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No	Authors	Title	Journal	Volume	Page Number	Year	DOI
1	S. Sahu, L. R. Widger, M. G. Quesne, S. P. de Visser, H. Matsumura, P. Moenne-Loccoz, M. A. Siegler, and D. P. Goldberg	Secondary Coordination Sphere Influence on the Reactivity of Nonheme Iron(II) Complexes: An Experimental and DFT Approach	J. Am. Chem. Soc.	135	10590-10593	2013	10.1021/ja402688t
2	L. R. Widger, Y. Jiang, M. Siegler, D. Kumar, R. Latifi, S. P. de Visser, G. N. L. Jameson, and D. P. Goldberg	Synthesis and Ligand Non-Innocence of Thiolate-Ligated (N4S) Iron(II) and Nickel(II) Bis(imino)pyridine Complexes	Inorg. Chem.	52	10467-10480	2013	10.1021/ic4013558
3	M. W. Stanford, F. R. Knight, K. S. A. Arachchige, P. S. Camacho, Sharon E. Ashbrook, M. Buehl, A. M. Z. Slawin and J. D. Woollins	Probing interactions through space using spin–spin coupling	Dalton Trans.	43	6548-6560	2014	10.1039/c4dt00408f
4	J. Schwabedissen, P. D. Lane, S. L. Masters, K. Hassler and D. A. Wann	Gas-phase structures of sterically crowded disilanes studied by electron diffraction and quantum chemical methods: 1,1,2,2-tetrakis(trimethylsilyl)disilane and 1,1,2,2-tetrakis(trimethylsilyl)dimethyldisilane	Dalton Trans.	43	10175-10182	2014	10.1039/C4DT00628C
5	M. Walker, A. J. A. Harvey, A. Sen and C. E. H. Dessent	Performance of M06, M06-2X, and M06-HF Density Functionals for Conformationally Flexible Anionic Clusters: M06 Functionals Perform Better than B3LYP for a Model System with Dispersion and Ionic Hydrogen-Bonding Interactions	J. Phys. Chem. A	117	12590-12600	2013	10.1021/jp408166m
6	K. Izod, J. M. Watson, W. Clegg and R. W. Harrington	Phosphido-borane and phosphido-bis(borane) complexes of the alkali metals, a comparative study	Inorg. Chem.	52	1466-1475	2013	10.1021/ic302205b
7	S. Koenig, N. F. Chilton, C. Maichle-moessmer, E. M. Pineda, T. Pugh, R. Anwander and R. A. Layfield	Fast magnetic relaxation in an octahedral dysprosium tetramethyl-aluminate complex	Dalton Trans.	43	3035–3038	2013	10.1039/C3DT52337C
8	R. J. Barber, J. K. Strange, C. Hill, O. L. Polyansky, G. C. Mellau, S. N. Yurchenko and J. Tennyson	ExoMol line lists - III. An improved hot rotation-vibration line list for HCN and HNC	MNRAS	437	1828-1835	2014	10.1093/mnras/stt2011
9	P. Guiglion, C. Butchosa and M. A.	Polymeric watersplitting photocatalysts; a	J. Mater. Chem.	2	11996-12004	2014	10.1039/C4TA02044

	Zwijnenburg	computational perspective on the water oxidation conundrum	A				H
10	X. Liu, J. M. Cole, P. C. Y. Chow, L. Zhang, Y. Tan, and T. Zhao	Dye aggregation and complex formation effects in 7-(diethylamino)-coumarin-3-carboxylic acid	J. Phys. Chem. C	118	13042–13051	2014	10.1021/jp409435v
11	X. Liu, D. Mao, J. M. Cole, and Z. Xu	Temperature insensitive fluorescence intensity in a coumarin monomer-aggregate coupled system	Chem. Commun.	50	9329-9332	2014	10.1039/C4CC04245J
12	L. Zhang and J. M. Cole	Tio2-assisted photoisomerization of azo dyes using self- assembled monolayers: Case study on para-methyl red towards solar-cell applications	ACS Applied Materials & Interfaces	6	3742–3749	2014	10.1021/am500308d
