PUBLICATIONS AND PRESENTATIONS REPORTED FROM USING NSCCS

Publications reported during the period of 1st February 2011 to 31st August 2016

No	Authors	Title	Journal	Volume	Page Number / Article Number	Year	DOI
1	J. G. Hill and J. A. Platts	Local electron correlation descriptions of the intermolecular stacking interactions between aromatic intercalators and nucleic acids	Chem. Phys. Lett.	479	279-283	2009	10.1016/j.cplett.2009.08.021
2	K. Gkionis and J. A. Platts	QM/MM investigation into binding of square-planar platinum complexes to DNA fragments	J. Biol. Inorg. Chem.	14	1165-1174	2009	10.1007/s00775-009-0560-2
3	J. A. Platts and K. Gkionis	NMR shielding as a probe of intermolecular interactions: ab initio and density functional theory studies	Phys. Chem. Chem. Phys.	11	10331-10339	2009	10.1039/b822560e
4	S. T. Mutter and J. A. Platts	Modulation of stacking interactions by transition metal coordination: ab initio benchmark studies	Chem. Eur. J.	16	5391-5399	2010	10.1002/chem.200902813
5	J. A. Platts and J. G. Hill	Non-Covalent Interactions using Local Correlation Methods: Energy Partitioning, Geometry Optimisation and Harmonic Frequency Calculations	Molec. Phys.	108	1497-1504	2010	10.1080/00268971003757977
6	J. A. Platts, J. Overgaard, C. Jones, B. B. Iversen and A. Stasch	First Experimental Characterisation of a Non-Nuclear Attractor in a Dimeric Magnesium(I) Compound	J. Phys. Chem. A	115	194-200	2011	10.1021/jp109547w
7	S. M. Hamilton, W. S. Hopkins, D. J. Harding, T. R. Walsh, P. Gruene, M. Haertelt, A. Fielicke, G. Meijer and S. R. Mackenzie	Infrared induced reactivity on the surface of isolated size-selected clusters: dissociation of N2O on rhodium clusters	J. Am. Chem. Soc.	132	1448-1449	2010	10.1021/ja907496c
8	G. Copeland, E. P. F. Lee, J. M. Dyke, W. K. Chow, D. K. W. Mok and F. T. Chau	Study of 2-H-Heptafluoropropane and Its Thermal Decomposition Using UV Photoelectron Spectroscopy and ab Initio Molecular Orbital Calculations	J. Phys. Chem. A	114	3540-3550	2010	10.1021/jp1000607
9	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	Franck-Condon simulation of the photoelectron spectrum of AsF2 and the photodetachment spectrum of AsF2- using ab initio calculations: Ionization energy and electron affinity of AsF2	Phys. Chem. Chem. Phys.	12	9075-9087	2010	10.1039/c003688a
10	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	Ab initio calculations on the (X)over-tilde B-2(1) and (A)over-bar (2)A(1) states of AsH2, and Franck-Condon simulation, including	J. Chem. Phys.	132	art. no. 234309	2010	10.1063/1.3442748

		anharmonicity, of the (A)over-tilde(0,0,0)-(X)over-tilde single vibronic level emission spectrum of AsH2					
11	D. A. Wann, A. R. Turner, J. R. Goerlich, L. J. Kettle, R. Schmutzler and D. W. H. Rankin	Gas-phase structures of 1-adamantylphosphines, PHn(1-Ad)3-n (n = 1-3)	Struct. Chem.	22	263-267	2011	10.1007/s11224-010-9695-6
12	D. A. Wann, C. N. Dickson, P. D. Lickiss, H. E. Robertson and D. W. H. Rankin	The gas-phase equilibrium structures of Si8O12(OSiMe3)8 and Si8O12(CHCH2)8	Inorg. Chem.	50	2988-2994	2011	10.1021/ic102457w
13	L. Varriale, N. Bhalla, N. M. Tonge, A. M. Ellis and T. G. Wright	Near-infrared Spectroscopy of LiNH3: First Observation of the Electronic Spectrum	J. Chem. Phys.	134	art no. 124304	2011	10.1063/1.3570824
14	C. L. Whalley, J. C. Gomez Martin, T. G. Wright and J. M. C. Plane	A Kinetic Study of Mg+ and Mg-containing Ions Reacting with O3, O2, N2, CO2, N2O and H2O: Implications for Magnesium Ion Chemistry in the Upper Atmosphere	Phys. Chem. Chem. Phys.	13	6352-6364	2011	10.1039/c0cp02637a
15	C. J. Evans, T. G. Wright and A. M. Gardner	Geometries and Bond Energies of the He-MX, Ne-MX and Ar-MX (M = Cu, Ag, Au; X = F, Cl) Complexes	J. Phys. Chem. A	114	4446-4454	2010	10.1021/jp912027y
16	A. M. Gardner, K. Gutsmiedl, T. G. Wright, W. H. Breckenridge, C. Y. N. Chapman and L. A. Viehland	Theoretical Study of Al+-RG (RG = He-Rn)	J. Chem. Phys.	133	art. no. 164302	2010	10.1063/1.3494602
17	A. M. Gardner, C. D. Withers, J. B. Graneek, T. G. Wright, L. A. Viehland and W. H. Breckenridge	Theoretical Study of M+-RG and M2+-RG Complexes and Transport of M+ through RG (M = Be and Mg; RG = He-Rn)	J. Phys. Chem. A	114	7631-7641	2010	10.1021/jp103836t
18	A. M. Gardner, R. J. Plowright, M. J. Watkins, T. G. Wright and W. H. Breckenridge	Theoretical study of the X (2)Sigma(+) states of the neutral CM-RG complexes (CM=coinage metal, Cu, Ag, and Au and RG=rare gas, He-Rn)	J. Chem. Phys.	132	art. no. 184301	2010	10.1063/1.3386239
19	L. A. Viehland, B. R. Gray and T. G. Wright	Interactions of Rare Gas Cations with Lighter Rare Gas Atoms	Molec. Phys.	108	547-555	2010	10.1080/00268971003604583

20	A. M. Gardner, C. D.Withers, T. G. Wright, K. I. Kaplan, C. Y. N. Chapman, L. A. Viehland, E. P. F. Lee and W. H. Breckenridge	Theoretical Study of the Bonding in Mn+-RG Complexes and the Transport of Mn+ Through RG (M = Ca, Sr, Ra; n = 1,2; RG = He-Rn)	J. Chem. Phys.	132	art. no. 054302	2010	10.1063/1.3297891
21	T. G. Wright and W. H. Breckenridge	Radii of Atomic Ions Determined From Diatomic Ion-He Bond Lengths	J. Phys. Chem. A	114	3182-3189	2010	10.1021/jp9091927
22	S. M. Hamilton, W. S. Hopkins, D. J. Harding, T. R. Walsh, M. Haertelt, C. Kerpal, P. Gruene, G. Meijer, A. Fielicke and S. R. Mackenzie	Infrared induced reactivity of N2O on small gas-phase rhodium clusters	J. Phys. Chem. A	115	2489-2497	2011	10.1021/jp201171p
23	D. K. W. Mok, E. P. F. Lee, F. T. Chau, and J. M. Dyke	Franck-Condon Simulation of the Photoelectron Spectrum of AsCl2 and the Photodetachment Spectrum of AsCl2- employing UCCSD(T)-F12a Potential Energy Functions: IE and EA of AsCl2	J. Comput. Chem.	32	1648-1660	2011	10.1002/jcc.21743
24	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	The enthalpies of formation of AsXn molecules, where X = H, F or Cl, and n = 1, 2 or 3, by RCCSD(T) and UCCSD(T)-F12x calculations	Phys. Chem. Chem. Phys.	13	9540-9553	2011	10.1039/c1cp20490d
25	D. A. Wann, S. L. Masters, H. E. Robertson, M. Green, R. J. Kilby, C. A. Russell, C. Jones and D. W. H. Rankin	Multiple bonding versus cage formation in organophosphorus compounds: the gas-phase structures of tricyclo-P3(CBut)2Cl and P[triple bond, length as m-dash]C-But determined by electron diffraction and computational methods	Dalton Trans.	40	5611-5616	2011	10.1039/c1dt10041f
26	A. Kerridge and N. Kaltsoyannis	All-electron CASPT2 study of Ce(eta(8)-C8H6)(2)	Comptes Rendus chimie	13	853-859	2010	10.1016/j.crci.2010.02.006
27	J. W. Emsley, P. Lesot, A. Lesage, G. De Luca, D. Merlet and G. Pileio	The conformation and orientational order of a 1,2-disubstituted ethane nematogenic molecule (I22) in liquid crystalline and isotropic phases studied by NMR spectroscopy	Phys. Chem. Chem. Phys.	12	2895-2914	2010	10.1039/b915587b
28	G. De Luca, J. W. Emsley, E. Salager and A. Lesage	A general strategy for obtaining 19F–19F and 13C–19F residual dipolar couplings in perfluorocarbons from the NMR spectroscopy of liquid crystalline samples	Phys. Chem. Chem. Phys.	12	7968-7976	2010	10.1039/c002817g
29	D. Cleland, G. H. Booth and A. Alavi	A study of electron affinites using the initiator approach to full configuration interaction quantum Monte Carlo	J. Chem. Phys.	134	art no. 024112	2011	10.1063/1.3525712

30	G. H. Booth and A. Alavi	Approaching chemical accuracy using full configuration-interaction quantum Monte Carlo: A study of ionization potentials	J. Chem. Phys.	132	art no. 174104	2010	10.1063/1.3407895
31	D. Cleland, G. H. Booth and A. Alavi	Survival of the Fittest: Accelerating convergence in full configuration-interaction Quantum Monte Carlo	J. Chem. Phys.	132	art no. 041103	2010	10.1063/1.3302277
32	G. H. Booth, A. J. W. Thom and A. Alavi	Fermion Monte Carlo without fixed nodes: a Game of Life, death and annihilation in Slater Determinant space	J. Chem. Phys.	131	art no. 054106	2009	10.1063/1.3193710
33	D. Kumar, L. Tahsini, S. P. de Visser, H. Y. Kang, S. J. Kim and W. Nam	Effect of porphyrin ligands on the regioselective dehydrogenation versus epoxidation of olefins by oxoiron(IV) mimics of cytochrome P450	J. Phys. Chem. A	113	11713-11722	2009	10.1021/jp9028694
34	C. S. Porro, D.Kumar and S. P. de Visser	Electronic properties of pentacoordinated heme complexes in cytochrome P450 enzymes: search for an Fe(I) oxidation state	Phys. Chem. Chem. Phys.	11	10219-10226	2009	10.1039/b911966c
35	S. P. de Visser	Trends in Substrate Hydroxylation Reactions by Heme and Nonheme Iron(IV)-Oxo Oxidants Give Correlations between Intrinsic Properties of the Oxidant with Barrier Height	J. Am. Chem. Soc.	132	1087-1097	2010	10.1021/ja908340j
36	K. A. Prokop, S. P. de Visser and D. P. Goldberg	Unprecedented Rate Enhancements of Hydrogen-Atom Transfer to a Manganese(V)-Oxo Corrolazine Complex	Angew. Chem. Int. Ed.	49	5091-5095	2010	10.1002/anie.201001172
37	D. Kumar, B. Karamzadeh, G. Narahari Sastry and S. P. de Visser	What Factors Influence the Rate Constant of Substrate Epoxidation by Compound I of Cytochrome P450 and Analogous Iron(IV)-Oxo Oxidants?	J. Am. Chem. Soc.	132	7656-7667	2010	10.1021/ja9106176
38	B. Karamzadeh, D. Kumar, G. Narahari Sastry, and S. P. de Visser	Steric Factors Override Thermodynamic Driving Force in Regioselectivity of Proline Hydroxylation by Prolyl-4-hydroxylase Enzymes	J. Phys. Chem. A	114	13234-13243	2010	10.1021/jp1089855
39	S. P. de Visser, R. Latifi, L. Tahsini and W. Nam	The Axial Ligand Effect on Aliphatic and Aromatic Hydroxylation by Non-heme Iron(IV)-oxo Biomimetic Complexes	Chem. Asian J.	6	493-504	2011	10.1002/asia.201000586
40	R. Latifi, L. Tahsini, B. Karamzadeh, N. Safari, W. Nam and S. P. de Visser	Manganese substituted Compound I of cytochrome P450 biomimetics: A comparative reactivity study of Mn-V-oxo versus Mn-IV-oxo species	Arch. Biochem. Biophys.	507	4-13	2011	10.1016/j.abb.2010.12.035
41	B. Shepperson, J. Liu, A. M. Ellis and S. Yang	Ionization of Doped Helium Nanodroplets: Residual Helium Attached to Diatomic Cations	J. Phys. Chem. A	115	7010-7016	2011	10.1021/jp112204e

