Publications reported during the period of 1st February 2013 to 31st January 2014

No	Authors	Title	Journal	Volume	Page Number	Year
1	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
2	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
3	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	045002	2013
4	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. J. Eur.	18	12411-12433	2012
5	Martijn A. Zwijnenburg, Ge Cheng, Tom O. McDonald, Kim. E. Jelfs, Jia-Xing Jiang, Shijie Ren, Tom Hasell, Frédéric Blanc, Andrew I. Cooper, and Dave J. Adams	Shedding Light on Structure–Property Relationships for Conjugated Microporous Polymers: The Importance of Rings and Strain	Macromolecules	46	7696	2013
6	Cristina Butchosa, Tom O. McDonald, Andrew I. Cooper, Dave J. Adams, and Martijn A. Zwijnenburg	Shining a Light on s-Triazine-Based Polymers	J. Phys. Chem. C	116	4314	2014
7	Ciarán R. S. Mooney, M. Eugenia Sanz, Adam R. McKay, Richard J. Fitzmaurice, Abil E. Aliev, Stephen Caddick, and Helen H. Fielding	Photodetachment Spectra of Deprotonated Fluorescent Protein Chromophore Anions	J. Phys. Chem. A	116	7943	2012
8	Ciarán R. S. Mooney, Daniel A. Horke, Adam S. Chatterley, Alexandra	Taking the green fluorescence out of the protein: dynamics of the isolated GFP chromophore anion	Chem. Sci.	4	921-927	2013

	Simperler, Helen H. Fielding and Jan R. R. Verlet					
9	Ewan R. Clark, Alessandro Del Grosso, and Dr. Michael J. Ingleson	The Hydride-Ion Affinity of Borenium Cations and Their Propensity to Activate H2 in Frustrated Lewis Pairs	Chem. Eur. J.	19	2462	2013
10	Lawson JR, Clark ER, Cade IA, Solomon SA, and Ingleson MJ	Haloboration of internal alkynes with boronium and borenium cations as a route to tetrasubstituted alkenes	Angew. Chem. Int. Ed.	52	7518	2013
11	Clark, E. R., Ingleson, M. J.	[(acridine)BCl2]+: A Borenium Cation That Is a Strong Boron- and Carbon-Based Lewis Acid	Organometallics	32	6712	2013
12	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	2013
13	Ma L, Takashima T, Koka J, Kimber HJ, Cox H, and Stace AJ	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
14	King AW, Longford F, Cox H	The stability of S-states of unit-charge Coulomb three-body systems: from H- to H2(+)	J Chem Phys	139	224306	2013
15	Tanja van Mourik, Victor I. Danilov, Vladimir V. Dailidonis, Noriyuki Kurita, Hajime Wakabayashi, and Takayuki Tsukamoto	A DFT study of uracil and 5-bromouracil in nanodroplets	Theor. Chem. Acc.	125	233	2010
16	Ruairidh S. Hunter, and Tanja van Mourik	DNA base stacking: The stacked uracil/uracil and thymine/thymine minima	J. Comp. Chem.	33	2161-2172	2012
17	Leeladee P, Jameson GN, Siegler MA, Kumar D, de Visser SP, Goldberg DP	Generation of a high-valent iron imido corrolazine complex and NR group transfer reactivity	Inorg. Chem.	52	4668-82	2013
18	Latifi R, Sainna MA, Rybak-Akimova EV, and de Visser SP	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
19	Skipper CV, Hamaed A, Antonelli DM, Kaltsoyannis N.	The Kubas interaction in M(II) (M = Ti, V, Cr) hydrazine-based hydrogen storage materials: a DFT study	Dalton Trans.	41	8515-8523	2012
20	Claire V. J. Skipper, David M. Antonelli, and Nikolas Kaltsoyannis	Are Metal-Metal Interactions Involved in the Rising Enthalpies Observed in The Kubas Binding of H2 to Hydrazine-Linked Hydrogen Storage Materials?	J. Phys. Chem. C	116	19134-19144	2012
21	D. A. Wann, P. D. Lane, H.	The gaseous structure of closo-9,12-(SH)2-1,2-C2B10H10, a modifier of	Dalton Trans.	42	12015-12019	2013

