

David E Woon

List of Publications by Year in descending order

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49
papers

15,721
citations

218677

26
h-index

223800

46
g-index

50
all docs

50
docs citations

50
times ranked

9559
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical kinetic studies of Venus chemistry. Formation and destruction of SCl, SCl ₂ , and HSCl. <i>Icarus</i> , 2021, 354, 114051.	2.5	4
2	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4342-4342.	3.1	0
3	Quantum Chemical Cluster Studies of Cation-ice Reactions for Astrochemical Applications: Seeking Experimental Confirmation. <i>Accounts of Chemical Research</i> , 2021, 54, 490-497.	15.6	11
4	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1680-1680.	2.5	0
5	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1973-1973.	2.6	0
6	The Formation of Glycolonitrile (HOCH ₂ CH ₂ CN) from Reactions of C ⁺ with HCN and HNC on Icy Grain Mantles. <i>Astrophysical Journal</i> , 2021, 906, 20.	4.5	9
7	Formation of methyl ketenimine (CH ₃ CH=CHNH) and ethylcyanide (CH ₃ CH ₂ CN) isomers through successive hydrogenations of acrylonitrile (CH ₂ =CHCN) under interstellar conditions: The role of CH ₃ CH=CHN radical in the activation of the cyano group chemistry. <i>Monthly Notices of the Royal Astronomical Society</i> , 2019, 485, 5210-5220.	4.4	10
8	High level ab initio calculations on ClF _n ⁺ (n = 1-6): Recoupled pair bonding involving a closed-shell central ion. <i>Computational and Theoretical Chemistry</i> , 2017, 1116, 73-85.	2.5	4
9	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	26
10	Quantum chemical protocols for modeling reactions and spectra in astrophysical ice analogs: the challenging case of the C ⁺ + H ₂ O reaction in icy grain mantles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28705-28718.	2.8	8
11	Bonding in PF ₂ Cl, PF ₃ Cl, and PF ₄ Cl: insight into isomerism and apicophilicity from ab initio calculations and the recoupled pair bonding model. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	8
12	Bonding in Sulfur-Oxygen Compounds HSO/SOH and SOO/SO: An Example of Recoupled Pair Bonding. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4444-4452.	5.3	24
13	The First Row Anomaly and Recoupled Pair Bonding in the Halides of the Late p-Block Elements. <i>Accounts of Chemical Research</i> , 2013, 46, 359-368.	15.6	47
14	High Level ab Initio Calculations for ClF _n ⁺ (n = 1-6) Ions: Refining the Recoupled Pair Bonding Model. <i>Journal of Physical Chemistry A</i> , 2013, 117, 4251-4266.	2.5	10
15	Insights into the Unusual Barrierless Reaction between Two Closed Shell Molecules, (CH ₃) ₂ S + F ₂ , and Its H ₂ S + F ₂ Analogue: Role of Recoupled Pair Bonding. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5247-5255.	2.5	15
16	A Theoretical Investigation of the Plausibility of Reactions between Ammonia and Carbonyl Species (Formaldehyde, Acetaldehyde, and Acetone) in Interstellar Ice Analogs at Ultracold Temperatures. <i>Journal of Physical Chemistry A</i> , 2011, 115, 5166-5183.	2.5	30
17	ION-ICE ASTROCHEMISTRY: BARRIERLESS LOW-ENERGY DEPOSITION PATHWAYS TO HCOOH, CH ₃ OH, AND CO ₂ ON ICY GRAIN MANTLES FROM PRECURSOR CATIONS. <i>Astrophysical Journal</i> , 2011, 728, 44.	4.5	23
18	Gaussian basis sets for use in correlated molecular calculations. VII. Valence, core-valence, and scalar relativistic basis sets for Li, Be, Na, and Mg. <i>Theoretical Chemistry Accounts</i> , 2011, 128, 69-82.	1.4	536

