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No	Authors	Title	Journal	Volume	Page Number	Year	DOI
1	G. A. Guirgis, J. S. Overby, T. J. Barker, M. H. Palmer, B. H. Pate and N. A. Seifert	The Molecular Structure of Methylfluoroisocyanato Silane: A Combined Microwave Spectral and Theoretical Study	J. Phys. Chem. A	119	652-658	2015	10.1021/jp511354j
2	T. G. Karabancheva, C. C. Lee, R. Donev, G. W. Black and C. Z. Christov	How Does Conformational Flexibility Influence Key Structural Features Involved in Activation of Anaplastic Lymphoma Kinase?	Mol. BioSyst.	10	1490-1495	2014	10.1039/C4MB00141A
3	T. G. Karabancheva-Christova, W. Singh and C. Z. Christov	Computational Study of the Structure, the Flexibility, and the Electronic Circular Dichroism of Staurosporine - a Powerful Protein Kinase Inhibitor	Z. Naturforsch. A	69	331-338	2014	10.5560/ZNA.2014-0021
4	A. Sen, T. F. M. Luxford, N. Yoshikawa and C. E. H. Dessent	Solvent evaporation versus proton transfer in nucleobase-Pt(CN)(4,6)(2-) dianion clusters: a collisional excitation and electronic laser photodissociation spectroscopy study	Phys. Chem. Chem. Phys.	16	15490-15500	2014	10.1039/c4cp00989d
5	A. Sen and C. E. H. Dessent	Mapping the UV Photophysics of Platinum Metal Complexes Bound to Nucleobases: Laser Spectroscopy of Isolated Uracil center dot Pt(CN)(4)(2-) and Uracil center dot Pt(CN)(6)(2-) Complexes	J. Phys. Chem. Lett.	5	3281-3285	2014	10.1021/jz501749j
6	A. Sen and C. E. H. Dessent	Communication: Photoactivation of nucleobase bound platinum(II) metal complexes: Probing the influence of the nucleobase	J. Chem. Phys.	141	art. no. 241101	2014	10.1063/1.4904259
7	A. Alwaaly, W. Clegg, R. A. Henderson, M. R. Probert and P. G. Waddell	Mechanisms and Rates of Proton Transfer to Coordinated Carboxydithioates: Studies on [Ni(S2CR){PhP(CH2CH2PPh2)2}] ⁺ (R = Me, Et, Bun or Ph)	Dalton Trans.	44	3307-3317	2015	10.1039/C4DT03543G
8	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, M. Biczysko, A. Baiardi, and P. Limaov-Vieira	Interpretation of the vacuum ultraviolet photoabsorption spectrum of iodobenzene by ab initio computations	J. Chem. Phys.	142	art. no. 134302	2015	10.1063/1.4916121

9	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, M. Biczysko, and A. Baiardi	The ionic states of iodobenzene studied by photoionization and ab initio configuration interaction and DFT computations	J. Chem. Phys.	142	art. no. 134301	2015	10.1063/1.4916120
10	C. Domene, P. Barbini and S. Furini	Bias-Exchange Metadynamics Simulations: An Efficient Strategy for the Analysis of Conduction and Selectivity in Ion Channels	J. Chem. Theory Comput.	11	1896-1906	2015	10.1021/ct501053x
11	C. R. S. Mooney, M. A. Parkes, A. Iskra and H. H. Fielding	Controlling Radical Formation in the Photoactive Yellow Protein Chromophore	Angew. Chem. Int. Ed.	54	1-5	2015	10.1002/anie.201500549
12	Q. R. Huang, J. R. Kingham and N. Kaltsoyannis	The strength of actinide-element bonds from the Quantum Theory of Atoms-in-Molecules	Dalton Trans.	44	2554-2566	2015	10.1039/c4dt02323d
13	J. Pang, N. S. Scrutton and M. J. Sutcliffe	Quantum Mechanics/Molecular Mechanics Studies on the Mechanism of Action of Cofactor Pyridoxal 5'-Phosphate in Ornithine 4,5-Aminomutase	Chem. Eur. J.	20	11390-11401	2014	10.1002/chem.201402759
14	M. Maniruzzaman, J. Pang, D. J. Morgan and D. Douroumis	Molecular modeling as a predictive tool for the development of solid dispersions	Mol. Pharm.	12	1040-1049	2015	10.1021/mp500510m
