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Experimental Charge Density studies of Ge(II) complexes using beamline I19

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Interest in the p-block elements has recently been stimulated by the need for new reagents for materials and electronics applications, as well as the intrinsic interest in the unprecedented structures and properties observed. For germanium the development of low-valent compounds, organometallics, multiply bonded species, radicals and clusters is of significant importance. We have probed the coordination chemistry of Ge(II) with a range of neutral ligands, few examples of which were reported until recently. They exhibit many striking features including diverse structural motifs and highly variable coordination numbers (between 3 and 8) [1] suggesting the Ge centre does not to have a strong stereochemical preference and small differences in steric and electronic properties of the donor ligands have a significant role. Bonding models have been used to rationalise the observed structures with a Ge-based lone pair occupying the stabilised Ge 4s orbital. However these models are not entirely satisfactory and experimental charge density studies could provide valuable insights into the structures and chemistry of these compounds. [GeCl2(2,2'-bipyridine)], 1, and [GeCl2(1,2-bis(dimethylphosphino)benzene], 2, were selected as targets for initial experimental charge density studies and data have been collected using 3 different experimental configurations of the small molecule single-crystal diffraction beamline I19 [2] at Diamond Light Source. Using a Rigaku Saturn 724+ CCD detector on a 4-circle kappa-geometry CrystalLogic goniometer, data for 1 were collected at λ=0.6889Å without bimorph focussing mirrors in place, and for 2 data were collected at both λ=0.6889Å with bimorph mirrors and λ=0.4859Å without mirrors giving data to 0.48 and 0.38 Å resolution respectively. Details of the analysis of the topology of the electron density will be presented with the insights gained into the bonding in these unusual complexes.

[1] *F. Cheng, J.M. Dyke, F. Ferrante, A.L. Hector, W. Levason, G. Reid, M. Webster and W. Zhang (2010), Dalton Trans, 39, 847-856.,* ***[2]*** *H. Nowell, S. A. Barnett, K. E. Christensen, S. J. Teat & D. R. Allan (2012). J. Synchrotron Rad. 19, 435-441.*

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