		and Their Clusters					
42	A. M. Gardner, K. A. Gutsmiedl, T. G. Wright, E. P. F. Lee, W. H. Breckenridge, S. Rajbhandari, C. Y. N. Chivone and L. A. Viehland	Theoretical Study of M+-RG Complexes (M = Ga, In; RG = He-Rn)	J. Phys. Chem. A	115	6979-6985	2011	10.1021/jp1122079
43	A. Kerridge and N. Kaltsoyannis	Quantum Chemical Studies of the Hydration of Sr2+ in Vacuum and Aqueous Solution	Chem. Eur. J.	17	5060-5067	2011	10.1002/chem.201003226
44	M. H. Palmer and I. C. Walker	The electronic states of buta-1,3-diene studied by ab initio configuration interaction and DFT methods, and electron energy loss spectroscopy	Chem. Phys.	373	159-169	2010	10.1016/j.chemphys.2010.04.016
45	G. A. Guirgis, Z. Wang, J. Lirjoni, M. H. Palmer, D. A. Obenchain, R. A. Peebles and S. A. Peebles	The molecular structure of difluoroisocyanato silane: a combined microwave spectral and theoretical study	J. Molec. Struct.	983	5-11	2010	10.1016/j.molstruc.2010.07.044
46	K. Kubiak and P.A. Mulheran	Molecular Dynamics Simulations of Hen Egg White Lysozyme Adsorption at a Charged Solid Surface	J. Phys. Chem. B	113	12189-12200	2009	10.1021/jp901521x
47	K. Kubiak-Ossowska and P.A. Mulheran	What Governs Protein Adsorption and Immobilization at a Charged Solid Surface?	Langmuir	26	7690-7694	2010	10.1021/la101276v
48	K. Kubiak-Ossowska and P.A. Mulheran	Mechanism of Hen Egg White Lysozyme Adsorption on a Charged Solid Surface	Langmuir	26	15954-15965	2010	10.1021/la102960m
49	T. J. Lin and P. J. O'Malley	An ONIOM Study of the Spin Density Distribution of the QA Site Plastosemiquinone in the Photosystem II Reaction Center	J. Phys. Chem. B	115	4227-4233	2011	10.1021/jp112163w
50	E. Martin, R. I. Samoilova, K. V. Narasimhulu, T. J. Lin, P. J. O'Malley, C. A. Colin and S. Dikanov	Hydrogen bonding and spin density distribution in the Q(B) semiquinone of bacterial reaction centers and comparison with the Q(A) site	J. Am. Chem. Soc.	133	5525-5537	2011	10.1016/j.bbabio.2012.06.091
51	K. Kubiak-Ossowska and P.A. Mulheran	Multiprotein Interactions during Surface Adsorption: a Molecular Dynamics Study of Lysozyme Aggregation at a Charged Solid Surface	J. Phys. Chem. B	115	8891-8900	2011	10.1021/jp1121239
52	P. S. Zuchowski and J. M. Hutson	Reactions of ultracold alkali-metal dimers	Phys. Rev. A	81	060703(R)	2010	10.1103/PhysRevA.81.060703

53	P. S. Zuchowski, J. Aldegunde and J. M. Hutson	Ultracold RbSr molecules can be formed by magnetoassociation	Phys. Rev. Lett.	105	153201	2010	10.1103/PhysRevLett.105.153201
54	T. W. Bentley and H. C. Harris	Solvolyses of Benzoyl Chlorides in Weakly Nucleophilic Media	Int. J. Mol. Sci.	12	4805-4818	2011	10.3390/ijms12084805
55	F. L. Mitchell, S. M. Miles, J. Neres, E. V. Bichenkova and R. A. Bryce	Tryptophan as a molecular shovel in the glycosyl transfer activity of Trypanosoma cruzi trans-sialidase	Biophysical J.	98	L38-L40	2010	10.1016/j.bpj.2010.01.006
56	I. Kirker and N. Kaltsoyannis	Does covalency really increase across the 5f series? A comparison of molecular orbital, natural population, spin and electron density analyses of AnCp(3) (An = Th-Cm; Cp = eta(5)-C(5)H(5))	Dalton Trans.	40	124-131	2011	10.1039/c0dt01018a
57	M. C. R. Cockett, M. Miyazaki, K. Tanabe and M. Fujii	Isomer selective IR-UV depletion spectroscopy of 4-fluorotoluene-NH3: evidence for pi-proton-acceptor and linear hydrogen-bonded complexes	Phys. Chem. Chem. Phys.	13	15633-15638	2011	10.1039/c1cp21545k
58	A. Kerridge and N. Kaltsoyannis	The coordination of Sr2+ by hydroxide: a density functional theoretical study	Dalton Trans.	40	11258-11266	2011	10.1039/c1dt10883b
59	C. Domene and S Furini	Molecular Dynamics Simulations of the TrkH Membrane Protein	Biochemistry	51	1559-1565	2012	10.1021/bi201586n
60	C. Boulho, P. Oulie, L. Vendier, M. Etienne, V. Pimienta, A. Locati, F. Bessac, F. Maseras, D. A. Pantazis and J. E. McGrady	C-H Bond Activation of Benzene by Unsaturated eta(2)-Cyclopropene and eta(2)-Benzyne Complexes of Niobium	J. Am. Chem. Soc.	132	14239-14250	2010	10.1021/ja1061505
61	C. Boulho, L. Vendier, M. Etienne, A. Locati, F. Maseras and J. E. McGrady	Aromatic versus Benzylic CH Bond Activation of Alkylaromatics by a Transient eta(2)-Cyclopropene Complex	Organometallics	30	3999-4007	2011	10.1021/om200199e
62	W. M. C. Sameera , C. J. McKenzie and J. E. McGrady	On the mechanism of water oxidation by a bimetallic manganese catalyst: A density functional study	Dalton Trans.	40	3859-3870	2011	10.1039/c0dt01362e
63	E. M. Zueva, W. M. C. Sameera, D. M. Pinero, I. Chakraborty, E. Devlin, P. Baran, K. Lebruskova, Y. Sanakis, J. E. McGrady and R. G. Raptis	Experimental and Theoretical Mossbauer Study of an Extended Family of [Fe(8)(mu(4)-O)(4)(mu-4-R-px)(12)X(4)] Clusters	Inorg. Chem.	50	1021-1029	2011	10.1021/ic101691q

64	S. T. Mutter and J. A. Platts	Density functional theory studies of interactions of ruthenium-arene complexes with base pair steps	J. Phys. Chem. A	115	11293-11302	2011	10.1021/jp2049487
65	S. Chakravorty, J. A. Platts and B. K. Das	Novel C-H center dot center dot center dot C contacts involving 3,5-dimethylpyrazole ligands in a tetracoordinate Co(II) complex	Dalton Trans.	40	11605-11612	2011	10.1039/c1dt10948k
66	R. J. Baker, P. E. Colavita, D. M. Murphy, J. A. Platts and J. D. Wallis	Fluorine-Fluorine Interactions in the Solid State: An Experimental and Theoretical Study	J. Phys. Chem. B	116	1435-1444	2012	10.1021/jp2099976
67	J. Overgaard, C. Jones, D. Dange and J. A. Platts	Experimental Charge Density Analysis of a Gallium(I) N-Heterocyclic Carbene Analogue	Inorg. Chem.	50	8418-8426	2011	10.1021/ic2009946
68	L. McDyre, E. Carter, K. J. Cavell, D. M. Murphy, J. A. Platts, K. Sampford, B. D. Ward, W. F. Gabrielli, M. J. Hanton and D. M. Smith	Intramolecular Formation of a Cr(I)(bis-arene) Species via TEA Activation of [Cr(CO)(4)(Ph(2)P(C(3)H(6))PPh(2))](+): An EPR and DFT Investigation	Organometallics	30	4505-4508	2011	10.1021/om2006062
69	R. M. Pinto, A. A. Dias, M. L. Costa, P. Rodrigues, M. T. Barros, J. S. Ogden and J. M. Dyke	Thermal Decomposition of Methyl 2-Azidopropionate Studied by UV Photoelectron Spectroscopy and Matrix Isolation IR Spectroscopy: Heterocyclic Intermediate vs Imine Formation	J. Phys. Chem. A	115	8447-8457	2011	10.1021/jp2036845
70	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	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(-)	J. Chem. Phys.	135	art. no. 124312	2011	10.1063/1.3640037
71	G. Copeland, M. V. Ghosh, D. E. Shallcross, C. J. Percival and J. M. Dyke	A study of the alkene-ozone reactions, 2,3-dimethyl 2-butene + O(3) and 2-methyl propene + O(3), with photoelectron spectroscopy: measurement of product branching ratios and atmospheric implications	Phys. Chem. Chem. Phys.	13	17461-17473	2011	10.1039/c1cp21922g
72	S. Beccaceci, N. Armata, J. S. Ogden, J. M. Dyke, L. Rhyman and P. Ramasami	A study of the atmospherically important reactions of dimethylsulfide (DMS) with I-2 and ICl using infrared matrix isolation spectroscopy and electronic structure calculations	Phys. Chem. Chem. Phys.	14	2399-2407	2012	10.1039/c2cp23392d
73	G. de Luca, J. W. Emsley,	The structure and conformations of mesogenic	Liq. Cryst.	39	211-219	2012	10.1080/02678292.