15	J. P. Harris, H. Dodson, W. H. Breckenridge and T. G. Wright	HM+-RG Complexes (M = Group 2 Metal; RG = Rare Gas): Physical vs. Chemical Interactions	J. Chem. Phys.	142	art. no. 154302	2015	10.1063/1.4918348
16	G. L. Gregory, M. Ulmann and A. Buchard	Synthesis of 6-membered cyclic carbonates from 1,3-diols and low CO ₂ pressure: a novel mild strategy to replace phosgene reagents	RSC Adv.	5	39404-39408	2015	10.1039/C5RA07290E
17	M. D. Jones, S. L. Hancock, P. McKeown, P. M. Schaefer, A. Buchard, L. H. Thomas, M. F. Mahon and J. P. Lowe	Zirconium complexes of bipyrrrolidine derived salan ligands for the isoselective polymerisation of rac-lactide	Chem. Commun.	50	15967-15970	2014	10.1039/c4cc07871c
18	D. M. Bittner, D. P. Zaleski, S. L. Stephens, D. P. Tew, N. R. Walker and A. C. Legon	A monomeric complex of ammonia and cuprous chloride: H ₃ N...CuCl isolated and characterised by rotational spectroscopy and ab initio calculations	J. Chem. Phys.	142	144302	2015	10.1063/1.4916391
19	M. D. Jones, L. Brady, P. McKeown, A. Buchard, P. M. Schaefer, L. H. Thomas, M. F. Mahon, T. J. Woodman and J. P. Lowe	Metal influence on the iso- and hetero-selectivity of complexes of bipyrrrolidine derived Salan ligands for the polymerisation of rac-lactide	Chem. Sci.	6	5034-5049	2015	10.1039/C5SC01819F
20	A. Alwaaly, W. Clegg, R. W. Harrington, A. L. Petrou and R. A.	Mechanism of proton transfer to coordinated thiolates: unexpected factors	Dalton Trans.	44	11977-11983	2015	10.1039/C5DT01716E

	Henderson	stabilize precursor intermediates					
21	K. Rix, G. H. Kelsall, K. Hellgardt and K. K. (Mimi) Hii	Chemo- and Diastereo-selectivities in the Electrochemical Reduction of Maleimides	ChemSusChem	8	665-671	2015	10.1002/cssc.201403184
22	S. Boonseng, G. W. Roffe, J. Spencer and H. Cox	The nature of the bonding in symmetrical pincer palladacycles	Dalton Trans.	44	7570-7577	2015	10.1039/C5DT00031A
23	M. J. Taylor, E. J. Coakley, M. P. Coles, H. Cox and J. R. Fulton	Beta-Diketiminato Organolead Complexes: Structures, ²⁰⁷ Pb NMR, and Hammett Correlations	Organometallics	34	2515-2521	2015	10.1021/om501223a
24	T. K. Lind, L. Darre, C. Domene, Z. Urbanczyk-Lipkowska, M. Cardenas and H. P. Wacklin	Antimicrobial peptide dendrimer interacts with phosphocholine membranes in a fluidity dependent manner: A neutron reflection study combined with molecular dynamics simulations	Biochim Biophys Acta	1848	2075-2084	2015	10.1016/j.bbamem.2015.05.015
25	A. Andrejeva, A. M. Gardner, J. B. Graneek, W. H. Breckenridge and T. G. Wright	Theoretical Study of M ⁺ -RG ₂ : (M ⁺ = Ca, Sr, Ba and Ra; RG= He-Rn)	<i>J. Phys. Chem. A</i>	119	5995-6005	2015	10.1021/jp511817g
26	D. M. Bittner, D. P. Zaleski, S. L. Stephens, N. R. Walker and A. C. Legon	The sigma-Hole interaction between sulfur hexafluoride and ammonia characterised by broadband rotational spectroscopy	Chem. Phys. Chem.	16	2630-2634	2015	10.1002/cphc.201500455
27	A. Mckechnie, G. H. Booth, A. J. Cohen and J. M. Cole	On the accuracy of density functional theory and wave function methods for calculating vertical ionization energies	J. Chem. Phys.	142	art. no. 194114	2015	10.1063/1.4921037
28	F. Sladojevich, A. L. Fuentes de Arriba, A. Ferrali, R. S. Paton and D. J. Dixon	Mechanistic investigations on the enantioselective Conia-ene reaction catalyzed by cinchona-derived amino urea pre-catalysts and Cu(I)	Chem. Eur. J.	19	14286-14295	2013	10.1002/chem.201200832
