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Nuclearity control in calix[4]arene-based zinc(ii) coordination complexes

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Abstract

© The Royal Society of Chemistry. Three zinc-based coordination complexes were selectively generated in the crystalline phase using a new flexible molecular "tweezers"calix[4]arene derivative ligand decorated with two appended carboxylic moieties and benzyl spacers (3-4H). Through the control of the metal/ligand ratio and the synthetic conditions, the coordination sphere around the zinc cations was found to be different, which influenced the nuclearity of the obtained complexes. The mononuclear complex (3-3H)2-Zn(DMF)2 was obtained, while two partially deprotonated ligands (3-3H)- cap the metallic cation, leading to a nontubular "8"-shaped structure with a metal/ligand ratio equal to 1/2. The dinuclear (3-2H)2-Zn2py4 complex displays a tubular structure with a metal/ligand ratio equal to 1/1, where two zinc cations act as a linear metal linker between two (3-2H)2- species, which adopts a cone conformation. Finally, the third trinuclear coordination complex (3-2H)4-Zn3(OH2) was obtained using (3-4H) and the highly coordinating sulfonylcalix[4]arene (4-4H), exhibiting a 3/1/1 metal/3/4 ratio. Thus, it has been demonstrated that under self-assembly conditions, the nuclearity of the new complexes based on zinc cations and calix[4]arene dicarboxylate (3-4H) can be tuned using different synthetic conditions: nature of solvent, crystallization method, use of a highly coordinating ligand (4-4H).

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