	A. Lesage and D. Merlet	molecules in the pre-transitional region of the isotropic phase: 5OCB and MBBA and their mixture					2011.631043
74	D. Kumar, G. N. Sastry and S. P. de Visser	Effect of the Axial Ligand on Substrate Sulfoxidation Mediated by Iron(IV)-Oxo Porphyrin Cation Radical Oxidants	Chem. Eur. J.	17	6196-6205	2011	10.1002/chem.201003187
75	R. Latifi, L. Tahsini, D. Kumar, G. N. Sastry, W. Nam and S. P. de Visser	Oxidative properties of a nonheme Ni(II)(O(2)) complex: Reactivity patterns for C-H activation, aromatic hydroxylation and heteroatom oxidation	Chem. Commun.	47	10674-10676	2011	10.1039/c1cc13993b
76	A. K. Vardhaman, C. V. Sastri, D. Kumar, and S. P. de Visser	Nonheme ferric hydroperoxo intermediates are efficient oxidants of bromide oxidation	Chem. Commun.	47	11044-11046	2011	10.1039/c1cc13775a
77	K. A. Prokop, H. M. Neu, S. P. de Visser, and D. P. Goldberg	A manganese(V)-oxo pi-cation radical complex: Influence of one-electron oxidation on oxygen-atom transfer	J. Am. Chem. Soc.	133	15874-15877	2011	10.1021/ja2066237
78	D. Kumar, G. N. Sastry, D. P. Goldberg and S. P. de Visser	Mechanism of S-oxygenation by a cysteine dioxygenase model complex	J. Phys. Chem. A	116	582-591	2012	10.1021/jp208230g
79	D. Kumar, G. N. Sastry and S. P. de Visser	Axial ligand effect on the rate constant of aromatic hydroxylation by iron(IV)-oxo complexes mimicking cytochrome P450 enzymes	J. Phys. Chem. B	116	718-730	2012	10.1021/jp2113522
80	R. Latifi, L. Tahsini, W. Nam and S. P. de Visser	Regioselectivity of aliphatic versus aromatic hydroxylation by a nonheme iron(II)-superoxo complex	Phys. Chem. Chem. Phys.	14	2518-2524	2012	10.1039/c2cp23352e
81	R. Latifi, J. S. Valentine, W. Nam and S. P. de Visser	Predictive studies of H-atom abstraction reactions by an iron(IV)-oxo corrole cation radical oxidant	Chem. Commun.	48	3491-3493	2012	10.1039/c2cc30365e
82	C. D. Withers, T. G. Wright, L. A. Viehland, L. Grossman, C. C. Kirkpatrick and E. P. F. Lee	Theoretical Study of Cl^--RG (rare gas) Complexes and Transport of Cl^- Through RG (RG = He-Rn)	J. Chem. Phys.	135	art. no. 024312	2011	10.1063/1.3598472
83	E. P. F. Lee, L. A. Viehland, R. Johnsen, W. H. Breckenridge and T. G. Wright	Interaction Potentials of Uranium Cations with Rare Gases (RG) and Transport of U^+ in RG (RG = He, Ne, Ar, Kr and Xe)	J. Phys. Chem. A	115	12126-12131	2011	10.1021/jp2076879
84	A. M. Gardner and T. G. Wright	Consistent Assignment of the Vibrations of Monosubstituted Benzenes	J. Chem. Phys.	135	art. no. 114305	2011	10.1063/1.3638266

85	J. P. Harris, A. M. Gardner and T. G. Wright, W. H. Breckenridge and L. A. Viehland	Interactions in the B^+-RG Complexes and Comparison with Be^+–RG (RG = He–Rn): Evidence for Chemical Bonding	J. Phys. Chem. A	116	4995-5007	2012	10.1021/jp303057x
86	R. A. Aitken, B. Fodi, M. H. Palmer, A. M. Z. Slawina and Jing Yang	Experimental and theoretical molecular and electronic structures of the N-oxides of pyridazine, pyrimidine and pyrazine	Tetrahedron	68	5845-5851	2012	10.1016/j.tet.2012.05.004
87	M. H. Palmer, P. J. Camp, S. Vronning Hoffmann, N. C. Jones, A. R. Head, D. L. Lichtenberger	The electronic states of 1,2,4-triazoles: a study of 1H- and 1-methyl-1,2,4-triazole by VUV photoabsorption and UV photoelectron spectroscopy and a comparison with ab initio configuration interaction computations'	J. Chem. Phys.	136	art. no. 094310	2012	10.1063/1.3692164
88	M. H. Palmer, S. Hoffmann, N. Jones, A. Head, D. Lichtenberger	The electronic states of 1,2,3-triazole studied by vacuum UV photoabsorption and UV photoelectron spectroscopy, and a comparison with ab initio configuration interaction methods	J. Chem. Phys.	134	art. no. 084309	2011	10.1063/1.3549812
89	M. G. Quesne and S. P. de Visser	Regioselectivity of substrate hydroxylation versus halogenation by a non-heme iron(IV)-oxo complex: Possibility of rearrangement pathways	J. Biol. Inorg. Chem.	17	841-852	2012	10.1007/s00775-012-0901-4
90	L. E. Gonzalez-Ovalle, M. G. Quesne, D. Kumar, D. P. Goldberg and S. P. de Visser	Axial and equatorial ligand effects on biomimetic cysteine dioxygenase model complexes	Org. Biomol. Chem.	10	5401-5409	2012	10.1039/c2ob25406a
91	P. Leeladee, R. A. Baglia, K. A. Prokop, R. Latifi, S. P. de Visser and D. P. Goldberg	Valence tautomerism in a high-valent manganese-oxo porphyrinoid complex induced by a Lewis acid	J. Am. Chem. Soc.	134	10397-10400	2012	10.1021/ja304609n
92	G. A. Guirgis, J. S. Overby, M. H. Palmer, R. A. Peebles, S. A. Peebles, L. F. Elmuti, D. A. Obenchain, B. H. Pate and N. A. Seifert	Molecular Structure of Methyldifluoroisocyanato Silane: A Combined Microwave Spectral and Theoretical Study	J. Phys. Chem. A	116	7822-7829	2012	10.1021/jp302519h
93	M. T. Lin, R. I. Samoilova, T.-J. Lin, K. Narasimhulu, R. B. Gennis, S. A. Dikanov and P. J. O'Malley	Interactions of Intermediate Semiquinone with Surrounding Protein Residues at the Q(H) Site of Wild-Type and D75H Mutant Cytochrome bo(3) from Escherichia coli	Biochemistry	51	3827-3838	2012	10.1021/bi300151q
94	T.-J. Lin and P. J.	Binding Site Influence on the Spin Density and	J. Phys. Chem. B	115	9311-9319	2011	10.1021/jp203484

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95	L. Rhyman, N. Armata, P. Ramasami and J. M. Dyke	A study of the atmospherically important reactions between dimethyl selenide (DMSe) and X2 (X = Cl, Br and I) with ab initio calculations	J. Phys. Chem. A	116	5595-5603	2012	10.1021/jp302750a
96	C. A. Taatjes, O. Welz, A. J. Eskola, J. D. Savee, D. Osborn, E. P. F. Lee, D. W. K. Mok, D. E. Shallcross, C. J. Percival and J. M. Dyke	Direct Measurement of Criegee Intermediate (CH_2OO) Reactions with Acetone, Acetaldehyde, and Hexafluoroacetone	Phys. Chem. Chem. Phys.	14	10391-10400	2012	10.1039/c2cp40294g
97	K. E. Riley, J. A. Platts, J. Rezac, P. Hobza and J. G. Hill	Assessment of the Performance of MP2 and MP2 Variants for the Treatment of Noncovalent Interactions	J. Phys. Chem. A	116	4159-4169	2012	10.1021/jp211997b
98	K. Izod, E. R. Clark, R. W. Harrington and W. Clegg	Hypervalent Sulfur-Functionalized Diphosphagermylene and Diphosphastannylene Compounds	Organometallics	31	246-255	2012	10.1021/om200832 7
99	S. Furini and C. Domene	Non-selective conduction in a mutated NaK channel with three cation-binding sites	Biophysical J.	103	2106-2114	2012	10.1016/j.bpj.2012. 10.004
100	S. M Hamilton, W. S. Hopkins, D. J. Harding, T. R. Walsh, M. Haertelt, C. Kerpal, P. Gruene, G. Meijer, A. Fielicke and S. R. Mackenzie	Infrared-Induced Reactivity of N2O on Small Gas-Phase Rhodium Clusters	J. Phys. Chem. A	115	2489-2497	2011	10.1021/jp201171p
101	A. C. Hermes, S. M. Hamilton, W. S. Hopkins, D. J. Harding, C. Kerpal, G. Meijer, A. Fielicke and S. R. Mackenzie	Effects of Coadsorbed Oxygen on the Infrared Driven Decomposition of N2O on Isolated Rh-5(+) Clusters	J. Phys. Chem. Lett.	2	3053-3057	2011	10.1021/jz2012963
102	A. C. Hermes, S. M. Hamilton, G. A. Cooper, C. Kerpal. D. J. Harding, G. Meijer, A. Fielicke and S. R. Mackenzie	Infrared driven CO oxidation reactions on isolated platinum cluster oxides, PtnOm	Faraday Discussion	157	213-225	2012	10.1039/c2fd20019h
103	E. Martin, A. Baldansuren, T.-J. Lin, R. I. Samoilova, C. A.	Hydrogen Bonding between the Q(B) Site Ubisemiquinone and Ser-L223 in the Bacterial Reaction Center: A Combined Spectroscopic and	Biochemistry	51	9086-9093	2012	10.1021/bi300834w

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104	C. Leidlmair, P. Bartl, H. Schoebel, S. Denifl, S. Yang, A. M. Ellis and P. Scheier	Ionization of Methane Clusters in Helium Nanodroplets	ChemPhysChem	13	469-476	2012	10.1002/cphc.201100880
105	B. Shepperson, J. Liu, A. M. Ellis and S. Yang	Communication: Electron impact ionization of binary H_2O/X clusters in helium nanodroplets: An *ab initio* perspective	J. Chem. Phys.	137	art. no. 201102	2012	10.1063/1.4769810
106	O. M. Roscioni, E. P. F. Lee and J. M.Dyke	Development and testing of a compact basis set for use in effective core potential calculations on rhodium complexes	J. Comput. Chem.	33	2049-2057	2012	10.1002/jcc.23034
107	R. M. Pinto, A. A. Dias, G. Levita, P. Rodrigues, M. T. Barros, J. M. Dyke and M. L. Costa	Pyrolysis of 3-azidopropionitrile studied by UV photoelectron and matrix-isolation IR spectroscopies: Formation of ketenimine H2C=C=NH	J. Molec. Struct.	1025	151-159	2012	10.1016/j.molstruc.2012.04.055
108	F. Innocenti, M. Eypper, S. Stranges, J. B. West, G. C. King and J. M. Dyke	Threshold photoelectron spectroscopy (TPES) of vibrationally excited nitrogen	J. Phys. B: At. Mol. Opt. Phys.	46	art. no. 045002	2013	10.1088/0953-4075/46/4/045002
109	E. P. F. Lee , D. K. W. Mok, D. E. Shallcross, C. J. Percival, D. L. Osborn, C. A. Taatjes and J. M. Dyke	Spectroscopy of the Simplest Criegee Intermediate CH2OO: Simulation of the First Bands in Its Electronic and Photoelectron Spectra	Chem. Eur. J.	18	12411-12433	2012	10.1002/chem.201200848
110	M. A. Zwijnenburg, G. Cheng, T. O. McDonald, K. E. Jelfs, J. X. Jiang, S. Ren, T. Hasell, F. Blanc, A. I. Cooper, and D. J. Adams	Shedding Light on Structure–Property Relationships for Conjugated Microporous Polymers: The Importance of Rings and Strain	Macromolecules	46	7696-7704	2013	10.1021/ma401311s
111	C. Butchosa, T. O. McDonald, A. I. Cooper, D. J. Adams, and M. A. Zwijnenburg	Shining a Light on s-Triazine-Based Polymers	J. Phys. Chem. C	116	4314-4324	2014	10.1021/jp411854f
112	C. R. S. Mooney, M. E. Sanz, A. R. McKay, R. J. Fitzmaurice, A. E. Aliev, S. Caddick, and H. H. Fielding	Photodetachment Spectra of Deprotonated Fluorescent Protein Chromophore Anions	J. Phys. Chem. A	116	7943-7949	2012	10.1021/jp3058349