29	C. Pubill-Ulldemolins, E. Fernandez, C. Bo and J. M. Brown	Origins of observed reactivity and specificity in the addition of B ₂ Cl ₄ and analogues to unsaturated compounds	Org. Biomol. Chem.	13	9619-9628	2015	10.1039/C5OB01280E
30	F. R. Knight, L. M. Diamond, K. S. Athukorala Arachchige, P. Sanz Camacho, R. A. M. Randall, S. E. Ashbrook, M. Buehl, A. M. Z. Slawin, and J. D. Woollins	Conformational Dependence of Through-Space Tellurium-Tellurium Spin-Spin Coupling in Peri-Substituted Bis(Tellurides)	Chem. Eur. J.	21	3613-3627	2015	10.1002/chem.201405599
31	A. Nordheider, E. Hupf, B. A. Chalmers, F. R. Knight, M. Buehl, S. Mebs, L. Checinska, E. Lork, P. Sanz	Peri-Substituted Phosphorus-Tellurium Systems-An Experimental and Theoretical Investigation of the P...Te through-Space	Inorg. Chem.	54	2435-2446	2015	10.1021/ic503056z

	Camacho, S. E. Ashbrook, K. S. Athukorala Arachchige, D. B. Cordes, A. M. Z. Slawin, J. Beckmann, and J. D. Woollins	Interaction					
32	R. Nasiri, V. M. Gun'ko and S. S. Sazhin	The effects of internal molecular dynamics on the evaporation/condensation of n-dodecane	Theor. Chem. Acc.	134	83	2015	10.1007/s00214-015-1681-z
33	L. Burroughs, L. Eccleshare, J. Ritchie, O. Kulkarni, B. Lygo, S. Simon Woodward and W. Lewis	One-Pot Cannizzaro Cascade Synthesis of ortho-Fused Cycloocta-2,5-dien-1-ones from 2-Bromo(hetero)aryl Aldehydes	Angew. Chem. Int. Ed.	54	10648-10651	2015	10.1002/anie.201505347
34	T. -I. Sohn, D. Kim and R. S. Paton	Substrate-Controlled Asymmetric Total Syntheses of Micro- cladallenes A, B, and C based on the Proposed Structures	Chem. Eur. J.	21	01-11	2015	10.1002/chem.201502592
35	Q. Wang, S. K. Ang, E. Ceh-Pavia, J. Pang and H. Lu	Role of tryptophan residues of Erv1: Trp95 and Trp183 are important for its folding and oxidase function	Biosci. Rep.	35	art:e00244	2015	10.1042/BSR20150144
36	S. Manzoor, A. Simperler and A. Korre	A theoretical study of the reaction kinetics of amines released into the atmosphere from CO ₂ capture	Int. J. Greenh. Gas Control	41	219-228	2015	10.1016/j.ijggc.2015.05.012
37	L. Ji, A. S. Faponle, M. G. Quesne, M. A. Sainna, J. Zhang, A. Franke, D. Kumar, R. van Eldik, W. Liu and S. P. de Visser	Drug Metabolism by Cytochrome P450 Enzymes: What Distinguishes the Pathways Leading to Substrate Hydroxylation Over Desaturation?	Chem. Eur. J.	21	9083-9092	2015	10.1002/chem.201500329
38	J. Iglesias-Fernandez, L. Darre, A. Kohlmeyer, R. K. Thomas, H. H. Shen and C. Domene	Surfactin at the Water/Air Interface and in Solution	Langmuir	31	11097-11104	2015	10.1021/acs.langmuir.5b02305
39	L. Darre, J. Iglesias, A. Kolh Meyer, H. Wacklin, and C. Domene	Molecular Dynamics Simulations and Neutron Reflectivity as an Effective Approach To Characterize Biological Membranes and Related Macromolecular Assemblies	J. Chem. Theory Comput.	11	4875-4884	2015	10.1021/acs.jctc.5b00635
40	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, M. Biczysko, A. Baiardi and K. Peterson	Interpretation of the photoelectron, ultraviolet, and vacuum ultraviolet photoabsorption spectra of bromobenzene by ab initio configuration interaction and DFT computations	J. Chem. Phys.	143	art. no. 164303	2015	10.1063/1.4933419
41	S. Kritikou and J. G. Hill	Auxiliary basis sets for density fitting in explicitly correlated calculations: The atoms H-Ar	J. Chem. Theory Comput.	11	5269-5276	2015	10.1021/acs.jctc.5b00816
42	M. R. Ranga Prabhat, J. Romanova,	The Role of Substituent Effects in Tuning	Angew. Chem.	54	7949-7953	2015	10.1002/anie.20150

