**Self-assembly of highly charged fullerene fragment: Structural mystery resolved.** Marina A. Petrukhina, Alexander V. Zabula, Alexander S. Filatov, Sarah N. Spisak. 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 coronulene tetraanion $C_{20}H_{10}^{-4}$, is now resolved [1]. Notably, the above coronulene 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 coronulene 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 carbocations in different solvent media will also be discussed and compared.

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

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**Exploring the solid state conformation and assembly of cyclic peptides derivatives.** Loredana Erra, Consigilia Tedesco, Giovanna Cerasuolo, Chiara De Cola, Brunello Nardone, Irene Izzo, Gavin Vaughan, Francesco De Riccardi. ESRF, 6 rue Jules Horowitz, BP220, 38043 Grenoble, France, Dipartimento di Chimica e Biologia, Universitá 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 treatment of several diseases [2]. The preference on the cyclic compounds over the linear ones has some rationale: 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 peptidomimetic 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 $\alpha$-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].

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.

**Keywords:** peptoids; conformation; crystal structure

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

**References**


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**Keywords:** peptoids; conformation; crystal structure