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114	E. R. Clark, A. Del Grosso, and M. J. Ingleson	The Hydride-Ion Affinity of Borenium Cations and Their Propensity to Activate H2 in Frustrated Lewis Pairs	Chem. Eur. J.	19	2462-2466	2013	10.1002/chem.201203318
115	J. R. Lawson, E. R. Clark, I. A. Cade, S. A. Solomon and M. J. Ingleson	Haloboration of internal alkynes with boronium and borenium cations as a route to tetrasubstituted alkenes	Angew. Chem. Int. Ed.	52	7518-7522	2013	10.1002/anie.201302609
116	E. R. Clark and M. J. Ingleson	[(acridine)BCl2]+: A Borenium Cation That Is a Strong Boron- and Carbon-Based Lewis Acid	Organometallics	32	6712-6717	2013	10.1021/om400463r
117	G. Roffe and H. Cox	Computational Study of the Coordination of Methane to First Row Transition Metal Diction Complexes	J. Phys. Chem. A	117	3017-3024	2013	10.1021/jp309739s
118	L. Ma, T. Takashima, J. Koka, H. J. Kimber, H. Cox, and A. J. Stace	Conformation-resolved UV spectra of Pb(II) complexes: a gas phase study of the sandwich structures [Pb(toluene)2]2+ and [Pb(benzene)2]2+	J. Chem. Phys.	138	164301	2013	10.1063/1.4801440
119	A. W. King, F. Longford and H. Cox	The stability of S-states of unit-charge Coulomb three-body systems: from H- to H2(+)	J. Chem. Phys.	139	art. no. 224306	2013	10.1063/1.4834036
120	T. van Mourik, V. I. Danilov, V. V. Dailidonis, N. Kurita, H. Wakabayashi and T. Tsukamoto	A DFT study of uracil and 5-bromouracil in nanodroplets	Theor. Chem. Acc.	125	233-244	2010	10.1007/s00214-009-0630-0
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122	P. Leeladee, G. N. Jameson, M. A. Siegler, D. Kumar, S. P. de Visser and D. P. Goldberg	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity	Inorg. Chem.	52	4668-4682	2013	10.1021/ic400280x
123	R. Latifi, M. A. Sainna, E. V. Rybak-Akimova and S. P. de Visser	Does hydrogen-bonding donation to manganese(IV)-oxo and iron(IV)-oxo oxidants affect the oxygen-atom transfer ability? A computational study.	Chem. Eur. J.	19	4058-4068	2013	10.1002/chem.201202811
124	C. V. Skipper, A. Hamaed, D. M. Antonelli and N. Kaltsoyannis	The Kubas interaction in M(II) (M = Ti, V, Cr) hydrazine-based hydrogen storage materials: a DFT study	Dalton Trans.	41	8515-8523	2012	10.1039/c2dt30383c

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126	D. A. Wann, P. D. Lane, H. E. Robertson, T. Base and D. Hnyk	The gaseous structure of closo-9,12-(SH)2-1,2-C2B10H10, a modifier of gold surfaces, as determined using electron diffraction and computational methods.	Dalton Trans.	42	12015-12019	2013	10.1039/c3dt51393a
127	D. A. Wann, D.W. H. Rankin, P. D. McCaffrey, J. M. L. Martin and R. J. Mawhorter	Equilibrium Gas-Phase Structures of Sodium Fluoride, Bromide, and Iodide Monomers and Dimers	J. Phys. Chem. A	118	1927-1935	2014	10.1021/jp411202t
128	T. G. Karabencheva-Christova, U. Carlsson, K. Balali-Mood, G. W. Black and C. Z. Christov	Conformational Effects on the Circular Dichroism of Human Carbonic Anhydrase II: A Multilevel Computational Study	PLOS ONE	8	e56874	2013	10.1371/journal.pone.0056874
129	M. Maniruzzaman, D. J. Morgan, A. P. Mendham, J. Pang, M. J. Snowden and D. Douroumis	Drug-polymer intermolecular interactions in hot-melt extruded solid dispersions	International Journal of Pharmaceutics	443	199-208	2013	10.1016/j.ijpharm.2012.11.048
130	D. A. Wann, P. D. Lane, H. E. Robertson, J. Holub and D. Hnyk	Structures of, and related consequences of deprotonation on, two Cs-symmetric arachno nine-vertex heteroboranes, 4,6-X2B7H9 (X = CH2; S) studied by gas electron diffraction/quantum chemical calculations and GIAO/NMR	Inorg. Chem.	52	4502-4508	2013	10.1021/ic302776d
131	D. A. Wann, A. Bil, P. D. Lane, H. E. Robertson, D. W. H. Rankin and E. Block	Gas-phase structures of dithietane derivatives, including an electron diffraction study of 1,3-dithietane 1,1,3,3-tetraoxide	Struct. Chem.	24	827-835	2013	10.1007/s11224-012-0179-8
132	A. M. Reilly, D. A. Wann, M. J. Gutmann, M. Jura, C. A. Morrison and D. W. H. Rankin	Predicting anisotropic displacement parameters using molecular dynamics: density functional theory plus dispersion modelling of thermal motion in benzophenone	J. Appl. Cryst.	46	656-662	2013	10.1107/S0021889813006225
133	S. L. Masters, S. J. Atkinson, M. Hölbling and K. Hassler	Gas-phase molecular structure of 1,1,1,2-tetrabromo-2,2-dimethyldisilane: theoretical and experimental investigation of a super-halogenated disilane and computational investigation of the F, Cl and I analogues	Struct. Chem.	24	1201-1206	2013	10.1007/s11224-012-0152-6

134	S. L. Masters, G. V. Girichev and S. A. Shylkov	The re-determination of the molecular structure of antimony(III) oxide using very-high-temperature gas electron diffraction (VHT-GED)	Dalton Trans.	42	3581-3586	2013	10.1039/c2dt32790b
135	S. J. Atkinson, H. E. Robertson, M. Hoelbling, W.-W. Du Mont, C. Mitrofan, K. Hassler and S. L. Masters	Do halogen and methyl substituents have electronic effects on the structures of simple disilanes? An experimental and theoretical study of the molecular structures of the series X3SiSiMe3 (X = H, F, Cl and Br)	Struct. Chem.	24	851-857	2013	10.1007/s11224-013-0213-5
136	A. Kurbangalieva, D. Carmichael, K. K. (Mimi) Hii, A. Jutand and J. M. Brown	Oxidative Addition to Palladium(0) Diphosphine Complexes: Observations of Mechanistic Complexity with Iodobenzene as Reactant	Chem. Eur. J.	20	1116-1125	2014	10.1002/chem.201301937
137	J. A. Raskatov, A. L. Thompson, A. R. Cowley, T. D. W. Claridge and J. M. Brown	Chiral recognition in contact ion-pairs; observation, characterization and analysis	Chem. Sci.	4	3140-3147	2013	10.1039/c3sc51096d
138	T. Gehring, M. Quaranta, B. Odell, D. G. Blackmond and J. M. Brown	Observation of a Transient Intermediate in Soai's Asymmetric Autocatalysis: Insights from 1H NMR Turnover in Real Time	Angew. Chem. Int. Ed.	51	9539-9542	2012	10.1002/anie.201203398
139	F. L. Thorp-Greenwood, J. A. Platts and M. P. Coogan	Experimental and theoretical characterisation of phosphorescence from rhenium polypyridyl tricarbonyl complexes	Polyhedron	67	505-512	2014	10.1016/j.poly.2013.09.033
140	K. M. Sharples, E. Carter, C. E. Hughes, K. D. M. Harris, J. A. Platts and D. M. Murphy	An ENDOR and DFT analysis of hindered methyl group rotations in frozen solutions of bis(acetylacetonato)-copper(II)	Phys. Chem. Chem. Phys.	15	15214-15222	2013	10.1039/c3cp52464g
141	V. E. Pritchard, F. L. Thorp-Greenwood, R. G. Balasingham, C. F. Williams, B. M. Kariuki, J. A. Platts, A. J. Hallett and M. P. Coogan	Simple Polyphenyl Zirconium and Hafnium Metallocene Room-Temperature Lumophores for Cell Imaging	Organometallics	32	3566-3569	2013	10.1021/om400212y
142	K. E. Henry, R. G. Balasingham, A. R. Vortherms, J. A. Platts, J. F. Valliant, M. P. Coogan, J. Zubieta and	Emission wavelength variation with changes in excitation in a Re(I)/bisthiazolate ligand complex that breaks Kasha's law	Chem. Sci.	4	2490-2495	2013	10.1039/c3sc22070b

