Inclusion Compounds of Plant Growth Regulators in Cyclodextrins

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As a part of a systematic investigation of the inclusion compounds of plant growth regulators in Cyclodextrins (CDs) we report here the crystal structures of the complexes of 4-chlorophenoxyacetic acid (4CPA) encapsulated in *β*-CD (4CPA/*β*-CD) and in heptakis(2,3,6-tri-*O*-methyl)-*β*-CD (4CPA/TM*β*CD). 4CPA is considered as a sufficiently safe plant growth regulator, exhibiting only slightly toxic qualities and it is fairly used in the food industry.

The 4CPA/*β*-CD complex crystallizes as a dimer in the space group *C*2 in the Tetrad packing mode. A review on the packing modes of the dimeric *β*-CD inclusion compounds indicates that close correspondence of unit-cell dimensions is a necessary, but not a sufficient condition for isostructurality.

The 4CPA/TMβCD inclusion complex crystallizes in the space group $P2_1$ and its asymmetric unit contains two crystallographically independent complexes exhibiting different orientations. These complexes exhibit also different conformations related to the different orientation of the guests inside the cavities. It is noted that the complexation process induces striking differences between the hosts of the two complexes though the guest molecules retain the same conformation. Thus, we conclude that the same guest having the same conformation does not inevitably cause a definite conformation of the host.

[1] Tsorteki F., Bethanis K., Pinotsis N., Giastas P., Mentzafos D., *Acta Cryst. B., Accepted 7 February 2005*.

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