13	L. Zhang, J. M. Cole, and C. Dai	Variation in optoelectronic properties of azo dye- sensitized tio2 semiconductor interfaces with different adsorption anchors: Carboxy- late, sulfonate, hydroxyl and pyridyl groups	ACS Applied Materials & Interfaces	6	7535–7546	2014	10.1021/am502186k
14	W. B. Cross, S. Razak, K. Singh, A. J. Warner	C(sp3)-H activation without a directing group: regioselective synthesis of N-ylide or N-heterocyclic carbene complexes controlled by the choice of metal and ligand	Chem. Eur. J.	20	1-8	2014	10.1002/chem.201403860
15	D. J. Shepherd, P. A. Broadwith, B. S. Dyson, R. S. Paton and J. W. Burton	Structure reassignment of laurefurenynes A and B by computation and total synthesis	Chem. Eur. J.	19	12644-12648	2013	10.1002/chem.201302349
16	J. P. Harris, D. R. Manship, W. H. Breckenridge and T. G. Wright	Comparison of the interactions in the rare gas hydride and Group 2 metal hydride anions	J. Chem. Phys.	140	084304	2014	10.1063/1.4865749
17	J. P. Harris, H. Dodson, W. H. Breckenridge and T. G. Wright	HM+ and HM+-He (M = Group 2 metal): chemical or physical interactions?	J. Chem. Phys.	141	094306	2014	10.1063/1.4894227
18	A. M. Gardner, A. M. Green, V. M. Tamé-Reyes, K. L. Reid, J. A. Davies, V. H. K. Parks (née Wilton) and T. G. Wright	The 700-1500 cm-1 region of the S1 (A 1B2) state of toluene studied with resonance- enhanced multiphoton ionization (REMPI), zero-kinetic-energy (ZEKE) spectroscopy and time-resolved slow-electron velocity-map imaging (tr-SEVI) spectroscopy	J. Chem. Phys.	140	114038	2014	10.1063/1.4867970
19	J. M. Brown	Origins of Stabilization and Evidence for Charge Delocalization in the Bicyclo[3.2.1]octadienyl Anion and	Aust. J. Chem.	67	1296–1300	2014	10.1071/CH14244

		Related Species					
20	A. V. Protchenko, D. Dange, J. Harmer, C. Y. Tang, A. D. Schwarz, M. J. Kelly, N. Phillips, K. H. Birjkumar, C. Jones, N. Kaltsoyannis, P. Mountford and S. Aldridge	Thermally robust monomeric MX_2 radicals (M = Ga, In, Tl)	Nature Chemistry	6	315-319	2014	10.1038/nchem.1870
21	M. L. Petrus, R. K. M. Bouwer, U. Lafont, S. Athanasopoulos, N. C. Greenham and T. J. Dingemans	Small-molecule azomethines: organic photovoltaics via Schiff base condensation chemistry	J. Mater. Chem. A	2	9474-9477	2014	10.1039/C4TA01629G
22	A. V. Protchenko, K. H. Birjkumar, D. Dange, A. D. Schwarz, D. Vidovic, C. Jones, N. Kaltsoyannis, P. Mountford and S. Aldridge	A stable two-coordinate acyclic silylene	J. Am. Chem. Soc.	134	6500–6503	2012	10.1021/ja301042u
23	A. V. Protchenko, A. D. Schwarz, C. Jones, N. Kaltsoyannis, P. Mountford and S. Aldridge	A generic one-pot route to acyclic two-coordinate silylenes from Si(IV) precursors: synthesis and structural characterization of a silylsilylene	Angew. Chem. Int. Ed.	52	568–571	2013	10.1002/anie.201208554
24	S. Bui, D. von Stetten, P. G. Jambrina, T. Prangé, N. Colloc'h, D. de Sanctis, A. Royant, E. Rosta and R. A. Steiner	Direct Evidence for a Peroxide Intermediate and a Reactive Enzyme–Substrate–Dioxygen Configuration in a Cofactor-free Oxidase	Angew. Chem. Int. Ed.	53	1-6	2014	10.1002/anie.201405485
