

Daniel K W Mok

List of Publications by Year in descending order

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52
papers

1,223
citations

471061

17
h-index

377514

34
g-index

52
all docs

52
docs citations

52
times ranked

1132
citing authors

#	ARTICLE	IF	CITATIONS
1	Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate CH ₃ CHOO. <i>Science</i> , 2013, 340, 177-180.	6.0	379
2	A new method of calculation of Franck-Condon factors which includes allowance for anharmonicity and the Duschinsky effect: Simulation of the He photoelectron spectrum of ClO ₂ . <i>Journal of Chemical Physics</i> , 2000, 113, 5791-5803.	1.2	103
3	Direct Measurements of Unimolecular and Bimolecular Reaction Kinetics of the Criegee Intermediate (CH ₃) ₂ COO. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4-15.	1.1	87
4	Spectroscopy of the Simplest Criegee Intermediate CH ₂ OO: Simulation of the First Bands in Its Electronic and Photoelectron Spectra. <i>Chemistry - A European Journal</i> , 2012, 18, 12411-12423.	1.7	54
5	Anti-inflammatory activities and mechanisms of action of the petroleum ether fraction of <i>Rosa multiflora</i> Thunb. hips. <i>Journal of Ethnopharmacology</i> , 2011, 138, 717-722.	2.0	44
6	Simulation of \tilde{X}^1B_1 CF ₂ single vibronic level emissions: Including anharmonic and Duschinsky effects. <i>Journal of Chemical Physics</i> , 2001, 115, 5816-5822.	1.2	40
7	Use of the ultraviolet absorption spectrum of CF ₂ to determine the spatially resolved absolute CF ₂ density, rotational temperature, and vibrational distribution in a plasma etching reactor. <i>Journal of Chemical Physics</i> , 2004, 120, 9499-9508.	1.2	35
8	HBx-K130M/V131I Promotes Liver Cancer in Transgenic Mice via AKT/FOXO1 Signaling Pathway and Arachidonic Acid Metabolism. <i>Molecular Cancer Research</i> , 2019, 17, 1582-1593.	1.5	29
9	The Singlet-Triplet Separation in CF ₂ : State-of-the-Art Ab Initio Calculations and Franck-Condon Simulations Including Anharmonicity. <i>ChemPhysChem</i> , 2005, 6, 2037-2045.	1.0	28
10	A Combined Ab Initio/Franck-Condon Study of the \tilde{X}^1B_1 Single-Vibronic-Level Emission Spectrum of CCl ₂ and the Photodetachment Spectrum of CCl ₂ ⁻ . <i>ChemPhysChem</i> , 2005, 6, 2046-2059.	1.0	28
11	Petroleum ether extractive of the hips of <i>Rosa multiflora</i> ameliorates collagen-induced arthritis in rats. <i>Journal of Ethnopharmacology</i> , 2014, 157, 45-54.	2.0	28
12	Franck-Condon simulation of the single vibronic level emission spectra of HSiF and DSiF including anharmonicity. <i>Journal of Chemical Physics</i> , 2004, 120, 1292-1305.	1.2	26
13	Difluorocarbene Studied with Threshold Photoelectron Spectroscopy (TPES): Measurement of the First Adiabatic Ionization Energy (AIE) of CF ₂ . <i>Chemistry - A European Journal</i> , 2008, 14, 11452-11460.	1.7	23
14	Ab Initio Calculations on PO ₂ and Anharmonic Franck-Condon Simulations of Its Single-Vibrational-Level Emission Spectra. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10130-10138.	1.1	20
15	\tilde{X}^1A_1 , \tilde{A}^3B_1 , and \tilde{A}^1B_1 States of SiCl ₂ : Ab Initio Calculations and Simulation of Emission Spectra. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4925-4932.	1.1	19
16	Rate coefficients of the CF ₃ CHFCF ₃ + H reaction at different temperatures calculated by transition state theory with <i>ab initio</i> and DFT reaction paths. <i>Journal of Computational Chemistry</i> , 2013, 34, 545-557.	1.5	18
17	Reaction between CH ₃ O ₂ and BrO Radicals: A New Source of Upper Troposphere Lower Stratosphere Hydroxyl Radicals. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4618-4632.	1.1	18
18	Rate Coefficients of the Cl + CH ₃ C(O)OCH ₃ reaction at different temperatures calculated by Transition-State Theory with <i>ab initio</i> and Density Functional Theory Reaction Paths. <i>Journal of Physical Chemistry A</i> , 2014, 118, 2040-2055.	1.1	17

