Publications reported during the period of 1st February 2012 to 31st January 2013

No	Authors	Title	Journal	Volume	Page Number	Year
1	C. Domene and S Furini	Molecular Dynamics Simulations of the TrkH Membrane Protein	Biochemistry	51	1559–1565	2012
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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	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
11	R. M. Pinto, A. A. Dias, M. L. Costa, P. Rodrigues, M. T. Barros, J. S. Ogden and	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

	J. M. Dyke					
12	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
13	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
14	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
15	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	Biophys. J.	98	L38-L40	2010
16	G. de Luca, J. W. Emsley, A. Lesage and D. Merlet	The structure and conformations of mesogenic molecules in the pre-transitional region of the isotropic phase: 5OCB and MBBA and their mixture	Liq. Cryst.	39	211-219	2012
17	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
18	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
19	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
20	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
21	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
22	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
23	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
24	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

25	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
26	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
27	A. M. Gardner and T. G. Wright	Consistent Assignment of the Vibrations of Monosubstituted Benzenes	J. Chem. Phys.	135	art. no. 114305	2011
28	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
29	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	88	5845-5851	2012
30	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
31	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
32	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
33	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
34	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
35	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

36	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
37	T.-J. Lin and P. J. O'Malley	Binding Site Influence on the Spin Density and EPR Parameters of the Phyllosemiquinone Anion Free Radical of Photosystem I	J. Phys. Chem. B	115	9311-9319	2011
38	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
39	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 (CH2OO) Reactions with Acetone, Acetaldehyde, and Hexafluoroacetone	Phys. Chem. Chem. Phys.	14	10391-10400	2012
40	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
41	K. Izod, E. R. Clark, R. W. Harrington and W. Clegg	Hypervalent Sulfur-Functionalized Diphosphagermylene and Diphosphastannylene Compounds	Organometallics	31	246-255	2012
42	S. Furini and C. Domene	Non-selective conduction in a mutated NaK channel with three cation-binding sites	Biophysical J.	103	2106-2114	2012
43	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
44	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
45	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
46	E. Martin, A. Baldansuren, T.-J. Lin, R. I. Samoilova, C.	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

	A. Wraight, S. A. Dikanov, and P. J. O'Malley	Computational Perspective				
47	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
48	B. Shepperson, J. Liu, A. M. Ellis and S. Yang	Communication: Electron impact ionization of binary H2O/X clusters in helium nanodroplets: An ab initio perspective	J. Chem. Phys.	137	201102	2012