	R. J. Curry, S. R. P. Silva and P. D. Jarowski	Metallophilic Interactions and Emission Energy of bis-4-(2-Pyridyl)-1,2,3-triazolato platinum(II) Complexes	Int. Ed.				2390
43	M. S. Inkpen, S. Du, M. Hildebrand, A. J. P. White, N. M. Harrison, T. Albrecht and N. J. Long	The Unusual Redox Properties of Fluoroferrocenes Revealed through a Comprehensive Study of the Haloferrocenes	Organometallics	34	5461-5469	2015	10.1021/acs.organo met.5b00811
44	W. D. Tuttle, R. L. Thorington, L. A. Viehland and T. G. Wright	Interaction Potentials, Spectroscopy and Transport Properties of C+(2Pj) and C+(4Pj) with Helium	Molec. Phys.	113	3767-3782	2015	10.1080/00268976.2015.1061153
45	A. Andrejeva, W. H. Breckenridge and T. G. Wright	A Surprisingly Simple Electrostatic Model Explains Bent Versus Linear Structures in M+-RG2 Species (M = Group 1 Metal, Li-Fr; RG = Rare Gas, He-Rn)	J. Phys. Chem. A	119	10959-20970	2015	10.1021/acs.jpca.5b08045
46	X. Tong, P. K. Busk, L. Lange and J. Pang	New insights into the molecular mechanism of methanol-induced inactivation of Thermomyces lanuginosus lipase: A molecular dynamics simulation study	Mol. Simul.	42	435-445	2015	10.1080/08927022.2015.1059938
47	J. P. F. Nunes, J. Holub, D. W. H. Rankin, D. A. Wann and D. Hnyk	A computational analysis of the apparent nido vs. hypho conflict: are we dealing with six- or eight-vertex open-face diheteroboranes?	Dalton Trans.	44	11819-11826	2015	10.1039/C5DT01460C
48	Y. V. Vishnevskiy, D. S. Tikhonov, C. G. Reuter, N. W. Mitzel, D. Hnyk, J. Holub, D. A. Wann, P. D. Lane, R. J. F. Berger and S. A. Hayes	Influence of Antipodally Coupled Iodine and Carbon Atoms on the Cage Structure of 9,12-I2-closo-1,2-C2B10H10: An Electron Diffraction and Computational Study	Inorg. Chem.	54	11868-11874	2015	10.1021/acs.inorgchem.5b02102
49	R. N. Straker, Q. Peng, A. Mekareeya, R. S. Paton and E. A. Anderson	Computational Ligand Design-guided Enantio- and Diastereoselective Cycloisomerization	Nature Communications	7	art. no. 10109	2015	10.1038/ncomms10109
50	W. A. Cortopassi, R. Simion, C. E. Hornsby, T. C. C. Franca and R. S. Paton	Dioxygen binding in the active site of histone demethylase JMJD2A and the role of protein environment	Chem. Eur. J.	21	18983-18992	2015	10.1002/chem.201502983
51	K. E. Jackson, C. L. Mortimer, B. Odell, J. M. McKenna, T. D. W. Claridge, R. S. Paton and D. M. Hodgson	α - and α' -Lithiation-Electrophile trapping of N-thiopivaloyl and N-t-butoxythiocarbonyl α -substituted Azetidines: rationalisation of the regiodivergence using NMR and computation	J. Org. Chem.	80	9838-9846	2015	10.1021/acs.joc.5b01804

52	A. D. Gammack Yamagata, S. Datta, L. Stegbauer, R. S. Paton and D. J. Dixon	Enantioselective Intramolecular Organocatalytic Michael Addition Reactions to α,β -Unsaturated Esters; A Desymmetrization Strategy to the Morphan Scaffold	Angew. Chem. Int. Ed.	127	4981-4985	2015	10.1002/ange.201411924
53	L. Simon, and R. S. Paton	Origins of asymmetric phosphazene organocatalysis: computations reveal a common mechanism for nitro- and phospho-aldol additions	J. Org. Chem.	80	2756-2766	2015	10.1021/acs.joc.5b00063
54	C. P. Johnston, A. Kothari, T. Sergeieva, S. I. Okovytyy, K. E. Jackson, R. S. Paton, R. S. and M. D. Smith	Catalytic Enantioselective Synthesis of Indanes via Cation-Directed 5- <i>Endo-Trig</i> Cyclization	Nature Chem.	7	171-178	2015	10.1038/nchem.2150
55	R. D. Richardson, M. G. J. Baud, C. E. Weston, H. S. Rzepa, M. K. Kuimova and M. J. Fuchter	Dual wavelength asymmetric photochemical synthesis with circularly polarized light	Chem. Sci.	6	3853-3862	2015	10.1039/c4sc03897e