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19	The enthalpies of formation of AsX _n molecules, where X = H, F or Cl, and n = 1, 2 or 3, by RCCSD(T) and UCCSD(T)-F12x calculations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 9540.	1.3	15
20	DFT and ab initio calculations on two reactions between hydrogen atoms and the fire suppressants 2-H heptafluoropropane and CF ₃ Br. <i>Journal of Computational Chemistry</i> , 2007, 28, 1582-1592.	1.5	14
21	An Ab Initio Study of the Low-Lying Electronic States of YO ₂ and Franck-Condon Simulation of the First Photodetachment Band of YO ₂ ⁺ . <i>Journal of Physical Chemistry A</i> , 2008, 112, 4511-4520.	1.1	14
22	Franck-Condon simulation of the single-vibronic-level emission spectra of HPCl/DPCl and the chemiluminescence spectrum of HPCl, including anharmonicity. <i>Journal of Chemical Physics</i> , 2004, 121, 1810-1823.	1.2	13
23	Ab initio calculations on low-lying electronic states of TeO ₂ and Franck-Condon simulation of the (1)B ₂ ← X ₁ TeO ₂ absorption spectrum including anharmonicity. <i>Journal of Chemical Physics</i> , 2004, 121, 2962-2974.	1.2	12
24	Ab initio calculations on the X ¹ and A ³ states of HPO and Franck-Condon simulation of the single vibronic level emission spectra of HPO and DPO. <i>Journal of Chemical Physics</i> , 2007, 127, 214305.	1.2	10
25	A combined ab initio and Franck-Condon factor simulation study on the photodetachment spectrum of ScO ₂ ⁺ . <i>Journal of Computational Chemistry</i> , 2009, 30, 337-345.	1.5	10
26	A theoretical study of the atmospherically important radical reaction BrO + HO ₂ ; the product channel O ₂ (a ¹ g) + HOBr is formed with the highest rate. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30554-30569.	1.3	10
27	Ab Initio Calculations on the (1)2 ¹ Excited State and Low-Lying Quartet States of GaN ₂ : A Simulation of Its LIF Spectrum. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9533-9542.	1.1	9
28	Ab Initio Calculations and Franck-Condon Simulation of the Absorption Spectra of GeCl ₂ Including Anharmonicity. <i>ChemPhysChem</i> , 2005, 6, 719-731.	1.0	9
29	Ab initio calculations on the X ¹ and A ² states of AsH ₂ , and Franck-Condon simulation, including anharmonicity, of the A ¹ (0,0,0)-X ¹ single vibronic level emission spectrum of AsH ₂ . <i>Journal of Chemical Physics</i> , 2010, 132, 234309.	1.2	9
30	Ab initio calculations on the and states of AlNC and simulation of the AlNC- emission spectra. <i>Journal of Computational Chemistry</i> , 2001, 22, 1896-1906.	1.5	8
31	A combined ab initio and Franck-Condon factor simulation study on the photodetachment spectrum of HfO ₂ ⁺ . <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 7270.	1.3	7
32	Simulation of the single-vibronic-level emission spectrum of HPS. <i>Journal of Chemical Physics</i> , 2014, 140, 194311.	1.2	7
33	Ab initio calculations on SCl ₂ and low-lying cationic states of SCl ₂ ⁺ : Franck-Condon simulation of the UV photoelectron spectrum of SCl ₂ . <i>Journal of Chemical Physics</i> , 2006, 125, 104303.	1.2	6
34	Ab initio calculations on SF ₂ and its low-lying cationic states: Anharmonic Franck-Condon simulation of the uv photoelectron spectrum of SF ₂ . <i>Journal of Chemical Physics</i> , 2006, 125, 104304.	1.2	6
35	An ab initio study on the ground and low-lying doublet electronic states of SbO ₂ . <i>Journal of Chemical Physics</i> , 2006, 125, 064307.	1.2	6
36	Ab initio calculations on SnCl ₂ and Franck-Condon factor simulations of its A ¹ -X ¹ and B ¹ -X ¹ absorption and single-vibronic-level emission spectra. <i>Journal of Chemical Physics</i> , 2007, 127, 024308.	1.2	6