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143	S. T. Mutter, K. Gkionis and J. A. Platts	QM/MM description of platinum-DNA interactions: Comparison of binding and DNA distortion of five drugs	RSC Adv.	3	4066-4073	2013	10.1039/c3ra23041d
144	J. A. Platts, J. G. Hill , K. Eugene Riley , J. Rezac and P. Hobza	Basis set dependence of interaction energies computed using composite post-MP2 methods	J. Chem. Theory Comput.	9	330-337	2013	10.1021/ct300842d
145	M. Walker, A. Sen, A. J. A. Harvey, and C. E. H. Dessent	Complexation of anions to gas-phase amino acids: Conformation is critical in determining if the global minimum is canonical or zwitterionic	Chem. Phys. Lett.	588	43-46	2013	10.1016/j.cplett.2013.09.074
146	A. Kerridge	A RASSCF study of free base, magnesium and zinc porphyrins: accuracy versus efficiency	Phys. Chem. Chem. Phys.	15	2197-2209	2013	10.1039/c2cp43982d
147	A. Kerridge	Oxidation state and covalency in f-element metallocenes (M = Ce, Th, Pu): a combined CASSCF and topological study	Dalton Trans.	42	16428-16436	2013	10.1039/c3dt52279b
148	A. Andrejeva, A. M. Gardner, J. B. Graneek, R. J. Plowright, W. H. Breckenridge and T. G. Wright	Theoretical Study of M+-RG2 (M+ = Li, Na, Be, Mg; RG = He-Rn)	J. Phys. Chem. A	117	13578-13590	2013	10.1021/jp4075652
149	A. M. Gardner, A. M. Green, V. M. Tame-Reyes, V. H. K. Wilton and T. G. Wright	Vibrations of the Low Energy States of Toluene (X1A1 and A1B2) and the toluene cation (X2B1)	J. Chem. Phys.	138	art. no. 134303	2013	10.1063/1.4796204
150	J. A. Davies, A. M. Green, A. M. Gardner, C. D. Withers, T. G. Wright and K. L. Reid	Critical Influences on the Rate of Intramolecular Vibrational Redistribution: a Comparative Study of Toluene, Tolune-d3 and p-Fluorotoluene	Phys. Chem. Chem. Phys.	16	430-443	2014	10.1039/c3cp53055h
151	O. V. Ershova, J. Klos, J. P. Harris, A. M. Gardner, V. M. Tame-Reyes, A. Andrejeva, M. H. Alexander, N. A. Besley and T. G. Wright	Interaction of NO 3pπ Rydberg State with Ar: Potential Energy Surfaces and Spectroscopy	J. Chem. Phys.	138	art. no. 214313	2013	10.1063/1.4808027
152	V. M. Tame-Reyes, A. M. Gardner, J. P. Harris, J. McDaniel and T. G. Wright	Spectroscopy of the A State of NO-alkane Complexes (alkane = methane, ethane, propane and n-butane)	J. Chem. Phys.	137	art. no. 214307	2012	10.1063/1.4768811

153	E. Packard, D. D. Pascoe, J. Maddaluno, T. P. Goncalves and D. C. Harrowven	Organoytterbium Ate Complexes Extend the Value of Cyclobutenediones as Isoprene Equivalents	Angew. Chem. Int. Ed.	125	13314-13317	2013	10.1002/anie.201307193
154	X. Liu, J. M. Cole, P. G. Waddell and T. C. Lin	Molecular origins of commercial laser dye functionality in azacoumarins and quinolones: LD 425, LD 489 and LD 473	Acta Crystallographica B	67	560-568	2011	10.1107/S0108768111037311
155	X. Liu, J. M. Cole, P. G. Waddell, T. C. Lin, J. Radia and A. Zeidler	Molecular origins of optoelectronic properties in coumarin dyes: towards designer solar-cell and laser applications	J. Phys. Chem. A	116	727-737	2012	10.1021/jp209925y
156	J. M. Cole, K. F. Bowes, I. P. Clark, A. Zeidler, A. W. Parker, I. R. Laskar and T.-M. Chen	Material Profiling for Photocrystallography: Relating Single-Crystal Photophysical and Structural Properties of Luminescent Bis-Cyclometalated Iridium-Based Complexes	Crystal Growth & Design	17	1826-1837	2013	10.1021/cg301386s
157	T. C. Lin, J. M. Cole, A. P. Higginbotham, A. J. Edwards, R. O. Piltz, J. P-Moreno, J-Y. Seo, J-S. Lee, K. Clays and O-P. Kwon	Molecular origins of the high-performance non-linear optical susceptibility of a phenolic polyene chromophore: molecular charge-densities, hydrogen-bonding and ab initio calculations	J. Phys. Chem. C	117	9416-9430	2013	10.1021/jp400648q
158	T. A. Merz, P. G. Waddell and J. M. Cole	Systematic Molecular Design of p-phenylene Lasing Properties	J. Phys. Chem. C	117	8429-8426	2013	10.1021/jp401004m
159	X. Liu, J. M. Cole, P. G. Waddell, T. C. Lin and S. McKechnie	Molecular Origins of Optoelectronic Properties in Coumarins 343, 314T, 445 and 522B	J. Phys. Chem. C	117	14130-14141	2013	10.1021/jp400614e
160	X. Liu, J. M. Cole and K. S. Low	Molecular Origins of Dye Aggregation and Complex Formation Effects in Coumarin 343	J. Phys. Chem. C	117	14723-14730	2013	10.1021/jp4024266
161	X. Liu, Z. Xu and J. M. Cole	Molecular Design of UV-vis Absorption and Emission Properties in Organic Fluorophores: Towards Larger Bathochromic Shifts, Enhanced Molar Extinction Coefficients and Greater Stokes Shifts	J. Phys. Chem. C	117	16584-16595	2013	10.1021/jp404170w
162	L. Zhang, J. M. Cole, P. G. Waddell, K. S. Low and X. Liu	Relating Electron Donor and Carboxylic Acid Anchoring Substitution Effects in Azo Dyes to Dye-sensitized Solar Cell Performance	ACS Sustainable Chem. Eng.	1	1440-1452	2013	10.1021/sc400183t
163	L. Zhang, J. M. Cole and X. Liu	Tuning Solvatochromism of Azo Dyes with Intramolecular Hydrogen Bonding in Solution and on Titanium Dioxide Nanoparticles	J. Phys. Chem. C	117	26316-26323	2013	10.1021/jp4088783
164	M. H. Palmer, S. V. Hoffmann, N. Jones, E.	The electronic states of pyridine-N-oxide studied by VUV photoabsorption and ab initio	J. Chem. Phys.	138	art. no. 214317	2013	10.1063/1.4807841

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165	K. Izod, D. G. Rayner, S. M. El-Hamruni, R. W. Harrington and U. Baisch	Stabilization of a Diphosphagermylene through ppi-ppi Interactions with a Trigonal-Planar Phosphorus Center	Angew. Chem. Int. Ed.	53	3636-3640	2014	10.1002/anie.201308002
166	A.W. Potts, D.M.P. Holland, I. Powis, L. Karlsson, A.B. Trofimov and I.L. Bodzuk	A study of the valence shell electronic structure and photoionisation dynamics of meta-dichlorobenzene and meta-bromochlorobenzene	Chem. Phys.	415	84-97	2013	10.1016/j.chemphys.2012.12.031
167	I. Powis, A. B. Trofi,ov, I. L. Bodzuk, D. M. P. Holland, A. W. Potts and L. Karlsson	A study of the valence shell electronic structure and photoionisation dynamics of para-dichlorobenzene and para-bromochlorobenzene	Chem. Phys.	415	291-308	2013	10.1016/j.chemphys.2012.09.026
168	M. Staniforth, S. Daly, K. L. Reid and I. Powis	A generic pi* shape resonance observed in energy-dependent photoelectron angular distributions from two-colour, resonant multiphoton ionization of difluorobenzene isomers	J. Chem. Phys.	139	art. no. 064304	2013	10.1063/1.4817324
169	C. S. Lehmann, N. B. Ram, I. Powis and M. H. Janssen	Imaging photoelectron circular dichroism of chiral molecules by femtosecond multiphoton coincidence detection	J. Chem. Phys.	139	art. no. 234307	2013	10.1063/1.4844295
170	M. H. M. Janssen and I. Powis	Detecting chirality in molecules by imaging photoelectron circular dichroism	Phys. Chem. Chem. Phys.	16	856-871	2014	10.1039/c3cp53741b
171	G. A. Garcia, L. Nahon, S. Daly and I. Powis	Vibrationally induced inversion of photoelectron forward-backward asymmetry in chiral molecule photoionization by circularly polarized light	Nature Communications	4	2132	2013	10.1038/ncomms3132
172	M. Tia, B. C. de Miranda, S. Daly, F. Gaie-Levrel, G. A. Garcia, I. Powis and L. Nahon	Chiral Asymmetry in the Photoionization of Gas Phase Amino Acid Alanine at Lyman-α Radiation Wavelength	J. Phys. Chem. Lett.	4	2698-2704	2013	10.1021/jz4014129
173	A. K. H. Hirsch, P. Reutenauer, M. Le Moignan, S. Ulrich, P. J. Boul, J. M. Harrowfield, P. D. Jarowski and J-M. Lehn	Theoretical and Structural Analysis of Long C-C Bonds in the Adducts of Polycyanoethylene and Anthracene Derivatives and Their Connection to the Reversibility of Diels-Alder Reactions	Chem. Eur. J.	20	1073-1080	2014	10.1002/chem.201303276

174	C. A. Taatjes, O. Welz, A. J. Eskola, J. D. Savee, A. M. Scheer, D. E. Shallcross, B. Rotavera, E. P. F. Lee, J. M. Dyke, D. K. W. Mok, D. L. Osborn and C. J. Percival	Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate CH3CHOO	Science	340	177-180	2013	10.1126/science.1234689
175	M. Ng, D. K. Mok, E. P. Lee and J. M. Dyke	Rate coefficients of the CF3CHFCF3 + H → CF3CFCF3 + H2 reaction at different temperatures calculated by transition state theory with ab initio and DFT reaction paths	J. Comput. Chem.	34	545-557	2013	10.1002/jcc.23163
176	C. Kerpal, D. J. Harding, A. C. Hermes, G. Meijer, S. R. Mackenzie and A. Fielicke	Structures of Platinum Oxide Clusters in the Gas Phase	J. Phys. Chem. A	117	1233-1239	2013	10.1021/jp3055137
177	S. Roy, R. J. Large, A. M. Akande, A. Kshatri, T. I. Webb, C. Domene, G. P. Sergeant, N. G. McHale, K. D. Thornbury and M. A. Hollywood	Development of GoSlo-SR-5-69, a potent activator of large conductance Ca2+-activated K+ (BK) channels	Eur. J. Med. Chem.	75	426-437	2014	10.1016/j.ejmech.2014.01.035
178	D. Botten, G. Fugallo, F. Fraternali and C. Molteni	A Computational Exploration of the Interactions of the Green Tea Polyphenol (-)-Epigallocatechin 3-Gallate with Cardiac Muscle Troponin C	PLOS ONE	8	e70556	2013	10.1371/journal.pone.0070556
179	F. Comitani, N. Cohen, D. Botten, J. A. Ashby, S. C.R. Lummis and C. Molteni	Insights into the binding of GABA to the insect RDL receptor from atomistic simulations: a comparison of models	J. Comput. Aided Mol. Des.	28	35-48	2014	10.1007/s10822-013-9704-0
180	H. M. Betts, S. I. Pascu, A. Buchard, P. D. Bonnitcha and J. R. Dilworth	One-pot synthesis, characterisation and kinetic stability of novel side-bridged pentaazamacrocyclic copper(II) complexes	RSC Adv.	4	12964-12970	2014	10.1039/c3ra47450j
181	S. Furini, P. Barbini and C. Domene	Effects of the Protonation State of the EEEE Motif of a Bacterial Na(+)-channel on Conduction and Pore Structure	Biophysical J.	106	2175-2183	2014	10.1016/j.bpj.2014.04.005
182	A. K. Vardhaman, P. Barman, S. Kumar, C. V. Sastri, D. Kumar and S. P. de Visser	Comparison of the Reactivity of Nonheme Iron(IV)-Oxo versus Iron(IV)-Imido Complexes: Which is the Better Oxidant?	Angew. Chem. Int. Ed.	52	12288-12292	2013	10.1002/anie.201305370

