

Poster Sessions

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Human MutT homolog-1 (hMTH1) hydrolyzes a variety of oxidized nucleoside triphosphates such as 8-oxo-dGTP, 2-oxo-dATP and 2-oxo-ATP to their corresponding monophosphates and prevents replicational and transcriptional errors caused by their misincorporations into DNA and RNA. We have determined crystal structures of hMTH1 complexed with 8-oxo-dGTP and 2-oxo-dATP and found that hMTH1 recognizes the two different oxidized nucleotides, 8-oxo-dGTP and 2-oxo-dATP, by the exchange of the protonation site between the neighboring Asp residues (Asp119 and Asp120) in the active site pocket. To our knowledge, this is a very novel mechanism for expression of broad substrate specificity by enzymes. In this study, we investigated the pH dependence of substrate-active site interactions in the crystal structures of the hMTH1-8-oxo-dGTP and hMTH1-2-oxo-dATP complexes. Under the crystallization condition with ammonium sulfate as precipitate, the hMTH1-8-oxo-dGTP crystals over pH 7.0 reveal that the substrate binding mode is altered toward an inactive form, in which the triphosphate group is located far from the catalytic residues in the Nudix motif. In the hMTH1-2-oxo-dATP crystals, electron densities for 2-oxo-dATP disappear at pH8.0. These are suggested that the deprotonation of Asp119 in the hMTH1-8-oxo-dGTP crystals and Asp120 in the hMTH1-2-oxo-dATP crystals occurs at these pHs.

Keywords: genome stability, broad substrate specificity, pH-dependence

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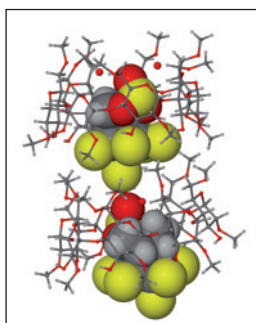
Inclusion of the insecticide endosulfan in cyclodextrins

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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 2θ values. The peaks do not match those of the pure crystalline guest material but do show



The asymmetric unit showing only the major disordered guest component

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.

[1] E. Morillo, in *Cyclodextrins and their Complexes* ed. H. Dodziuk. John Wiley & Sons, Weinheim, 2006, 16.3, 459-467

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180° Domain detection by surface phase sensitive second harmonic generation microscopy of polar materials

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Phase Sensitive Second Harmonic Generation Microscopy (PS-SHM) technique [1], [2] was developed to map 180° domains of polarization. Domain contrast is achieved by using the interference effect between SHG responses of a sample and a homogeneous reference material. Previously it was shown [1] that interpretation of domain mapping is simple if the crystal thickness is homogeneous and in the range of or below the coherence length l_c . Our objective is to demonstrate experimentally, that PS-SHM technique can be performed using a sufficiently flat surface of samples irrespective of their thickness. This is offering most feasible conditions to investigate various as grown materials, and especially those which could not be obtained in μm thick layers.

Using the PS-SHM technique in transmission mode, we have demonstrated [3] either a mono- or bi-polar state for different nonlinear optical crystals such as *N,N*-dimethyl-2-acetamido-4-nitroaniline (DAN), 2-cyclo-octylamino-5-nitropyridine (COANP), a channel-type inclusion compound of perhydrotriphenylene (PHTP) / *N,N*-dimethyl-3-nitroaniline (DMNA), potassium dihydrogen phosphate (KH_2PO_4) crystals stained by dyes and the zeolite $\text{AlPO}_4\text{-5}$ loaded by 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4*H*-pyran (DCM). For all these cases a phase contrast was found irrespective of thickness and surface quality.

In this work, we have demonstrated that the application of PS-SHM can be realized under non phase matching conditions of samples much thicker than the coherence length. Further development is exploring the possibility to perform PS-SHM under reflection.

[1] P. Rechsteiner, J. Hulliger, M. Flörsheimer, *Chem. Mater.* 2000, 12, 3296-3300. [2] S. Kluge, F. Budde, I. Dohnke, *Appl. Phys. Lett.* 2002, 81, 247-249. [3] H. Aboulfadl, J. Hulliger, *Cryst. Growth Des.* to be published 2011.

Keywords: microscopy, phase contrast, polarity

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Molecular recognition and cluster size in supersaturated solutions of NaClO_3

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