

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	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
2	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
3	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
4	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
5	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
6	Pathways to Glycine and Other Amino Acids in Ultraviolet-irradiated Astrophysical Ices Determined via Quantum Chemical Modeling. <i>Astrophysical Journal</i> , 2002, 571, L177-L180.	4.5	171
7	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
8	Theory of Hypervalency: Recoupled Pair Bonding in SF _n (n = 1-6). <i>Journal of Physical Chemistry A</i> , 2009, 113, 7915-7926.	2.5	81
9	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
10	The Rate of the Reaction between CN and C ₂ H ₂ at Interstellar Temperatures. <i>Astrophysical Journal</i> , 1997, 477, 204-208.	4.5	49
11	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
12	Benchmark calculations with correlated molecular wave functions. IX. The weakly bound complexes Ar-H ₂ and Ar-HCl. <i>Journal of Chemical Physics</i> , 1998, 109, 2233-2241.	3.0	46
13	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. <i>Chemical Physics</i> , 2006, 331, 67-76.	1.9	43
14	Bonding in ClF _n (n = 1-7) Molecules: Further Insight into the Electronic Structure of Hypervalent Molecules and Recoupled Pair Bonds. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12645-12654.	2.5	42
15	A comparison between polar covalent bonding and hypervalent recoupled pair bonding in diatomic chalcogen halide species {O,S,Se} - {F,Cl,Br}. <i>Molecular Physics</i> , 2009, 107, 991-998.	1.7	42
16	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
17	Recoupled Pair Bonding in PF _n (n = 1-5). <i>Journal of Physical Chemistry A</i> , 2010, 114, 8845-8851.	2.5	41
18	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. <i>Journal of Physical Chemistry A</i> , 2001, 105, 9478-9481.	2.5	40

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19	Why HOC[TSUP]+[/TSUP] Is Detectable in Interstellar Clouds: The Rate of the Reaction between HOC[TSUP]+[/TSUP] and H[TINF]2[/TINF]. <i>Astrophysical Journal</i> , 1996, 463, L113-L115.	4.5	39
20	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
21	An ab initio benchmark study of the H+CO ⁺ HCO reaction. <i>Journal of Chemical Physics</i> , 1996, 105, 9921-9926.	3.0	36
22	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. <i>International Journal of Quantum Chemistry</i> , 2002, 88, 226-235.	2.0	35
23	IS HO ^{<sup>+</sup><sub>2</sub> A DETECTABLE INTERSTELLAR MOLECULE?. <i>Astrophysical Journal</i>, 2009, 697, 601-609.}	4.5	35
24	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
25	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. <i>Icarus</i> , 2009, 202, 642-655.	2.5	32
26	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
27	Electron Affinity of NO. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11185-11188.	2.5	26
28	Thom H. Dunning, Jr.: Contributions to chemical theory and computing. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	26
29	Bonding in Sulfur ⁺ Oxygen Compounds ⁺ HSO/SOH and SOO/OSO: An Example of Recoupled Pair π Bonding. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4444-4452.	5.3	24
30	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
31	Hypervalency and recoupled pair bonding in the p-block elements. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 7-12.	2.5	23
32	Computational Confirmation of the Carrier for the "XCN" Interstellar Ice Band: OCN - Charge Transfer Complexes. <i>Astrophysical Journal</i> , 2004, 601, L63-L66.	4.5	22
33	A correlated ab initio study of the $\tilde{A}^2\Pi^+$ transition in MgCCH. <i>Chemical Physics Letters</i> , 1997, 274, 299-305.	2.6	16
34	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
35	Photoionization in ultraviolet processing of astrophysical ice analogs at cryogenic temperatures. <i>Advances in Space Research</i> , 2004, 33, 44-48.	2.6	14
36	Quantum Chemical Evaluation of the Astrochemical Significance of Reactions between S Atom and Acetylene or Ethylene. <i>Journal of Physical Chemistry A</i> , 2007, 111, 11249-11253.	2.5	13

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37	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
38	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
39	Formation of methyl ketenimine ($\text{CH}_3\text{CH}=\text{C}=\text{NH}$) and ethylcyanide ($\text{CH}_3\text{CH}_2\text{C}\equiv\text{N}$) isomers through successive hydrogenations of acrylonitrile ($\text{CH}_2=\text{CH}-\text{C}\equiv\text{N}$) under interstellar conditions: The role of $\text{CH}_3\text{C}\equiv\text{N}$ 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
40	A correlated ab initio study of the $X^1\Sigma^+$ and $A^1\Sigma^+$ states of MgCH_3 . <i>Journal of Chemical Physics</i> , 1996, 104, 9495-9498.	3.0	9
41	The Formation of Glycolonitrile (HOCH_2CN) from Reactions of C^+ with HCN and HNC on Icy Grain Mantles. <i>Astrophysical Journal</i> , 2021, 906, 20.	4.5	9
42	Bonding in PF_2Cl , PF_3Cl , and PF_4Cl : 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
43	Quantum chemical protocols for modeling reactions and spectra in astrophysical ice analogs: the challenging case of the $\text{C}^+ + \text{H}_2\text{O}$ reaction in icy grain mantles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28705-28718.	2.8	8
44	Ab Initio Modeling of $(\text{LiF})_2$ and $(\text{LiF})_2(\text{H}_2\text{O})$. <i>The Journal of Physical Chemistry</i> , 1994, 98, 8831-8833.	2.9	6
45	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
46	Theoretical kinetic studies of Venus chemistry. Formation and destruction of SCl , SCl_2 , and HSCl . <i>Icarus</i> , 2021, 354, 114051.	2.5	4
47	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4342-4342.	3.1	0
48	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry A</i> , 2021, 125, 1680-1680.	2.5	0
49	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1973-1973.	2.6	0