25	A. Kerridge	f-orbital covalency in the actinocenes (An=Th-Cm): multiconfigurational studies and topological analysis	RSC Adv.	4	12078-12086	2014	10.1039/C3RA47088A
26	K. Izod, C. Wills, E. Anderson, R. W. Harrington and M. R. Probert	Insights into the Stability and Structures of Phosphine-Boranes and Their α-Metalated Derivatives	Organometallics	33	5283-5294	2014	10.1021/om5005995
27	P. D. Jarowski and Y. Mo	Two States Are Not Enough: Quantitative Evaluation of the Valence-Bond Intramolecular Charge-Transfer Model and Its Use in Predicting Bond Length Alternation Effects	Chem. Eur. J.	20	1-8	2014	10.1002/chem.201404978
28	M. Ng, D. K. W. Mok, J. M. Dyke and E. P. F. Lee	Decomposition reactions of hexafluoropropylene oxide (HFPO): Rate coefficients calculated at different temperatures using ab initio and DFT reaction paths	J. Fluorine Chem.	259	29-37	2014	10.1016/j.jfluchem.2013.11.013
29	R. Chow, M. Ng, D. K. W. Mok, E. P. F. Lee and J. M. Dyke	Rate Coefficients of the Cl + CH3C(O)OCH3 -> HCl + CH3C(O)OCH2	J. Phys. Chem. A	118	2040-2055	2014	10.1021/jp5000864

		Reaction at Different Temperatures Calculated by Transition-State Theory with ab Initio and Density Functional Theory Reaction Paths					
30	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	Simulation of the single-vibronic-level emission spectrum of HPS	J. Chem. Phys.	140	art. no. 194311	2014	10.1063/1.4875806
31	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	Simulated photodetachment spectra of AIH(2)(-)	J. Chem. Phys.	139	art. no. 014301	2014	10.1063/1.4811671
32	G. Copeland, E. P. F. Lee, R. G. Williams, A. T. Archibald, D. E. Shallcross and J. M. Dyke	Determination of the Photolysis Rate Coefficient of Monochlorodimethyl Sulfide (MClDMS) in the Atmosphere and Its Implications for the Enhancement of SO2 Production from the DMS + Cl-2 Reaction	Environ. Sci. Technol.	48	1557-1565	2014	10.1021/es402956r
33	O. M. Roscioni, J. M. Dyke and J. Evans	Structural Characterization of Supported Rh-I(CO)(2)/gamma-Al2O3 Catalysts by Periodic DFT Calculations	J. Phys. Chem. C	117	19464-19470	2013	10.1021/jp405549k
34	W. G. Roeterdink, J.. Bulthuis, E. P. F. Lee, D. Ding and C. A. Taatjes	Hexapole transmission spectrum of formaldehyde oxide	Chem. Phys. Lett.	598	96-101	2014	10.1016/j.cplett.2014.03.009
35	C. J. Percival, O. Welz, A. J. Eskola, J. D. Savee, D. L. Osborn, D. O. Topping, D. Lowe, S. R. Utembe, A. Bacak, G. McFiggans, M. C. Cooke, X. Ping, A. T. Archibald, M. E. Jenkin, R. G. Derwent, I. Riipinen, D. K. W. Mok, E. P. F. Lee, J. M. Dyke, C. A. Taatjes and D. E. Shallcross	Regional and global impacts of Criegee intermediates on atmospheric sulphuric acid concentrations and first steps of aerosol formation	Faraday Discussions	165	45-73	2013	10.1039/c3fd00048f
36	J. B. Greenwood, J. Miles, S. D. Camillis, P. Mulholland, L. Zhang, M. A. Parkes, H. C. Hailes and H. H. Fielding	Resonantly Enhanced Multiphoton Ionization Spectrum of the Neutral Green Fluorescent Protein Chromophore	J. Phys. Chem. Lett.	5	3588-3592	2014	10.1021/jz5019256
37	A. Alwaaly and R. A. Henderson	Sterics level the rates of proton transfer to [Ni(XPh){PhP(CH2CH2PPh2)2}]+ (X = O, S or Se)	Chem. Commun.	50	9669-9671	2014	10.1039/c4cc04197f