183	S. M. Pratter, C. Konstantinovics, C. L. M. DiGiuro, E. Leitner, D. Kumar, S. P. de Visser, G. Grogan and G. D. Straganz	Inversion of Enantioselectivity of a Mononuclear Non-Heme Iron(II)-dependent Hydroxylase by Tuning the Interplay of Metal-Center Geometry and Protein Structure	Angew. Chem. Int. Ed.	52	9677-9681	2013	10.1002/anie.201304633
184	S. P. de Visser	Differences in chemical properties and reactivity patterns of mono- and dioxomanganese(V) porphyrins as revealed by density functional theory	J. Porph. Phthalocyanines	17	954-963	2013	10.1142/S1088424613500661
185	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
186	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
187	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
188	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
189	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
190	K. Izod, J. M. Watson, W.	Phosphido-borane and phosphido-bis(borane)	Inorg. Chem.	52	1466-1475	2013	10.1021/ic302205b

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191	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
192	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
193	P. Guiglion, C. Butchosa and M. A. Zwijnenburg	Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation conundrum	J. Mater. Chem. A	2	11996-12004	2014	10.1039/C4TA02044H
194	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
195	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
196	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
197	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
198	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
199	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
200	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	art. no. 084304	2014	10.1063/1.4865749

201	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	art. no. 094306	2014	10.1063/1.4894227
202	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	art. no. 114038	2014	10.1063/1.4867970
203	J. M. Brown	Origins of Stabilization and Evidence for Charge Delocalization in the Bicyclo[3.2.1]octadienyl Anion and Related Species	Aust. J. Chem.	67	1296–1300	2014	10.1071/CH14244
204	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
205	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
206	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
207	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
208	S. Bui, D. von Stetten, P. G. Jambrina, T. Prangé, N. Colloc'h, D. de	Direct Evidence for a Peroxide Intermediate and a Reactive Enzyme–Substrate–Dioxygen Configuration in a Cofactor-free Oxidase	Angew. Chem. Int. Ed.	53	13710–13714	2014	10.1002/anie.201405485

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209	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
210	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
211	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
212	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
213	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 Reaction at Different Temperatures Calculated by Transition-State Theory with ab Initio and Density Functional Theory Reaction Paths	J. Phys. Chem. A	118	2040-2055	2014	10.1021/jp5000864
214	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
215	D. K. W. Mok, E. P. F. Lee, F. T. Chau and J. M. Dyke	Simulated photodetachment spectra of AlH(2)(-)	J. Chem. Phys.	139	art. no. 014301	2014	10.1063/1.4811671
216	G. Copela165nd, 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
217	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
218	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
219	C. J. Percival, O. Welz, A.	Regional and global impacts of Criegee	Faraday Discussions	165	45-73	2013	10.1039/c3fd00048

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220	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
221	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
222	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
223	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 solvating agents	Chem. Eur. J.	19	8136-8143	2013	10.1002/chem.201300062
224	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
225	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
226	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
227	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
228	C. Lapthorn, T. J. Dines, B. Z. Chowdhry, G. L.	Can ion mobility mass spectrometry and density functional theory help elucidate protonation	Rapid Commun. Mass Spectrom.	27	2399-2410	2013	10.1002/rcm.6700

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229	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
230	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
231	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
232	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
233	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
234	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
235	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
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237	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
238	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
239	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
240	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
241	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
242	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
243	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
244	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
245	I. Powis	Communication: The influence of vibrational parity in chiral photoionization dynamics	J. Chem. Phys.	140	art. no. 111103	2014	10.1063/1.4869204
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247	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

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249	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
250	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
251	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
252	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
253	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
254	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
255	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
256	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
257	G. A. Guirgis, J. S. Overby, T. J. Barker, M. H. Palmer, B. H. Pate	The Molecular Structure of Methylfluoroisocyanato Silane: A Combined Microwave Spectral and Theoretical Study	J. Phys. Chem. A	119	652-658	2015	10.1021/jp511354j

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258	L. Burroughs, J. Ritchie, M. Ngwenya, D. Khan, W. Lewis and S. Woodward	Anionic Sigmatropic-Electrocyclic-Chugaev Cascades: Accessing 12-aryl-5-(methylthio(carbonyl)thio)tetracenes and a Related Anthra[2,3-b]thiophene	Beilstein J. Org. Chem.	11	273-279	2015	10.3762/bjoc.11.31
259	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
260	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	119	1600-1608	2015	10.1021/jp507744u
261	T. G. Karabencheva, 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
262	T. G. Karabencheva-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
263	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
264	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
265	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
266	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
267	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C.	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

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268	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
269	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
270	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
271	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
272	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
273	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
274	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
275	G. L. Gregory, M. Ulmann and A. Buchard	Synthesis of 6-membered cyclic carbonates from 1,3-diols and low CO2 pressure: a novel mild strategy to replace phosgene reagents	RSC Adv.	5	39404-39408	2015	10.1039/C5RA07290E
276	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 bipyrrolidine derived salan ligands for the isoselective polymerisation of rac-lactide	Chem. Commun.	50	15967-15970	2014	10.1039/c4cc07871c
277	D. M. Bittner, D. P. Zaleski, S. L. Stephens, D. P. Tew, N. R. Walker	A monomeric complex of ammonia and cuprous chloride: H3N···CuCl isolated and characterised by rotational spectroscopy and ab initio	J. Chem. Phys.	142	144302	2015	10.1063/1.4916391

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278	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 bipyrrolidine derived Salan ligands for the polymerisation of rac-lactide	Chem. Sci.	6	5034-5049	2015	10.1039/C5SC01819F
279	A. Alwaaly, W. Clegg, R. W. Harrington, A. L. Petrou and R. A. Henderson	Mechanism of proton transfer to coordinated thiolates: unexpected factors stabilize precursor intermediates	Dalton Trans.	44	11977-11983	2015	10.1039/C5DT01716E
280	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
281	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
282	M. J. Taylor, E. J. Coakley, M. P. Coles, H. Cox and J. R. Fulton	Beta-Diketiminato Organolead Complexes: Structures, 207Pb NMR, and Hammett Correlations	Organometallics	34	2515-2521	2015	10.1021/om501223a
283	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
284	A. Andrejeva, A. M. Gardner, J. B. Graneek, W. H. Breckenridge and T. G. Wright	Theoretical Study of M+−RG2: (M+= Ca, Sr, Ba and Ra; RG= He–Rn)	J. Phys. Chem. A	119	5995-6005	2015	10.1021/jp511817g
285	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	ChemPhysChem	16	2630-2634	2015	10.1002/cphc.201500455
286	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
287	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

288	C. Pubill-Ulldemolins, E. Fernanez, C. Bo and J. M. Brown	Origins of observed reactivity and specificity in the addition of B2Cl4 and analogues to unsaturated compounds	Org. Biomol. Chem.	13	9619-9628	2015	10.1039/C5OB01280E
289	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
290	A. Nordheider, E. Hupf, B. A. Chalmers, F. R. Knight, M. Buehl, S. Mebs, L. Checinska, E. Lork, P. Sanz Camacho, S. E. Ashbrook, K. S. Athukorala Arachchige, D. B. Cordes, A. M. Z. Slawin, J. Beckmann, and J. D. Woollins	Peri-Substituted Phosphorus-Tellurium Systems-An Experimental and Theoretical Investigation of the P...Te through-Space Interaction	Inorg. Chem.	54	2435-2446	2015	10.1021/ic503056z
291	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
292	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
293	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-Nov	2015	10.1002/chem.201502592
294	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
295	S. Manzoor, A. Simperler and A. Korre	A theoretical study of the reaction kinetics of amines released into the atmosphere from CO2 capture	Int. J. Greenh. Gas Control	41	219-228	2015	10.1016/j.ijggc.2015.05.012
296	L. Ji, A. S. Faponle, M. G. Quesne, M. A. Sainna, J. Zhang, A. Franke, D.	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

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297	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
298	L. Darre, J. Iglesias, A. Kolhmeyer, 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
299	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
300	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
301	M. R. Ranga Prabhath, J. Romanova, R. J. Curry, S. R. P. Silva and P. D. Jarowski	The Role of Substituent Effects in Tuning Metallophilic Interactions and Emission Energy of bis-4-(2- Pyridyl)-1,2,3-triazolatoplatinum(II) Complexes	Angew. Chem. Int. Ed.	54	7949-7953	2015	10.1002/anie.201502390
302	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.organomet.5b00811
303	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
304	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
305	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	Mol. Simul.	42	435-445	2015	10.1080/08927022.2015.1059938

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306	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
307	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
308	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	308
309	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	309
310	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	310
311	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	311
312	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	312
313	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-Endo-Trig Cyclization	Nature Chem.	7	171-178	2015	313
314	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

315	J. Romanova, M. R. Ranga Prabhath, 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
316	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
317	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
318	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
319	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
320	M. J. D. Champion, J. M. Dyke, W. Levason, M. E. Light, D. Pugh, H. Bhakhoa, L. Rhyman, P. Ramasami, and G. Reid	Sodium Thioether Macrocyclic Chemistry: Remarkable Homoleptic Octathia Coordination to Na+	Inorg. Chem.	54	2497-2499	2015	10.1021/acs.inorgchem.5b00156
321	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 CH3O2 and BrO Radicals: A New Source of Upper Troposphere Lower Stratosphere Hydroxyl Radicals	J. Phys. Chem. A	119	4618-4632	2015	10.1021/jp5108203
322	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
323	M. A. H. Khan, S. M. P. Gillespie, B. Razis, P. Xiao, M. T. Davies-	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

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324	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
325	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
326	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
327	A. K. King, A. Buchard, M. F. Mahon and R. L. Webster	Facile, Catalytic Dehydrocoupling of Phosphines Using - Diketiminate Iron(II) Complexes	Chem. Eur. J.	21	15960-15963	2015	10.1002/chem.201503399
328	A. Draksharapu, D. Angelone, M. G. Quesne, S. K. Padamati, L. Gómez, R. Hage, M. Costas, W. R. Browne and S. P. de Visser	Identification and spectroscopic characterization of nonheme iron(III) hypochlorite intermediates	Angew. Chem. Int. Ed.	54	4357-4361	2015	10.1002/anie.201411995
329	D. Sahoo, M. G. Quesne, S. P. de Visser and S. P. Rath	Hydrogen bonding interactions trigger a spin-flip in iron(III)-porphyrin complexes	Angew. Chem. Int. Ed.	54	4796-4800	2015	10.1002/anie.201411399
330	M. A. Sainna, D. Sil, D. Sahoo, B. Martin, S. P. Rath, P. Comba and S. P. de Visser	Spin-state ordering in hydroxo-bridged diiron(III)bisporphyrin complexes	Inorg. Chem.	54	1919-1930	2015	10.1021/ic502803b
331	M. Sallmann, S. Kumar, P. Chernev, J. Nehrkorn, A. Schnegg, D. Kumar, H. Dau, C. Limberg, and S. P. de Visser	Structure and mechanism leading to formation of the cysteine sulfinate product complex of a biomimetic cysteine dioxygenase model	Chem. Eur. J.	21	7470-7479	2015	10.1002/chem.201500644