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19	Hypervalency and recoupled pair bonding in the p-block elements. Computational and Theoretical Chemistry, 2011, 963, 7-12.	2.5	23
20	Recoupled Pair Bonding in PF ₅ (n = 1 ⁺ 5). Journal of Physical Chemistry A, 2010, 114, 8845-8851.	2.5	41
21	Modeling chemical growth processes in Titan's atmosphere 2. Theoretical study of reactions between C ₂ H and ethene, propene, 1-butene, 2-butene, isobutene, trimethylethene, and tetramethylethene. Icarus, 2009, 202, 642-655.	2.5	32
22	Bonding in ClF ₇ (n = 1 ⁺ 7) Molecules: Further Insight into the Electronic Structure of Hypervalent Molecules and Recoupled Pair Bonds. Journal of Physical Chemistry A, 2009, 113, 12645-12654.	2.5	42
23	A comparison between polar covalent bonding and hypervalent recoupled pair bonding in diatomic chalcogen halide species {O,S,Se} Å— {F,Cl,Br}. Molecular Physics, 2009, 107, 991-998.	1.7	42
24	Theory of Hypervalency: Recoupled Pair Bonding in SF ₆ (n = 1 ⁺ 6). Journal of Physical Chemistry A, 2009, 113, 7915-7926.	2.5	81
25	IS HO ⁺ ₂ A DETECTABLE INTERSTELLAR MOLECULE?. Astrophysical Journal, 2009, 697, 601-609.	4.5	35
26	Electron Affinity of NO. Journal of Physical Chemistry A, 2007, 111, 11185-11188.	2.5	26
27	Quantum Chemical Evaluation of the Astrochemical Significance of Reactions between S Atom and Acetylene or Ethylene. Journal of Physical Chemistry A, 2007, 111, 11249-11253.	2.5	13
28	Modeling chemical growth processes in Titan's atmosphere: 1. Theoretical rates for reactions between benzene and the ethynyl (C ₂ H) and cyano (CN) radicals at low temperature and pressure. Chemical Physics, 2006, 331, 67-76.	1.9	43
29	Photoionization in ultraviolet processing of astrophysical ice analogs at cryogenic temperatures. Advances in Space Research, 2004, 33, 44-48.	2.6	14
30	Computational Confirmation of the Carrier for the "XCN" Interstellar Ice Band: OCN - Charge Transfer Complexes. Astrophysical Journal, 2004, 601, L63-L66.	4.5	22
31	Pathways to Glycine and Other Amino Acids in Ultraviolet-irradiated Astrophysical Ices Determined via Quantum Chemical Modeling. Astrophysical Journal, 2002, 571, L177-L180.	4.5	171
32	Ab initio quantum chemical studies of reactions in astrophysical ices. 4. Reactions in ices involving HCOOH, CH ₂ NH, HCN, HNC, NH ₃ , and H ₂ O. International Journal of Quantum Chemistry, 2002, 88, 226-235.	2.0	35
33	Ab Initio Quantum Chemical Studies of Reactions in Astrophysical Ices 3. Reactions of HOCH ₂ NH ₂ Formed in H ₂ CO/NH ₃ /H ₂ O Ices. Journal of Physical Chemistry A, 2001, 105, 9478-9481.	2.5	40
34	Benchmark calculations with correlated molecular wave functions. IX. The weakly bound complexes ArH ₂ and ArHCl. Journal of Chemical Physics, 1998, 109, 2233-2241.	3.0	46
35	The Rate of the Reaction between CN and C ₂ H ₂ at Interstellar Temperatures. Astrophysical Journal, 1997, 477, 204-208.	4.5	49
36	A correlated ab initio study of the $\tilde{A}^2\hat{1}\tilde{\lambda}^2\hat{1}^+$ transition in MgCCH. Chemical Physics Letters, 1997, 274, 299-305.	2.6	16

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37	The Rate of the Reaction between C ₂ H and C ₂ H ₂ at Interstellar Temperatures. <i>Astrophysical Journal</i> , 1997, 489, 109-112.	4.5	35
38	Why HOC ⁺ Is Detectable in Interstellar Clouds: The Rate of the Reaction between HOC ⁺ and H ₂ . <i>Astrophysical Journal</i> , 1996, 463, L113-L115.	4.5	39
39	Ab initio investigation of the N ₂ -HF complex: Accurate structure and energetics. <i>Journal of Chemical Physics</i> , 1996, 104, 5883-5891.	3.0	41
40	A correlated ab initio study of the X ¹ Σ ⁺ and A ¹ Σ ⁺ states of MgCH ₃ . <i>Journal of Chemical Physics</i> , 1996, 104, 9495-9498.	3.0	9
41	An ab initio benchmark study of the H+CO ⁺ →HCO reaction. <i>Journal of Chemical Physics</i> , 1996, 105, 9921-9926.	3.0	36
42	AB Initio Characterization of MgCCH, MgCCH ⁺ , and MgC ₂ and Pathways to Their Formation in the Interstellar Medium. <i>Astrophysical Journal</i> , 1996, 456, 602.	4.5	50
43	On the Stability of Interstellar Carbon Clusters: The Rate of the Reaction between C ₃ and O. <i>Astrophysical Journal</i> , 1996, 465, 795.	4.5	37
44	A correlated ab initio study of linear carbon-chain radicals C _n H (n = 2-7). <i>Chemical Physics Letters</i> , 1995, 244, 45-52.	2.6	129
45	Gaussian basis sets for use in correlated molecular calculations. V. Core-valence basis sets for boron through neon. <i>Journal of Chemical Physics</i> , 1995, 103, 4572-4585.	3.0	2,622
46	Ab Initio Modeling of (LiF) ₂ and (LiF) ₂ (H ₂ O). <i>The Journal of Physical Chemistry</i> , 1994, 98, 8831-8833.	2.9	6
47	Benchmark calculations with correlated molecular wave functions. V. The determination of accurate ab initio intermolecular potentials for He ₂ , Ne ₂ , and Ar ₂ . <i>Journal of Chemical Physics</i> , 1994, 100, 2838-2850.	3.0	175
48	Gaussian basis sets for use in correlated molecular calculations. IV. Calculation of static electrical response properties. <i>Journal of Chemical Physics</i> , 1994, 100, 2975-2988.	3.0	2,382
49	Gaussian basis sets for use in correlated molecular calculations. III. The atoms aluminum through argon. <i>Journal of Chemical Physics</i> , 1993, 98, 1358-1371.	3.0	8,623