38	A. E. Sheshenev, E. V. Boltukhina, A. J. P. White and K. K. Hii	Methylene-bridged bis(imidazoline)-derived 2-oxopyrimidinium salts as catalysts for asymmetric Michael reactions	Angew. Chem. Int. Ed.	52	6988-6991	2013	10.1002/anie.201300614
39	A. E. Sheshenev, E. V. Boltukhina, A. A. Grishina, I. Cisarova, I. M. Lyapkalo and K. K. Hii	New chiral zwitterionic phosphorus heterocycles: Synthesis, structure, properties and application as chiral	Chem. Eur. J.	19	8136-8143	2013	10.1002/chem.201300062

		solvating agents					
40	A. E. Sheshenev, E. V. Boltukhina and K. K. Hii	Levonantradol: asymmetric synthesis and structural analysis	Chem. Commun.	49	3685-3687	2013	10.1039/C3CC41388H
41	A. Buchard, D. R. Carbery, M. G. Davidson, P. K. Ivanova, B. J. Jeffery, G. I. Kociok-Koehn and J. P. Lowe	Preparation of Stereoregular Isotactic Poly(mandelic acid) through Organocatalytic Ring-Opening Polymerization of a Cyclic O-Carboxyanhydride	Angew. Chem. Int. Ed.	53	13858-13861	2014	10.1002/anie.201407525
42	M. M. Law, J. T. Fraser-Smith and C. U. Perotto	The potential energy surface of isomerising disilyne	Phys. Chem. Chem. Phys.	14	6922–6936	2012	10.1039/c2cp40605e
43	M. M. Law and C. U. Perotto	The vibrational bound states of isomerising disilyne	J. Chem. Phys.	139	art. no. 064308	2013	10.1063/1.4817533
44	C. Lapthorn, T. J. Dines, B. Z. Chowdhry, G. L. Perkins and F. S. Pullen	Can ion mobility mass spectrometry and density functional theory help elucidate protonation sites in 'small' molecules?	Rapid Commun. Mass Spectrom.	27	2399-2410	2013	10.1002/rcm.6700
45	S. P. de Visser, M. G. Quesne, B. Martin, P. Comba and U. Ryde	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes	Chem. Commun.	50	262-282	2014	10.1039/C3CC47148A
46	M. G. Quesne, R. Latifi, L. E. Gonzalez-Ovalle, D. Kumar and S. P. de Visser	Quantum mechanics/molecular mechanics study on the oxygen binding and substrate hydroxylation step in AlkB repair enzymes	Chem. Eur. J.	20	435-446	2014	10.1002/chem.201303282
47	L. R. Widger, Y. Jiang, T. Yang, A. C. McQuilken, M. A. Siegler, H. Matsumura, P. Moenne-Loccoz, D. Kumar, S. P. de Visser and D. P. Goldberg	Thioether-ligated iron(II) and iron(III)-hydroperoxo/alkylperoxo complexes with an H-bond donor in the second coordination sphere	Dalton Trans.	43	7522-7532	2014	10.1039/C4DT00281D
48	H. M. Neu, M. G. Quesne, T. Yang, K. A. Prokop-Prigge, K. M. Lancaster, J. Donohoe, S. DeBeer, S. P. de Visser and D. P. Goldberg	Dramatic influence of an anionic donor on the oxygen-atom-transfer reactivity of an Mn(V)-oxo complex	Chem. Eur. J.	20	14584-14588	2014	10.1002/chem.201404349
49	S. Sahu, M. G. Quesne, C. G. Davies, M. Duerr, I. Ivanovic-Burmazovic, M. A. Siegler, G. N. L. Jameson, S. P. de Visser and D. P. Goldberg	Direct observation of a non-heme iron(IV)-oxo complex that mediates aromatic C-F hydroxylation	J. Am. Chem. Soc.	136	13542-13545	2014	10.1021/ja507346t
50	H. M. Neu, T. Yang, R. A. Baglia, T. H. Yosca, M. T. Green, M. G. Quesne, S. P. de Visser and D. P. Goldberg	Oxygen-atom transfer reactivity of axially ligated Mn(V)-Oxo complexes: Evidence for enhanced electrophilic and nucleophilic pathways	J. Am. Chem. Soc.	136	13845-13852	2014	10.1021/ja507177h

