{O})_{n-1}$ ( $n = 1, 2, \text{ and } 3$ ) reactions for primordial atmospheres of Venus and Earth. Monthly Notices of the Royal Astronomical Society, 2018, 475, 3191-3200.	4.4	4
16	Valence Band Structure of Coupled Diluted Magnetic Quantum Dots. Journal of Superconductivity and Novel Magnetism, 2010, 23, 121-125.	1.8	3
17	A multireference configuration interaction study of CuB and CuAl molecular constants and photoionization spectra. Journal of Chemical Physics, 2013, 139, 124316.	3.0	3
18	Thermochemical and kinetics studies of the $\text{CH}_3\text{SH} + \text{S}$ (3P) hydrogen abstraction and insertion reactions. Journal of Molecular Modeling, 2014, 20, 2449.	1.8	3

#	ARTICLE	IF	CITATIONS
19	Could HCN Be Responsible for the Formamide Synthesis in Earth's Primitive Atmosphere?. Astrophysical Journal, Supplement Series, 2019, 245, 11.	7.7	3
20	Spin-density calculation via the graphical unitary group approach. Molecular Physics, 2023, 121, .	1.7	3
21	Thermochemical and Kinetics of the $\text{CH}_3\text{OH} + \text{S}^4\text{N}$ Reactional System. Journal of Physical Chemistry A, 2018, 122, 5905-5910.	2.5	2
22	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
23	Tunneling Enhancement of the Gas-Phase $\text{CH} + \text{CO}_2$ Reaction at Low Temperature. Journal of Physical Chemistry A, 2020, 124, 10717-10725.	2.5	1
24	Reply to "Comment on "Thermochemical and Kinetics of the $\text{CH}_3\text{OH} + \text{S}^4\text{N}$ Reactional System". Journal of Physical Chemistry A, 2019, 123, 967-969.	2.5	0