

Chirality matters: crowded macrocycles as tectons for inclusion systems

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Chiral but symmetric cyclic polyazamacrocycles represent a very promising class of compounds of shapes resembling geometric figures [1,2]. Single macrocycle molecules can be used as effective ligands and catalysts in asymmetric transformations, while in the condensed phase macrocyclic molecules interact non-covalently to form porous higher-order structures: from discrete molecular cages through amorphous molecular aggregates to crystalline materials. Moreover, these materials show the ability to specifically absorb guest molecules [3]. At the same time, they have the advantage of high thermal and chemical stability and moisture resistance. These properties mean that the spectrum of applications for crystalline materials based on macrocycles can be much broader than for coordination materials or dynamic covalent systems such as MOFs or COFs.

It has been shown that the nature of the π -electron moiety and the functional groups present in the aromatic linkers control the stoichiometry of the formed products and are crucial for further use of these macrocycles as supramolecular tectons [4]. Given that the chemistry of chiral and conformationally stable macrocyclic polyimines containing bulky or sterically demanding substituents is still at an early stage of research, we have focused on highly crowded macrocycles as molecules with significant potential in crystal engineering (Figure 1)[4]. We studied both optically active and racemic forms of macrocycles. We have shown how changes in the steric requirements of the substituents and the conditions of the crystallization process affect the crystal structure of the studied compounds. The packing of these compounds in the crystal lattice and, above all, their ability to form inclusion systems will be discussed.

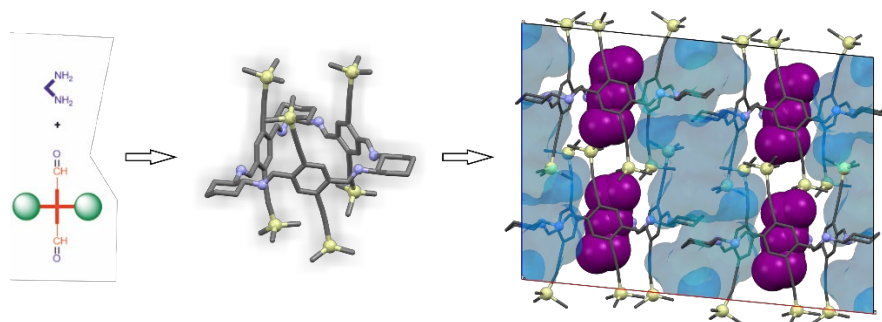


Figure 1. Preparation, molecular structure and crystal packing of sterically crowded model macrocycle.

- [1] Gawroński, J., H. Kołbon, H., Kwit, M., Katrusiak, A. (2000) *J. Org. Chem.*, **65**, 5768.
- [2] Kwit, M., Grajewski, J., Skowronek, P., Zgorzelak, M., Gawroński, J. (2019) *Chem. Rec.*, **19**, 213-237.
- [3] Zhang, G., Zhu, X., Alimi, L.O., Liu, X., Chen, A., Moosa, B.M., Khashab, N.M. (2024) *J. Mater. Chem. A*, **12**, 6875.
- [4] Prusinowska, N., Bardziński, M., Janiak, A., Skowronek, P., Kwit, M. (2018) *Chem. Asian J.*, **13**, 2691.

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