

## Poster Presentation

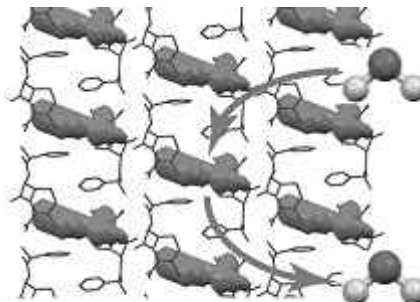
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### *Hydration and Dehydration Transformation Mechanism of Cefaclor Pseudopolymorphs*

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Hydration/dehydration phase transitions of active pharmaceutical ingredients (API) are often accompanied with changes of physicochemical properties, such as solubility, stability, and bioavailability. Therefore, three dimensional structural investigation of the hydration / dehydration mechanism of API is important for pharmaceutical research and development. By relative humidity control, Cefaclor hydrate crystal dehydrates non-stoichiometrically from dihydrate to anhydrous form A. Unexpectedly, its monohydrate form transformed into new 1.9 hydrate by slurry treatment (methanol / water) which dehydrated into another anhydrous form B through hemihydrate by heating. In this study, these hydration and dehydration pseudo-polymorphic transitions of Cefaclor are investigated by the crystal structure analyses. Crystal structures of anhydrous and partially dehydrated forms were determined by structure determination from powder diffraction data technique because such dehydration phase transitions were resulted in a disintegration of single crystal form. In the first dehydration route, hydrates and the anhydrous form A have similar crystal structure, which is referred as 'isomorphic desolvation'. Interestingly, the anhydrous form A has void spaces which corresponds to the water molecule position in the hydrate form. Thus, in hydration / dehydration phase transitions, water molecules move in and out of the void without changing the crystal structures, and the anhydrous form A can hydrate even in low R.H. condition. In the second route, the 1.9 hydrate, hemihydrate and the anhydrate form B have three crystallographically independent molecules forming similar T-shape building block pattern. There are tunnel spaces along b axis between the blocks. In the hydration / dehydration process, the blocks slide each other to open and close the channel. This mechanism explains another non-stoichiometric dehydration in this route.



**Isomorphic Desolvate**

**Keywords:** Hydration/Dehydration, Cefaclor, Powder structure analysis