MS31-03 | ENERGY STUDIES OF SINGLE CRYSTAL TO SINGLE CRYSTAL TRANSFORMATIONS IN CYCLIC PEPTOIDS

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Biological processes rely on the control of the dynamic behaviour of biomolecules: the intrinsic flexibility of proteins enables accurate guest recognition and specific substrate conversion. Cyclic peptoids are cyclic *N*-substituted polyglycines, as peptidomimetic compounds they feature useful biological activities and novel chemical properties both in solution and in the solid state [1].

Recently, we reported that a cyclic hexapeptoid strategically decorated by propargyl and methoxyethyl side chains undergoes a reversible single-crystal to single-crystal transformation upon guest release/uptake. The transformation consists in a drastic conformational change, where two propargyl side chains move by 113° and form a CH-pi zipper, which reversibly opens and closes, allowing for guest sensing [2]

We continued the structural characterization of cyclic hexapeptoids [4] and discovered new solid state transformations either triggered by temperature changes or by guest molecules [3].

Here we will report the results of *in-situ* X-ray crystallography, conformational energy studies and energy framework analysis of cyclic peptoids.

These findings highlight that the solid state assembly of the macrocycles determines their solid state dynamic behaviour and pave the way to the design and synthesis of artificial systems able to mimic biological functions.

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[3] Macedi, E. et al. (2017). CrystEngComm, 19, 4704-4708.
[4] Tedesco, C. et al. (2017). Acta Cryst. B73, 399-412.