	E. Robertson, T. Base and D. Hnyk	gold surfaces, as determined using electron diffraction and computational methods.				
22	Derek A. Wann, David W. H. Rankin, Philip D. McCaffrey, Jan M. L. Martin, and Richard J. Mawhorter	Equilibrium Gas-Phase Structures of Sodium Fluoride, Bromide, and Iodide Monomers and Dimers	J. Phys. Chem. A	118	1927-1935	2014
23	Tatyana G. Karabencheva-Christova, Uno Carlsson, Kia Balali-Mood, Gary W. Black, Christo Z. Christov	Conformational Effects on the Circular Dichroism of Human Carbonic Anhydrase II: A Multilevel Computational Study	PLOS ONE	8	56874	2013
24	Mohammed Maniruzzaman, David J. Morgan, Andrew P. Mendham, Jiayun Pang, Martin J. Snowden, Dennis Douroumis	Drug-polymer intermolecular interactions in hot-melt extruded solid dispersions	International Journal of Pharmaceutics	466	199-208	2014
25	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
26	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
27	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
28	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
29	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
30	S. J. Atkinson, H. E. Robertson, M. Hoelbling, W.-W. Du Mont, C. Mitrofan, K. Hassler and S.	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

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31	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
32	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
33	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	Angewandte Chemie International Edition	51	9539-9542	2012
34	Flora L. Thorp-Greenwood, James A. Platts, Michael P. Coogan	Experimental and theoretical characterisation of phosphorescence from rhenium polypyridyl tricarbonyl complexes	Polyhedron	67	505-512	2014
35	K. M. Sharples, E. Carter, C. E. Hughes, K. D. M. Harris, J. A. Platts 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	15124	2013
36	V.E. Pritchard, F.L. Thorp-Greenwood, R.G. Balasingham, C.F. Williams, B.M. Kariuki, J.A. Platts, A.J. Hallett, M.P. Coogan	Simple Polyphenyl Zirconium and Hafnium Metallocene Room-Temperature Lumophores for Cell Imaging	Organometallics	32	3566	2013
37	K. E. Henry, R. G. Balasingham, A. R. Vortherms, J. A. Platts, J. F. Valliant, M. P. Coogan, J. Zubieta, R. P. Doyle	Emission wavelength variation with changes in excitation in a Re(I)/bisthiazolate ligand complex that breaks Kasha's law	Chem. Sci.	4	2490	2013
38	S. T. Mutter, K. Gkionis, 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
39	J.A. Platts, J. G. Hill , K. Eugene Riley , J. Řezáč , P. Hobza	Basis set dependence of interaction energies computed using composite post-MP2 methods	J. Chem. Theory Comput.	9	330	2013
40	Martin Walker, Ananya Sen, Andrew J.A. Harvey, and Caroline E.H. Dessent	Complexation of anions to gas-phase amino acids: Conformation is critical in determining if the global minimum is canonical or zwitterionic	Chemical Physics Letters	588	43-46	2013

41	A. Kerridge	A RASSCF study of free base, magnesium and zinc porphyrins: accuracy versus efficiency	Phys. Chem. Chem. Phys.	15	2197	2013
42	A. Kerridge	Oxidation state and covalency in f-element metallocenes (M = Ce, Th, Pu): a combined CASSCF and topological study	Dalton Trans.	42	16428	2013
43	Anna Andrejeva, Adrian M. Gardner, Jack B. Graneek, Richard J. Plowright, W. H. Breckenridge, and Timothy G. Wright	Theoretical Study of M+-RG2 (M+ = Li, Na, Be, Mg; RG = He-Rn)	J. Phys. Chem. A	117	13578-13590	2013
44	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	134303	2013
45	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
46	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	214313	2013
47	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	214307	2012
48	Emma Packard, David D. Pascoe, Jacques Maddaluno, Theo P. Goncalves, and David C. Harrowven	Organoytterbium Ate Complexes Extend the Value of Cyclobutenediones as Isoprene Equivalents	Angew. Chem.	125	13314-13317	2013
49	X. Liu, J. M. Cole, P. G. Waddell, 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
50	X. Liu, J. M. Cole, P. G. Waddell, T. C. Lin, J. Radia, 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
51	J. M. Cole, K. F. Bowes, I.	Material Profiling for Photocrystallography: Relating Single-Crystal	Crystal Growth & Design	17	1826-1837	2013

