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Publications reported during the period of 1<sup>st</sup> February 2016 to 31<sup>st</sup> January 2017

No	Authors	Title	Journal	Volume	Page Number	Year	DOI
1	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
2	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
3	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
4	M. Sallmann, S. Kumar, P. Chernev, J. Nehr Korn, A. Schnegg, D. Kumar, H. Dau, C. Limberg, and S. P. de Visser	Structure and mechanism leading to formation of the cysteine sulfinic acid product complex of a biomimetic cysteine dioxygenase model	Chem. Eur. J.	21	7470-7479	2015	10.1002/chem.201500644
5	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
6	I. A. Cade and M. J. Ingleson	syn-1,2-carboboration of Alkynes with Borene Cations	Chem. Eur. J.	20	12874-12880	2014	10.1002/chem.201403614
7	J. J Dunsford, E. R. Clark and M. J. Ingleson	Direct C(sp <sup>2</sup> )-C(sp <sup>3</sup> ) 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
8	I. A. Cade, W. Y. Chau, I. Vitorica-Yrezabal and M. J. Ingleson	1,1/1,2 Isomerisation in Lewis base adducts of B <sub>2</sub> cat <sub>2</sub>	Dalton Trans.	44	7506-7511	2015	10.1039/C5DT00645G

9	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
10	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
11	W. Singh, T. Karabancheva-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
12	W. Singh, T. Karabancheva-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
13	W. Singh, T. Karabancheva-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
14	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
15	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
16	A. C. Behrle, A. Kerridge and J. R. Walensky	Dithio- and Diselenophosphate Thorium(IV) and Uranium(IV) Complexes: Molecular and Electronic Structures, Spectroscopy, and	Inorg. Chem.	54	11625-11636	2015	10.1021/acs.inorgchem.5b01342

		Transmetalation Reactivity					
17	L. A. Viehland, R. Johnsen, B. R. Gray and T. G. Wright	Transport properties of He <sup>+</sup> in helium	J. Chem. Phys.	144	art. no. 074306	2016	10.1063/1.4941775
18	A. Andrejeva, W. D. Tuttle, J. P. Harris and T. G. Wright	Assignment of the Vibrations of the S <sub>0</sub> , S <sub>1</sub> , and D <sub>0</sub> <sup>+</sup> States of Perhydrogenated and Perdeuterated Isotopologues of Chlorobenzene	J. Chem. Phys.	143	art. no. 104312	2015	10.1063/1.4932052
19	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 S <sub>0</sub> , S <sub>1</sub> and D <sub>0</sub> <sup>+</sup> states of bromobenzene and the S <sub>0</sub> and D <sub>0</sub> <sup>+</sup> states of iodobenzene	J. Chem. Phys.	143	art. no. 244320	2015	10.1063/1.4938501
20	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
21	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
22	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
23	J. M. Cole, K. S. Low, Y. Gong	Discovery of Black Dye Crystal Structure Polymorphs: Implications for Dye	ACS Appl. Mater. Interfaces	7	27646-27653	2015	10.1021/acsami.5b07364

		Conformational Variation in Dye-Sensitized Solar Cells					
24	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
25	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 <sup>-</sup> · MI (M = Na, K, Cs) anionic salt microclusters	J. Chem. Phys.	143	art. no. 101103	2015	10.1063/1.4930919
26	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
27	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
28	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
29	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 H <sub>2</sub> O <sub>2</sub> with Threshold Photoelectron Spectroscopy (TPES) and Electronic Structure Calculations: Re-determination of the first Adiabatic Ionization Energy (AIE)	J. Phys. Chem. A	120	5220-5229	2016	10.1021/acs.jpca.6b01039
30	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.	12	3398-3406	2016	10.1021/acs.jctc.6b00303

