Influence of environmental humidity on organization and molecular dynamics of heteromacrocyclic assemblies.

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Streszczenie

1D and 2D NMR study, Car–Parrinello molecular dynamics, as well as classical molecular dynamics were employed to investigate *three derivatives of* benzodiazacoronands (achiral compounds which are able to form single crystals with a planar chirality) with intention to explain all subtle effects important during their preorganization, the step anticipating formation of crystals. The experimental study was carried out in two solvents: chloroform and DMSO either containing traces of water (commercial samples) or carefully dried over molecular sieves. Both methods revealed that environmental humidity has a dramatic influence on topology of solute–solvent interactions. Damping of the macrocycle dynamics by its diverse types of interactions with water molecules was shown by computational means. In the most spectacular experiment, we have proved that in chloroform-*d* during the low temperature measurements traces of water dramatically change the spectral pattern, leading to isochronous NMR signals of the AB spin system of benzodiazacoronand. The temperature of isochronous point (TIP) strongly depends on the benzodiazacoronand/water (BW) ratio. This observation opens a pathway to a new strategy based on variable temperature crystallizations and fitting of BW ratio with hope to optimize conditions for formation of chiral crystals.

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