332	E. R. Clark and M. J. Ingleson	N-Methylacridinium Salts: Carbon Lewis Acids in Frustrated Lewis Pairs for sigma bond activation and catalytic reductions	Angew. Chem. Int. Ed.	53	11306-11309	2014	10.1002/anie.201406122
333	I. A. Cade and M. J. Ingleson	syn-1,2-carboboration of Alkynes with Borenium Cations	Chem. Eur. J.	20	12874-12880	2014	10.1002/chem.201403614
334	J. J Dunsford, E. R. Clark and M. J. Ingleson	Direct C(sp2)-C(sp3) Cross-Coupling of Diaryl Zinc Reagents with Benzylic, Primary, Secondary, and Tertiary Alkyl Halides	Angew. Chem. Int. Ed.	54	5688-5692	2015	10.1002/anie.201411403
335	I. A. Cade, W. Y. Chau, I. Vitorica-Yrezabal and M. J. Ingleson	1,1/1,2 Isomerisation in Lewis base adducts of B2cat2	Dalton Trans.	44	7506-7511	2015	10.1039/C5DT00645G
336	L. D. Curless, E. R. Clark, J. Cid, A. Del Grosso and M. J. Ingleson	Complete reductive cleavage of CO facilitated by highly electrophilic borocations	Chem. Commun.	51	10903-10906	2015	10.1039/C5CC03504J
337	D. L. Crossley, I. A. Cade, E. R. Clark, A. Escande, M. J. Humphries, S. M. King, I. Vitorica-Yrezabal, M. J. Ingleson and M. L. Turner	Enhancing electron affinity and tuning band gap in donor-acceptor organic semiconductors by benzothiadiazole directed C-H borylation	Chem. Sci.	6	5144-5151	2015	10.1039/C5SC01800E
338	W. Singh, T. Karabencheva-Christova, G. Black, L. Dover and C. Christov	Conformational Dynamics, Ligand Binding and Effects of Mutations in NirE S-Adenosyl-L-Methionine-Dependent Uroporphyrinogen III Methyltransferase	Sci. Rep.	6	art. no. 20107	2016	10.1038/srep20107
339	W. Singh, T. Karabencheva-Christova, O. Sparagano, G. Black, P. Petrov and C. Christov	Dimerization and Ligand Binding and in TyrosylProtein Sulfotransferase - 2 are influenced by Molecular Motions	RSC Adv.	6	18542-18548	2016	10.1039/C6RA01899H
340	W. Singh, T. Karabencheva-Christova, O. Sparagano, G. Black and C. Christov	Conformational Flexibility and Structure-Function Relationships in TyrosylProtein Sulfotransferase	RSC Adv.	6	11344-11352	2016	10.1039/C5RA25365A
341	L. Burroughs, J. Ritchie and S. Woodward	Understanding Anionic Chugaev Elimination in Pericyclic Tetracene Formation	Tetrahedron	72	1686-1689	2016	10.1016/j.tet.2016.02.025
342	P. Di Pietro and A. Kerridge	U−Oyl Stretching Vibrations as a Quantitative Measure of the Equatorial Bond Covalency in Uranyl Complexes: A Quantum-Chemical Investigation	Inorg. Chem.	55	573-583	2016	10.1021/acs.inorgchem.5b01219

343	A. C. Behrle, A. Kerridge and J. R. Walensky	Dithio- and Diselenophosphinate Thorium(IV) and Uranium(IV) Complexes: Molecular and Electronic Structures, Spectroscopy, and Transmetalation Reactivity	Inorg. Chem.	54	11625-11636	2015	10.1021/acs.inorgchem.5b01342
344	L. A. Viehland, R. Johnsen, B. R. Gray and T. G. Wright	Transport properties of He+ in helium	J. Chem. Phys.	144	art. no. 074306	2016	10.1063/1.4941775
345	A. Andrejeva, W. D. Tuttle, J. P. Harris and T. G. Wright	Assignment of the Vibrations of the S0, S1, and D0+ States of Perhydrogenated and Perdeuterated Isotopologues of Chlorobenzene	J. Chem. Phys.	143	art. no. 104312	2015	10.1063/1.4932052
346	A. Andrejeva, W. D. Tuttle, J. P. Harris and T. G. Wright	Resonance-enhanced multiphoton ionization (REMPI) spectroscopy of bromobenzene and its perdeuterated isotopologue: assignment of the vibrations of the S0, S1 and D0+ states of bromobenzene and the S0 and D0+ states of iodobenzene	J. Chem. Phys.	143	art. no. 244320	2015	10.1063/1.4938501
347	A. Andrejeva, A. M. Gardner, W. D. Tuttle and T. G. Wright	Consistent assignment of the vibrations of symmetric and asymmetric para-disubstituted benzene molecules	J. Mol. Spectros.	321	28-29	2016	10.1016/j.jms.2016.02.004
348	M. Grazia Concilio, A. J. Fielding, R. Bayliss, S. G. Burgess	Density functional theory studies of MTSL nitroxide side chain conformations attached to an activation loop	Theor. Chem. Acc.	135	97	2016	10.1007/s00214-016-1859-z
349	M. H. Palmer, T. Ridley, S. V. Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, M. Biczysko, A. Baiardi, and K. A. Peterson	Combined theoretical and experimental study of the valence, Rydberg, and ionic states of chlorobenzene	J. Chem. Phys.	144	art. no. 124302	2016	10.1063/1.4944078
350	J. M. Cole, K. S. Low, Y. Gong	Discovery of Black Dye Crystal Structure Polymorphs: Implications for Dye Conformational Variation in Dye-Sensitized Solar Cells	ACS Appl. Mater. Interfaces	7	27646-27653	2015	10.1021/acsami.5b07364
351	H. Bhakhoa, L. Rhyman, E. P. F. Lee, P. Ramasami and J. M. Dyke	Can Cyclen Bind Alkali Metal Azides? A DFT Study as a Precursor to Synthesis	Chem. Eur. J.	22	4469-4482	2016	10.1002/chem.201504607
352	A. J. A. Harvey, N. Yoshikawa, J.-G. Wang, and C. E. H. Dessent	Communication: Evidence for dipole-bound excited states in gas-phase I− · MI (M = Na, K, Cs) anionic salt microclusters	J. Chem. Phys.	143	art. no. 101103	2015	10.1063/1.4930919

353	A. Sen, E. M. Matthews, G.-L. Hou, X.-B. Wang, and C. E. H. Dessent	Photoelectron Spectroscopy of the Hexachloroplatinate Dianion Bound to Uracil, Thymine, Cytosine and Adenine: Nucleobase Decay Dynamics Observed via Cluster Photodetachment	J. Chem. Phys.	43	art. no. 184307	2015	10.1063/1.4935171
354	A. Nash, H. L. Birch, N. H. de Leeuw	Mapping intermolecular interactions and active site conformations: from human MMP-1 crystal structure to molecular dynamics free energy calculations	J. Biomol. Struct. Dyn.			2016	10.1080/07391102.2016.1153521
355	G. Pepe, J. M Cole, P. G. Waddell, and S. McKechnie	Molecular Engineering of Cyanine Dyes to Design a Panchromatic Response	Mol. Syst. Des. Eng.	1	86-98	2016	10.1039/c6me00014b
356	L. Schio, M. Alagia, A. A. Dias, S. Falcinelli, V. Zhaunerchyk, E. P. F.Lee, D. K. W. Mok, S. Stranges and J. M. Dyke	A Study of H2O2 with Threshold Photoelectron Spectroscopy (TPES) and Electronic Structure Calculations: Re-determination of the first Adiabatic Ionization Energy (AIE)	J. Phys. Chem. A			2016	10.1021/acs.jpca.6b01039
357	F. Comitani, V. Limongelli and C. Molteni	The free energy landscape of GABA binding to a pentameric ligand-gated ion channel and its disruption by mutations	J. Chem. Theory Comput.			2016	10.1021/acs.jctc.6b00303
358	M. Gregson, E. Lu, F. Tuna, E. J. L. McInnes, C. Hennig, A. C. Scheinostm, J. McMaster, W. Lewis, A. J. Blake, A. Kerridge and S. T. Liddle	Emergence of comparable covalency in isostructural cerium(IV)– and uranium(IV)–carbon multiple bonds	Chem. Sci.	7	3286-3297	2016	10.1039/C6SC00278A
359	P. Guiglion, E. Berardo, C. Butchosa, M. C. C. Wobbe and M. A. Zwijnenburg	Modelling materials for solar fuel synthesis by artificial photosynthesis; predicting the optical, electronic and redox properties of photocatalysts	J. Phys. Condens. Matter.	28	074001	2016	10.1088/0953-8984/28/7/074001
360	P. Guiglion, C. Butchosa and M. A. Zwijnenburg	Polymer Photocatalysts for Water Splitting: Insights from Computational Modeling	Macromol. Chem. Phys.	217	344-353	2016	10.1002/macp.201500432
361	M. A. Zwijnenburg, E. Berardo, W. J. Peveler, and K. E. Jelfs	Amine molecular cages as supramolecular fluorescent explosive sensors; a computational perspective	J. Phys. Chem. B	120	5063-5072	2016	10.1021/acs.jpcb.6b03059
362	R. S. Sprick, B. Bonillo, R. Clowes, P. Guiglion, N. J. Brownbill, B. J. Slater, F. Blanc, M. A.	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts	Angew. Chem. Int. Ed.	55	1792-1796	2016	10.1002/anie.201510542

