Inclusion of the insecticide endosulfan in cyclodextrins

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Most agrochemicals are highly insoluble in water, highly toxic and have reduced stability against chemical and photolytic degradation which makes them environmentally hazardous [1]. Endosulfan is an organochlorine insecticide and acaricide with a combination of these poor physical properties. Improving these physical properties has been attempted by complexing endosulfan with native and derivatised cyclodextrins (CDs).

Solid state inclusion complexes have been formed with β-CD, γ-CD and a derivatised CD known as DIMEB (heptakis(2,6-di-O-methyl)-β-CD). The single crystal X-ray structures of both the β-CD complex and the DIMEB complex of the symmetrical β-endosulfan isomer have been elucidated. The asymmetric unit of the DIMEB-β-endosulfan complex contains two DIMEB molecules with a disordered guest molecule situated in each (Figure). This complex shows a novel packing arrangement as the DIMEB molecules pack head-to-tail in infinite columns with adjacent columns parallel to one another rather than anti-parallel.

An amorphous CD, randomly methylated β-CD (RAMEB), was also investigated for inclusion with endosulfan using PXRD. Kneading experiments between RAMEB and endosulfan resulted in a semi-crystalline material with distinct peaks at low 20 values. The peaks do not match those of the pure crystalline guest material but do show some similarity to the DIMEB-β-endosulfan complex PXRD pattern.

An understanding of the host-guest interactions forms an essential part of complex characterisation needed for developing new agrochemical formulations.


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