MS43-O4 **Self-assembly of highly charged fullerene fragment: Structural mystery resolved.** Marina A. Petrukhina,[a] Alexander V. Zabula,[a] Alexander S. Filatov,[a] Sarah N. Spisak.[a] *[a]Department of Chemistry, University at Albany, State University of New York, Albany, NY 12222, USA*
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The long-standing mystery behind the structure formed by the highly reduced smallest fullerene fragment, the corannulene tetraanion $C_{20}H_{10}^{4-}$, is now resolved [1]. Notably, the above corannulene anion having one electron per five carbon atoms is more electron rich than the hexaanion of C_{60}^{6-} (one electron per ten carbon atoms). The first single-crystal X-ray diffraction analysis of its lithium salt reveals the formation of a sandwich-type supramolecular aggregate with a high degree of alkali metal intercalation. In contrast to the previously proposed model based on in situ NMR spectroscopy study, it is now revealed that five Li^+ ions are sandwiched between the two tetrareduced corannulene decks to form the supramolecular dimer in the solid state. The latter also exists in solutions, as revealed by ^{7}Li NMR spectroscopy. These results establish a new paradigm for lithium intercalation between the curved carbon surfaces of buckybowls, fullerenes, and nanotubes. Structural deformations caused by adding multiple electrons to a bowl-shaped polyarene [2, 3] as well as self-assembly of the resulting non-planar carboanions in different solvent media will also be discussed and compared.

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Keywords: curved polyarene; multi-electron reduction; metal binding

MS43-O5 **Exploring the solid state conformation and assembly of cyclic peptoids derivatives.** Loredana Erra,[a] Consiglia Tedesco,[b] Giovanna Cerasuolo[b], Chiara De Cola,[b] Brunello Nardone,[b] Irene Izzo,[b] Gavin Vaughan,[a] Francesco De Riccardis[b] *[a]ESRF, 6 rue Jules Horowitz, BP220, 38043 Grenoble, France, [b]Dipartimento di Chimica e Biologia, Universitŕ di Salerno, via Ponte don Melillo, I-84084 Fisciano, Italy*
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The molecular conformation control is a key need in drug design: in fact, being inspired from the biological world, it is evident that the structure determines each single function a biological system expresses. The structure-function relation is the concept to keep in mind to achieve results in drug related research fields.[1] Over the years it has been proved that the polypeptides beeing chemically similar to the proteins, are the best candidates to interact with them: in particular, cyclic peptides form a class of compounds of crucial impact for the tratement of several diseases [2]. The preference on the cyclic compounds over the linear ones has some rationals: usually the conformational rigidity ensured by the cyclization corresponds to a better chemical stability together with an increased receptor selectivity. Indeed extensive efforts have been also devoted to synthetise peptidomimentic compounds having an increased proteolytic stability because of their abiotic character [3]. Among them an interesting class of molecules are the cyclo peptoids. In general peptoids are oligomers of *N*-substituted glycine. They differ from peptides because the side chain is attached to the backbone amide nitrogen instead of the á-carbon, the peptoid backbone is achiral and the lack of the amide proton prevents the formation of H-bonds involving this site. Moreover tertiary amide bonds can isomerise between *cis* and *trans* conformation [4]. Here we report and analyze the solid state molecular conformation and the crystal structure of two new derivatives: the cyclo hexa *N*-(benzyl) glycine **1** and cyclo [*N*-(benzyl)glycine-N-(*t*-butyldiphenylsilyloxyethyl)glycine]$_3$ **2** [5]. Moreover we compare our results with the few ones already reported [3] with the aim to rationalize how the chemical interactions inside the structures define both the molecular conformation and the general solid state assembly.

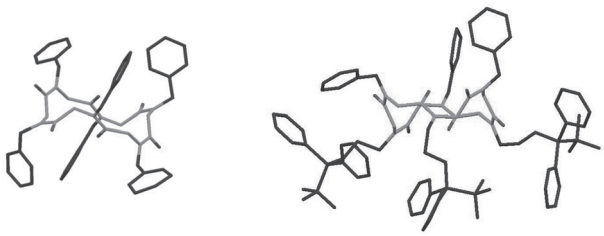

Fig. 1 Molecular structure as obtained by X-ray single crystal diffraction for the compounds **1** (left) and **2** (right).

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