51	B. Karamzadeh, D. Singh, W. Nam, D. Kumar and S. P. de Visser	Properties and reactivities of nonheme iron(IV)-oxo versus iron(V)-oxo: Long-range electron transfer versus hydrogen atom abstraction	Phys. Chem. Chem. Phys.	16	22611-22622	2014	10.1039/c4cp03053b
52	R. Jastrzebski, M. G. Quesne, B. M. Weckhuysen, S. P. de Visser and P. C. Bruijnincx	Experimental and computational evidence for the mechanism of intradiol catechol dioxygenation by non-heme iron(III) complexes	Chem. Eur. J.	20	15686-15691	2014	10.1002/chem.201404988
53	D. A. Wann, S. Young, K. Baetz, S. L. Masters, A. G. Avent, D. W. H. Rankin, and P. D. Lickiss	Structures of Tetrasilylmethane Derivatives C(SiXMe2)4 (X = H, F, Cl, Br) in the Gas Phase and their Dynamic Structures in Solution	Z. Naturforsch. B	69	1321-1332	2014	10.5560/ZNB.2014-4147
54	S. Kumar, A. S. Faponle, P. Barman, A. K. Vardhaman, C. V. Sastri, D. Kumar and S. P. de Visser	Long-range electron transfer triggers mechanistic differences between iron(IV)-oxo and iron(IV)-imido oxidants	J. Am. Chem. Soc.	136	17102–17115	2014	10.1021/ja508403w
55	A. S. Faponle, M. G. Quesne, C. V. Sastri, F. Banse and S. P. de Visser	Differences and comparisons of the properties and reactivities of iron(III)-hydroperoxo complexes with saturated coordination sphere	Chem. Eur. J.	20	1-17	2014	10.1002/chem.201404918
56	A. K. Vardhaman, P. Barman, S. Kumar, C. V. Sastri, D. Kumar and S. P. de Visser	Mechanistic insight into halide oxidation by non-heme iron complexes. Haloperoxidase versus halogenase activity	Chem. Commun.	49	10926-10928	2013	10.1039/c3cc46792a
57	M. G. Quesne, R. A. Ward and S. P. de Visser	Cysteine protease inhibition by nitrile-based inhibitors: A computational study	Front. Chem.	1	39.1-39.10	2013	10.3389/fchem.2013.00039
58	M. Tia, B. Cunha de Miranda, S. Daly, F. Gaie-Levrel, G. A. Garcia, L. Nahon and I. Powis	VUV Photodynamics and Chiral Asymmetry in the Photoionization of Gas Phase Alanine Enantiomers	J. Phys. Chem. A	118	2765-2779	2014	10.1021/jp5016142
59	G. A. Garcia, H. Dossmann, L. Nahon, S. Daly and I. Powis	Photoelectron circular dichroism and spectroscopy of trifluoromethyl- and methyl-oxirane: a comparative study	Phys. Chem. Chem. Phys.	16	16214-16224	2014	10.1039/C4CP01941E
60	S. Daly, I. Powis, M. Tia, G. A. Garcia and L. Nahon	Dissociative VUV photoionization of butanediol isomers	Int. J. Mass Spectrom.	376	46-53	2015	10.1016/j.ijms.2014.11.013
61	I. Powis	Communication: The influence of vibrational parity in chiral photoionization dynamics	J. Chem. Phys.	140	art. no. 111103	2014	10.1063/1.4869204
62	K. Izod, C. M. Dixon, R. W. Harrington, M. R. Probert	Impact of a rigid backbone on the structure of an agostically-stabilised dialkylstannylene: isolation of an unusual bridged stannyl-stannylene	Chem. Commun.	51	679-681	2015	10.1039/C4CC08740B

63	L. Darré, S. Furini and C. Domene	Permeation and Dynamics of an Open-Activated TRPV1 Channel	J. Mol. Biol.	427	537-549	2015	10.1016/j.jmb.2014.11.016