	P. Clark, A. Zeidler, A. W. Parker, I. R. Laskar, T.-M. Chen	Photophysical and Structural Properties of Luminescent Bis-Cyclometalated Iridium-Based Complexes				
52	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, 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
53	T. A. Merz, P. G. Waddell, J. M. Cole	Systematic Molecular Design of p-phenylene Lasing Properties	J. Phys. Chem. C	117	8429-8426	2013
54	X. Liu, J. M. Cole, P. G. Waddell, T. C. Lin, S. McKechnie	The Molecular Origins of Optoelectronic Properties in Coumarins 343, 314T, 445 and 522B	J. Phys. Chem. C	117	14130-41	2013
55	X. Liu, J. M. Cole, K. S. Low	Molecular Origins of Dye Aggregation and Complex Formation Effects in Coumarin 343	J. Phys. Chem. C	117	14723-30	2013
56	X. Liu, Z. Xu, 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
57	L. Zhang, J. M. Cole, P. G. Waddell, K. S. Low, 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
58	L. Zhang, J. M. Cole, X. Liu	Tuning Solvatochromism of Azo Dyes with Intramolecular Hydrogen Bonding in Solution and on Titanium Dioxide Nanoparticles	J. Phys. Chem. C	117	26316-23	2013
59	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	The Molecular Structure of Methyldifluoroisocyanato Silane: A Combined Microwave Spectral and Theoretical Study	J. Phys. Chem. A	116	7822-7829	2012
60	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
61	M. H. Palmer, S. Vronning Hoffmann, N. Jones, E. Smith, and D. Lichtenberger	The electronic states of pyridine-N-oxide studied by VUV photoabsorption and ab initio configuration interaction computations	J. Chem. Phys.	138	214317-1	2013
62	Keith Izod, Daniel G. Rayner, Salima M. El-Hamruni, Ross W. Harrington, and Ulrich	Stabilization of a Diphosphagermylene through ppi-ppi Interactions with a Trigonal-Planar Phosphorus Center	Angew. Chem. Int. Ed.	53	1	2014

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63	Potts, A. W. et al	A study of the valence shell electronic structure and photoionisation dynamics of meta-dichlorobenzene and meta-bromochlorobenzene	Chem. Phys.	415	84	2013
64	I. Powis et al	A study of the valence shell electronic structure and photoionisation dynamics of para-dichlorobenzene and para-bromochlorobenzene	Chem. Phys.	415	291	2013
65	M. Staniforth, S. Daly, K. L. Reid, and I. Powis	A generic π* shaperesonance observed in energy-dependent photoelectron angular distributions from two colour, resonant multiphoton ionization of difluorobenzene isomers	J. Chem. Phys.	139	064304	2013
66	Lehmann CS, Ram NB, Powis I, Janssen MH	Imaging photoelectron circular dichroism of chiral molecules by femtosecond multiphoton coincidence detection	J. Chem. Phys.	139	234307	2013
67	Maurice H. M. Janssen and Ivan Powis	Detecting chirality in molecules by imaging photoelectron circular dichroism	Phys. Chem. Chem. Phys.	16	856-871	2014
68	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	Nat. Commu.	4	2132	2013
69	M. Tia et al.	Chiral Asymmetry in the Photoionization of Gas Phase Amino Acid Alanine at Lyman-α Radiation Wavelength	J. Phys. Chem. Lett.	4	2698	2013
70	Anna K. H. Hirsch, Philippe Reutenauer, Marc Le Moignan, Sebastien Ulrich, Peter J. Boul, Jack M. Harrowfield, Peter D. Jarowski, and Jean-Marie 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
71	Craig A. Taatjes, Oliver Welz, Arkke J. Eskola, John D. Savee, Adam M. Scheer, Dudley E. Shallcross, Brandon Rotavera, Edmond P. F. Lee, John M. Dyke, Daniel K. W. Mok, David L. Osborn, Carl J. Percival	Direct Measurements of Conformer-Dependent Reactivity of the Criegee Intermediate CH3CHOO	Science	340	177-180	2013
72	Ng M, Mok DK, Lee EP, Dyke JM	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	545-57	2013
73	Christian Kerpal, Dan J. Harding, Alexander C.	Structures of Platinum Oxide Clusters in the Gas Phase	J. Phys. Chem.	117	1233-9	2013

	Hermes, Gerard Meijer, Stuart R. Mackenzie, and André Fielicke					
74	Subhrangsu Roy, Roddy J Large, Adebola Morayo Akande, Aravind Kshatri, Tim I Webb, Carmen Domene, Gerard P Sergeant, Noel G McHale, Keith D Thornbury, Mark A Hollywood	Development of GoSlo-SR-5-69, a potent activator of large conductance Ca< sup> 2+</sup>-activated K< sup>+</sup>(BK) channels	European journal of medicinal chemistry	75	426-437	2014