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37	Simulation of the single-vibronic-level emission spectra of HAsO and DAsO. Journal of Chemical Physics, 2016, 144, 184303.	1.2	6
38	Ab Initio Study of Low-Lying Electronic States of SnCl ₂ ⁺ . Journal of Physical Chemistry A, 2007, 111, 13193-13199.	1.1	5
39	High-level <i>ab initio</i> calculations on HGeCl and the equilibrium geometry of the \tilde{A}^3 state derived from Franck-Condon analysis of the single-vibronic-level emission spectra of HGeCl and DGeCl. Journal of Computational Chemistry, 2010, 31, 476-491.	1.5	5
40	Franck-Condon simulation of the photoelectron spectrum of AsF ₂ and the photodetachment spectrum of AsF ₂ ⁺ using <i>ab initio</i> calculations: ionization energy and electron affinity of AsF ₂ . Physical Chemistry Chemical Physics, 2010, 12, 9075.	1.3	5
41	Simulated photodetachment spectra of AlH ₂ ⁺ . Journal of Chemical Physics, 2013, 139, 014301.	1.2	5
42	A Study of H ₂ O ₂ with Threshold Photoelectron Spectroscopy (TPES) and Electronic Structure Calculations: Redetermination of the First Adiabatic Ionization Energy (AIE). Journal of Physical Chemistry A, 2016, 120, 5220-5229.	1.1	5
43	The Atmospherically Important Reaction of Hydroxyl Radicals with Methyl Nitrate: A Theoretical Study Involving the Calculation of Reaction Mechanisms, Enthalpies, Activation Energies, and Rate Coefficients. Journal of Physical Chemistry A, 2017, 121, 6554-6567.	1.1	5
44	Ab initio calculations on low-lying electronic states of SnCl ₂ ⁺ and Franck-Condon simulation of its photodetachment spectrum. Physical Chemistry Chemical Physics, 2008, 10, 834-843.	1.3	4
45	Franck-Condon simulation of the photoelectron spectrum of AsCl ₂ and the photodetachment spectrum of AsCl employing UCCSD(T)-F12a potential energy functions: IE and EA of AsCl ₂ . Journal of Computational Chemistry, 2011, 32, 1648-1660.	1.5	3
46	Franck-Condon simulation, including anharmonicity, of the photodetachment spectrum of P ₂ H ⁺ : Restricted-spin coupled-cluster single-double plus perturbative triple and unrestricted-spin coupled-cluster single-double plus perturbative triple -F12x potential energy functions of P ₂ H and P ₂ H ⁺ . Journal of Chemical Physics, 2011, 135, 124312.	1.2	3
47	A theoretical study of the mechanism of the atmospherically relevant reaction of chlorine atoms with methyl nitrate, and calculation of the reaction rate coefficients at temperatures relevant to the troposphere. Physical Chemistry Chemical Physics, 2015, 17, 7463-7476.	1.3	3
48	<i>ab initio</i> calculations on low-lying electronic states of SbO ₂ ⁺ and Franck-Condon simulation of its photodetachment spectrum. Journal of Chemical Physics, 2007, 127, 094306.	1.2	2
49	Schwann cell-specific Pten inactivation reveals essential role of the sympathetic nervous system activity in adipose tissue development. Biochemical and Biophysical Research Communications, 2020, 531, 118-124.	1.0	2
50	A theoretical study of the addition of CH ₂ OO to hydroxymethyl hydroperoxide and its implications on SO ₃ formation in the atmosphere. Physical Chemistry Chemical Physics, 2020, 22, 14130-14141.	1.3	2
51	Comment on "Impact of water on the BrO + HO ₂ gas-phase reaction: mechanism, kinetics and products" by N. T. Tsona, S. Tang and L. Du, Phys. Chem. Chem. Phys., 2019, 21, 20296. Physical Chemistry Chemical Physics, 2021, 23, 6309-6315.	1.3	1
52	Simulation of the photodetachment spectrum of H ₂ F ₂ ⁺ using coupled-cluster calculations. Journal of Chemical Physics, 2016, 145, 244303.	1.2	0