31	M. Gregson, E. Lu, F. Tuna, E. J. L. McInnes, C. Hennig, A. C. Scheinost, 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
32	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
33	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
34	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.jpcc.6b03059
35	R. S. Sprick, B. Bonillo, R. Clowes, P. Guiglion, N. J. Brownbill, B. J. Slater, F. Blanc, M. A. Zwijnenburg, D. J. Adams and A. I. Cooper	Visible-Light-Driven Hydrogen Evolution Using Planarized Conjugated Polymer Photocatalysts	Angew. Chem. Int. Ed.	55	1792-1796	2016	10.1002/anie.201510542
36	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
37	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.organo.6b00146
38	S. D. Ahn, A. C. Fisher, A.	Hydrodynamic Rocking Disc	Electroanalysis	28	1-12	2016	10.1002/elan.201

	Buchard, S. D. Bull, A. M. Bond and F. Marken	Electrode Study of the TEMPO-Mediated Catalytic Oxidation of Primary Alcohols	is			6	600141
39	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
40	D. S. Lee, M. J. Duran-Pena, L. Burroughs and S. Woodward	Efficient Preparation of TMS $\text{CCl}_2\text{Br}$ and Its Use in Dichlorocyclopropanation of Electron-Deficient Alkenes	Chem. Eur. J.	22	1-9	2016	10.1002/chem.201600607
41	M. M. Rafiee Fanoood, 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
42	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
43	D. M. Bittner, D. P. Zaleski, D. P. Tew, N. R. Walker and A. C. Legon	Highly Unsaturated Platinum and Palladium Carbenes PtC $_3$ and PdC $_3$ Isolated and Characterized in the Gas Phase	Angew. Chem. Int. Ed.	55	1-5	2016	10.1002/anie.201511646
44	D. M. Bittner, S. L. Stephens, D. P. Zaleski, D. P. Tew, N. R. Walker and A. C. Legon	Gas phase complexes of H $3\text{N}\cdots\text{CuF}$ and H $3\text{N}\cdots\text{CuI}$ studied by rotational spectroscopy and ab initio calculations: the effect of X (X = F, Cl, Br, I) in OC $\cdots\text{CuX}$ and H $3\text{N}\cdots\text{CuX}$	Phys. Chem. Chem. Phys.	18	13638-13645	2016	10.1039/C6CP01368F
45	M. H. Palmer, T. Ridley, S. Vronning Hoffmann, N. C. Jones, M. Coreno, M. de Simone, C. Grazioli, T. Zhang,	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

	M. Biczysko, A. Baiardi, and K. A. Peterson						
46	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
47	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
48	C. Jorgensen, L. Darré, V. Oakes, R. Torella, D. Pryde and C. Domene	Lateral Fenestrations in K <sup>+</sup> -Channels Explored Using Molecular Dynamics Simulations	Mol. Pharm.	13	2263-2273	2016	10.1021/acs.molpharmaceut.5b00942
49	F. A. Y. N. Schroeder, J. M. Cole, P. G. Waddell and S. McKechnie	Transforming Benzophenoxazine Laser Dyes into Chromophores for Dye-Sensitized Solar Cells: A Molecular Engineering Approach	Adv. Energy Mater.	5	art. no. 1401728	2015	10.1002/aenm.201401728
50	S. L. Benjamin, T. Kramer, W. Levason, M. E. Light, S. A. Macgregor and G. Reid	[Pd <sub>4</sub> (μ <sub>3</sub> -SbMe <sub>3</sub> ) <sub>4</sub> (SbMe <sub>3</sub> ) <sub>4</sub> ]: A Pd(0) Tetrahedron with μ <sub>3</sub> -Bridging Trimethylantimony Ligands	J. Am. Chem. Soc.	138	6964-6967	2016	10.1021/jacs.6b04060
51	J. Fanfrlík, J. Holub, , J. Řezáč, P. D. Lane, D. A. Wann, D. Hnyk, A. Růžička and P. Hobza	Competition between Halogen, Hydrogen and Dihydrogen Bonding in Brominated Carboranes	ChemPhysChem	17	3373-3376	2016	10.1002/cphc.201600848
52	J. L. McDonagh, D. S. Palmer, T. van Mourik and J. B. O. Mitchell	Are the Sublimation Thermodynamics of Organic Molecules Predictable?	J. Chem. Inf. Model.	56	2162-2179	2016	10.1021/acs.jcim.6b00033