	Zwijnenburg, D. J. Adams and A. I. Cooper						
363	P. Guiglion and M. A. Zwijnenburg	Contrasting the optical properties of the different isomers of oligophenylene	Phys. Chem. Chem. Phys.	17	17854-17863	2016	10.1039/C5CP01916H
364	S. Doherty, J. G. Knight, D. O. Perry, N. A. B. Ward, D. M. Bittner, W. McFarlane, C. Wills and M. R. Probert	Triaryl-Like MONO-, BIS-, and TRISKITPHOS Phosphines: Synthesis, Solution NMR Studies, and a Comparison in Gold-Catalyzed Carbon–Heteroatom Bond Forming 5-exo-dig and 6-endo-dig Cyclizations	Organometallics	35	1265-1278	2016	10.1021/acs.organomet.6b00146
365	S. D. Ahn, A. C. Fisher, A. Buchard, S. D. Bull, A. M. Bond and F. Marken	Hydrodynamic Rocking Disc Electrode Study of the TEMPO-Mediated Catalytic Oxidation of Primary Alcohols	Electroanalysis	28	1-12	2016	10.1002/elan.201600141
366	C. Romain, Y. Zhu, P. Dingwall, S. Paul, H. S. Rzepa, A. Buchard and C. K. Williams	Chemoselective Polymerizations from Mixtures of Epoxide, Lactone, Anhydride, and Carbon Dioxide	J. Am. Chem. Soc.	138	4120-4131	2016	10.1021/jacs.5b13070
367	D. S. Lee, M. J. Duran-Pena, L. Burroughs and S. Woodward	Efficient Preparation of TMSCCl2Br and Its Use in Dichlorocyclopropanation of Electron-Deficient Alkenes	Chem. Eur. J.	22	1-9	2016	10.1002/chem.201600607
368	M. M. Rafiee Fanood, M. H. M. Janssen, I. Powis	Enantioselective femtosecond laser photoionization spectrometry of limonene using photoelectron circular dichroism	Phys. Chem. Chem. Phys.	17	8614-8617	2015	10.1039/C5CP00583C
369	I. Powis, D. M. P. Holland, E. Antonsson, M. Patanen, C. Nicolas, C. Miron, M. Schneider, D. Y. Soshnikov, A. Dreuw, A. B. Trofimov	The influence of the bromine atom Cooper minimum on the photoelectron angular distributions and branching ratios of the four outermost bands of bromobenzene	J. Chem. Phys.	143	art. no. 144304	2015	10.1063/1.4931642
370	D. M. Bittner, D. P. Zaleski, D. P. Tew, N. R. Walker and A. C. Legon	Highly Unsaturated Platinum and Palladium Carbenes PtC3 and PdC3 Isolated and Characterized in the Gas Phase	Angew. Chem. Int. Ed.	55	1-5	2016	10.1002/anie.201511646
371	D. M. Bittner, S. L. Stephens, D. P. Zaleski, D. P. Tew, N. R. Walker and A. C. Legon	Gas phase complexes of H3N···CuF and H3N···CuI studied by rotational spectroscopy and ab initio calculations: the effect of X (X = F, Cl, Br, I) in OC···CuX and H3N···CuX	Phys. Chem. Chem. Phys.	18	13638-13645	2016	10.1039/C6CP01368F
372	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang, M.	Combined theoretical and experimental study of the valence, Rydberg and ionic states of fluorobenzene	J. Chem. Phys.	144	art. no. 204305	2016	10.1063/1.4949548

	Biczysko, A. Baiardi, and K. A. Peterson						
373	P. A. Cox, A. G. Leach, A. D. Campbell and G. C. Lloyd-Jones	Protodeboronation of Heteroaromatic, Vinyl, and Cyclopropyl Boronic Acids: pH–Rate Profiles, Autocatalysis, and Disproportionation	J. Am. Chem. Soc.	138	9145-9157	2016	10.1021/jacs.6b03283
374	C. Jorgensen, S. Furini and C. Domene	Energetics of Ion Permeation in an Open-Activated TRPV1 Channel	Biophysical J.	111	1-9	2016	10.1016/j.bpj.2016.08.009
375	C. Jorgensen, L. Darré, V. Oakes, R. Torella, D. Pryde and C. Domene	Lateral Fenestrations in K+‑Channels Explored Using Molecular Dynamics Simulations	Mol. Pharm.	13	2263-2273	2016	10.1021/acs.molpharmaceut.5b00942

Oral and Poster presentations reported during the period of 1st February 2011 to 31st August 2016

Oral presentations:

Presenter(s)	Title	Event
I. Powis	Plenary talk: Multi-photon-photoelectron circular dichroism on Camphor.	I Powis @"Stereodynamics 2012", Oct 22-26, 2012, Paris.
T. P. Gonçalves,* D. C. Harrowven		POC Meeting, Syngenta, May 2013.
T. Gonçalves	Modelling of Cyclobutanone Rearrangements in silico: Mechanistic Insights and Application to Total Synthesis	Talk 3, NSCCS User Meeting, London, Dec 2012.
C. E. Dessent	Biological Ions in the Gas-Phase: Developing New Techniques for Structural Characterization of Isolated Biomolecular Ions	King's College, London, Department of Chemistry Seminar, June 2013.
C. E. Dessent	Photoionisation and Photodetachment	Gordon Research Conference, Galveston, TX USA, February 2014.
C. E. Dessent	Can a halide ion induce zwitterion formation in a gas-phase amino acid?	Gordon Research Seminar, Ionic and Molecular Clusters, Il Ciocco, Italy, April 2014.
S. Manzoor, A. Korre, S. Durucan and A. Simperler	Atmospheric chemistry modelling of amine emissions from post combustion CO2 capture plants.	Platform presentation at the Greenhouse Gas Control Technologies Conference GHGT-12, Austin, Texas in October 2014.
A. G. Leach and G. M. Noonan	Boronic acids as agents of their own destruction: Experimental and computational studies of protodeboronation provide a predictive model	246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013.
N. Kaltsoyannis	Advancing the chemistry of the f elements	Dalton Discussion 14, Edinburgh, July 2014.
S. Marinakis and B. J. Howard	Zeeman effects in open-shell van der Waals complexes: the ArNO case	The 23rd International Conference on High Resolution Molecular Spectroscopy, 2-6 September 2014, Bologna, Italy.
C. E. Dessent	Invited lecture on Photodetachment and Photoionization	Gordon Research Conference, Galveston, USA, Feb 2014

A. Sen	Contributed talk on Atomic and Molecular Clusters	Gordon Research Conference, Il Ciocco, April 2014
T. Kraemer		ScotChem 2014, Heriot-Watt University.
T. Kraemer		WATOC2014 Congress, Santiago de Chile.
P. D. Jarowski	Conference talk	XXth International Workshop on Quantum Systems in Chemistry, Physics and Biology, Varna, Bulgaria (2015).
T. Markovic, A. Simperler, J. N. Harvey, R. Vilar and D. Weiss	Fractionation of ZN upon complexation with physiologically relevant ligands in plants. Abstracts no. 2013.	Goldschmidy Conference 2015, Prague, Czech Republic.
T. Markovic, J. N. Harvey, R. Vilar and D. Weiss	The Role of 2'-Deoxymugineic acid in Zn complexation and uptake in rice: coparative experimental and DFT study.	Agri Innovation 2015: Emerging Science and Technologies in Crop Research conference. SCI, April 2015, London, UK.
T. Markovic, A. Simperler, J. N. Harvey, R. Vilar and D. Weiss	Zn partitioning in coordination complexes relevant for plant physiology: a comparative experimental and ab initio study.	Geochemistry Group Research in Progress Meeting, National Oceanography Centre, March 2015, Southampton, UK.
T. Markovic, A. Simperler, J. N. Harvey, R. Vilar and D. Weiss	Zn efficiency in rice: The Role of 2'-Deoxymugineric acid.	Responding to Environmental Change meeting. NERC, March 2015, London, UK.
C. E. Dessent	An invited lecture at the University of Nottingham	University of Nottingham, May 2015.
A. Sen	A contributed talk on the platinum complex-nucleobase work	Assilomar Conference on Spectroscopy and Dynamics, January 2015
A. Sen	A contributed talk on the platinum complex-nucleobase work	American Physical Society Meeting in San Antonio, Texas, USA, March 2015.

Poster presentations:

Presenter(s)	**Title**	**Event**
I. Powis	Photoelectron Circular Dichroism(PECD): Alanine	at ICCESDETAIL and at the Stereodynamics 2012 conference in Paris.
J. Marchois, T. Gonçalves,* J. Maddaluno, D. Harrowven, C. Fressigne	Selectivity in the Addition of Organometallic Reagents to Unsymmetrical Squarates - An *In Silico* Stu	Poster 17, NSCCS User Meeting, London, Dec 2012.
C. E. Dessent	Can a halide ion induce zwitterion formation in the gas-phase arginine amino acid?	Gordon Research Conference, Gaseous Ions, Galveston, TX USA, February 2013.
C. E. Dessent	Can a halide ion induce zwitterion formation in a gas-phase amino acid?	Spectroscopy and Dynamics meeting, Oxford, January 2014.
S. Manzoor	A Theoretical Study of the Atmospheric Chemistry Mechanisms of Amines Emissions from Post Combustion CO2 Capture Technology	Atmospheric Chemical Mechanisms 2014, UC Davies, USA, 10-12 Dec 2014.
S. Manzoor, A. Simperler and A. Korre	Atmospheric chemistry modelling of amine emissions from post combustion CO2 capture plants	Departmental Away Day; 2014 Sept 30; Millennium Conference Centre, UK.
S. Manzoor, A. Simperler and A. Korre	Atmospheric chemistry modelling of amine emissions from post combustion CO2 capture plants	UKCCSRC Biannual Meeting; 2014 Sept 10-11; Cardiff University, UK.

S. Manzoor, A. Simperler and A. Korre	Atmospheric chemistry modelling of amine emissions from post combustion CO2 capture plants	NSCCS User Meeting; 2013 Dec 11; Imperial College London, UK.
S. Boonseng, G. W. Roffe, J. Spencer and H. Cox	The Nature of the Bonding in Symmetrical Pincer Palladacycles	MGMS and RSC MMG Young Modellers' Forum 2014, 28 Nov 2014, SOAS, London.
A. Sen	Poster on Atomic and Molecular Clusters	Gordon Research Conference, Il Ciocco, April 2014
C. E. Dessent	Presented poster	Spectroscopy and Dynamics Meeting in Oxford, Jan 2014
A. Harvey	Presented poster	Spectroscopy and Dynamics Meeting in Oxford, Jan 2014
E. Mathews	Presented poster	ANUMOCP meeting, Leeds, June 2015.
G. Mensa Bonsu	Presented poster	ANUMOCP meeting, Leeds, June 2015.
A. Harvey	Presented poster	RSC Annual Spectroscopy and Dynamics Meeting in Nottingham, January 2015.
E. Mathews	Presented poster	RSC Annual Spectroscopy and Dynamics Meeting in Nottingham, January 2015.
G. Mensa Bonsu	Presented poster	RSC Annual Spectroscopy and Dynamics Meeting in Nottingham, January 2015.
E. Mathews	Presented poster	Cold Ions and Molecules Meeting in Bad Honnef, June 2015.
A. Harvey	Presented poster	Cold Ions and Molecules Meeting in Bad Honnef, June 2015.

Other publications (book chapter/report/thesis) reported during the period of 1st February 2011 to 31st May 2016

Author(s)	Title	Details
Andrew Booth, Odd Gunnar Brakstad, Eirik Falck da Silva, Anna Korre, Saba Manzoor, Sevket Durucan, Alexandra Simperler, Kolbjørn Zahlsen, Astrid Hyldbakk, Kai Vernestad	Final Project Report: Fate of nitramine and nitrosamine emissions in air, water and soil environments around amine-based post combustion CO2 capture plants	A project called SOLVFate for Gassnova, MHI and ENEL.
James McDonagh	Computing the Aqueous Solubility of Organic Drug-like Molecules and Understanding Hydrophobicity	PhD thesis, University of St Andrews, 2014.
Maurice Tia	Dichroïsme Circulaire de Photoélectrons (PECD) sur des systèmes chiraux isolés	PhD thesis, Universite de Paris Sud, 2014.
Joseph Wellington, Andrew Kerridge and Nikolas Kaltsoyannis	Embedded Cluster Calculations of Water Adsorption on the UO2 (111) Surface – 16503	Proceedings of Waste Management 2016, conference in Phoenix, Arizona.
J. Romanova, M. R. Ranga Prabhath, Y. Sadik, P. D. Jarowski	Molecular design of organometallic materials: effect of the metallophilic interaction, ligand, metal and oxidation state	Book chapter for Prog. Theor. Chem. Phys., 2016