64	D. M. P. Holland, I. Powis, A. B. Trofimov, I. L.. Bodzuk, D. Y. Soshnikov, A. W. Potts and L. Karlsson	A study of the valence shell electronic structure and photoionization dynamics of ortho-dichlorobenzene, ortho-bromochlorobenzene and trichlorobenzene	Chem. Phys.	448	61-75	2015	10.1016/j.chemphys.2014.11.025
65	D. A. Wann, M. S. Robinson, K. Bätz, S. L. Masters, A. G. Avent and P. D. Lickiss	Structures of tetrasilylmethane derivatives (XMe2Si)2C(SiMe3)2 (X = H, Cl, Br) in the gas phase, and their dynamic structures in solution	J. Phys. Chem. A	119	786-795	2015	10.1021/jp511301s
66	S. Furini and C. Domene	DNA recognition process of the lactose repressor protein studied via metadynamics and umbrella sampling simulations	J. Phys. Chem. B	118	13059-13065	2014	10.1021/jp505885j
67	B. Apellániz, E. Rujas, P. Carravilla, J. Requejo-Isidro, N. Huarte, C. Domene and J. L. Nieva	Cholesterol-dependent membrane fusion induced by the gp41 membrane-proximal external region-transmembrane domain connection suggests a mechanism for broad HIV-1 neutralization	J. Virol.	88	13367-13377	2014	10.1128/JVI.02151-14
68	S. Doherty, J. G. Knight, N. A. B. Ward, D. M. Bittner, C. Wills, W. McFarlane, W. Clegg, and R. W. Harrington	Electron-Rich Trialkyl-Type Dihydro-KITPHOS Monophosphines: Efficient Ligands for Palladium-Catalyzed Suzuki–Miyaura Cross-Coupling. Comparison with Their Biaryl-Like KITPHOS Monophosphine Counterparts	Organometallics	32	1773-1788	2013	10.1021/om3011992
69	J. P. Harris, A. Andrejeva, Wi. D. Tuttle, I. Pugliesi, C. Schriever and T. G. Wright	Vibrations of the S1 state of fluorobenzene-h5 and fluorobenzene-d5 via resonance-enhanced multiphoton ionization (REMPI) spectroscopy	J. Chem. Phys.	141	art. no. 244315	2014	10.1063/1.4904706
70	O. V. Ershova, J. Kłos, N. A. Besley and T. G. Wright	Interaction of the NO 3p (C2) Rydberg State with RG (RG = Ne, Kr and Xe): Potential Energy Surfaces and Spectroscopy	J. Chem. Phys.	142	art. no. 034311	2015	10.1063/1.4905563
71	V. M. Gun'ko, R. Nasiri, and S. S. Sazhin	Effects of the surroundings and conformerisation of n-dodecane molecules on evaporation/condensation processes	J. Chem. Phys.	142	art. no. 034502	2015	10.1063/1.4905496
72	L. Burroughs, J. Ritchie, M. Ngwenya, D. Khan, W. Lewis and S.	Anionic Sigmatropic-Electrocyclic-Chugaev Cascades: Accessing 12-aryl-5-	Beilstein J. Org. Chem.	11	273-279	2015	10.3762/bjoc.11.31

	Woodward	(methylthio(carbonyl)thio)tetracenes and a Related Anthra[2,3-b]thiophene					
73	S. L. Masters, H. E. Robertson, D. A. Wann, M. Hölbling, K. Hassler, R. Bjornsson, S. Ó. Wallevik and I. Arnason	Molecular structure of 1,2-bis(trifluoromethyl)-1,1,2,2-tetramethyldisilane in the gas, liquid and solid phases – unusual conformational changes between phases	J. Phys. Chem. A		*Article ASAP*	2015	10.1021/jp507744u
74	E. N. Daley, C. M. Vogels, S. J. Geier, A. Decken, S. Doherty and S. A. Westcott	The Phosphinoboration Reaction	Angew. Chem. Int. Ed.	54	2121-2125	2015	10.1002/anie.201410033
75	G. Noonan and A. G. Leach	A mechanistic proposal for the protodeboronation of neat boronic acids: boronic acid mediated reaction in the solid state	Org. Biomol. Chem.	13	2555-2560	2015	10.1039/C4OB02543A