56	J. Romanova, M. R. Ranga Prabath, and P. D. Jarowski	Relationship between Metallophilic Interactions and Luminescent Properties in Pt(II) Complexes: TD-DFT Guide for the Molecular Design of Light-Responsive Materials	J. Phys. Chem. C	120	2002-2012	2016	10.1021/acs.jpcc.5b12132
57	D. Botten, G. Fugallo, F. Fraternali and C. Molteni	Structural Properties of Green Tea Catechins	J. Phys. Chem. B	119	12860-12867	2015	10.1021/acs.jpcb.5b08737
58	F. Comitani, C. Melis and C. Molteni	Elucidating Ligand Binding and Channel Gating Mechanisms in Pentameric Ligand-Gated Ion Channels by atomistic simulations	Biochem. Soc. Trans.	43	151-156	2015	10.1042/BST20140259
59	M. Ng, D. K. W. Mok, E.P. F. Lee, and J. M. Dyke	A theoretical investigation of the atmospherically important reaction between chlorine atoms and formic acid: determination of the reaction mechanism and calculation of the rate coefficient at different temperatures	Molec. Phys.	113	1511-1533	2015	10.1080/00268976.2014.980448
60	M. Ng, D. K. W. Mok, E. P. F. Lee, and J. M. Dyke	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	Phys. Chem. Chem. Phys.	17	7463-7476	2015	10.1039/c4cp06007e
61	M. J. D. Champion, J. M. Dyke, W.	Sodium Thioether Macrocyclic Chemistry:	Inorg. Chem.	54	2497-2499	2015	10.1021/acs.inorgch

	Levason, M. E. Light, D. Pugh, H. Bhakhoa, L. Rhyman, P. Ramasami, and G. Reid	Remarkable Homoleptic Octathia Coordination to Na ⁺					em.5b00156
62	D. E. Shallcross, K. E. Leather, A. Bacak, P. Xiao, E. P. F. Lee, M. Ng, D. K. W. Mok, J. M. Dyke, R. Hossaini, M. P. Chipperfield, M. A. H. Khan and C. J. Percival	Reaction between CH ₃ O ₂ and BrO Radicals: A New Source of Upper Troposphere Lower Stratosphere Hydroxyl Radicals	J. Phys. Chem. A	119	4618-4632	2015	10.1021/jp5108203
63	J. M. Dyke, W. Levason, M. E. Light, D. A. Pugh, G. Reid, H. Bhakhoa, P. Ramasami, and L. Rhyman	Aza-macrocyclic complexes of Group 1 cations: synthesis, structures and density functional theory study	Dalton Trans.	44	13853-13866	2015	10.1039/C5DT01865J
64	M. A. H. Khan, S. M. P. Gillespie, B. Razis, P. Xiao, M. T. Davies-Coleman, C. J. Percival, R. G. Derwent, J. M. Dyke, M.V. Ghosh, E. P. F. Lee, D. E. Shallcross	A modelling study of the atmospheric chemistry of DMS using the global model, STOCHEM-CRI	Atmospheric Environment	127	69-79	2016	10.1016/j.atmosenv.2015.12.028
65	J. C. Mullaney, S. L. Stephens, D. P. Zaleski, M. J. Sprawling, D. P. Tew, N. R. Walker, and A. C. Legon	An Isolated Complex of Ethyne and Gold Iodide Characterized by Broadband Rotational Spectroscopy and Ab initio Calculations	J. Phys. Chem. A	119	9636-9643	2015	10.1021/acs.jpca.5b06593
66	D. P. Zaleski, J. C. Mullaney, D. M. Bittner, D. P. Tew, N. R. Walker, and A. C. Legon	Interaction of a pseudo- π C-C bond with cuprous and argentous chlorides: Cyclopropane...CuCl and cyclopropane...AgCl investigated by rotational spectroscopy and ab initio calculations	J. Chem. Phys.	143	art. No. 164314	2015	10.1063/1.4934539
67	S. D. Ahn, A. Kolodziej, R. Malpass-Evans, M. Carta, N. B. McKeown, S. D. Bull, A. Buchard and F. Marken	Polymer of Intrinsic Microporosity Induces Host-Guest Substrate Selectivity in Heterogeneous 4-Benzoyloxy-TEMPO-Catalysed Alcohol Oxidations	Electrocatalysis	7	70-78	2016	10.1007/s12678-015-0284-8
68	A. K. King, A. Buchard, M. F. Mahon and R. L. Webster	Facile, Catalytic Dehydrocoupling of Phosphines Using - Diketiminato Iron(II) Complexes	Chem. Eur. J.	21	15960-15963	2015	10.1002/chem.201503399