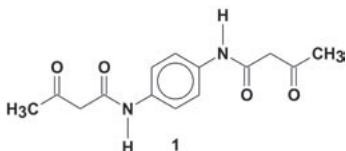


of organic azo pigments; it serves as a linker between two azo moieties [1]. Despite of its commercial importance, crystal structures of **1** are not known up to now. We were able to grow crystals from 1-butanol using re-crystallisation techniques. The X-ray structure analysis showed that the crystal was a monohydrate of **1**. We dried the powder of **1** at 120°C and measured its X-ray powder pattern. The powder was monophasic and we were able to determine the structure from the powder pattern using DASH [2] and TOPAS [3]. This polymorph turned out to be the anhydrous form. A third polymorphic form was obtained by drying the mono-hydrate at 70°C. The resulting powder pattern contained eight reflexions only, and the crystal structure could not be solved yet.

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[2] W. I. F. David, K. Shankland, J. van de Streek, E. Pidcock, W. D. S. Motherwell, J. C. Cole., *J. Appl. Cryst.*, **39**, 910-915 (2006).

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Keywords: polymorphism, organic compounds, powder structure determination

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Crystal structures of two insect recognition pheromones

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Social insects distinguish their nest mates from aliens via the recognition pheromones that are part of the complex mixture of waxy chemicals found on the cuticle. Among these, methyl-branched alkanes appear to act as pheromones, whereas straight-chain alkanes do not. Thus the stereochemistry associated with the methyl group, or the conformation of the molecule imposed by this group, may affect the binding of the molecule to the receptors in an insect's antennae. Enantiomerically pure methyl-branched alkanes have been synthesised and their crystal structures determined by high resolution powder diffraction, or by single crystal diffraction, using synchrotron radiation. 11-methyl nonacosane and 7-methylnonacosane are both monoclinic, space group $P2_1$, $Z = 2$, $a = 15.582 \text{ \AA}$, $b = 7.144 \text{ \AA}$, $c = 14.096 \text{ \AA}$, $\beta = 114.913^\circ$ and $a = 28.172 \text{ \AA}$, $b = 4.935 \text{ \AA}$, $c = 10.375 \text{ \AA}$, $\beta = 90.30^\circ$, respectively. The two compounds have distinct molecular packing arrangements in the structure. Moreover, molecules in 11-methylnonacosane are very straight, whereas 7-methylnonacosane molecules show a slight bend in the chain near the methyl group.

Keywords: alkanes, powder diffraction, synchrotron diffraction

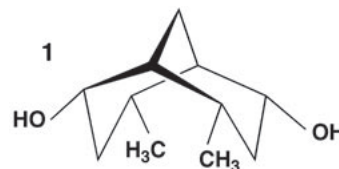
P06.09.33

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Five alternative crystal forms produced by crystallisation of a simple alicyclic dialcohol

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The simple racemic dialcohol **1** formed inclusion compounds in all recrystallisation experiments attempted by us. Many of these crystals are isostructural clathrates of stoichiometry 3(host).1(guest) that are formed in the cubic space group $Ia3$. However, two further inclusion crystal forms are also produced, namely 6(host).1(*p*-xylene) and 2(host).1(water), from these specific solvents. If the cubic crystals are sublimed, then the guest molecules are lost and solvent-free apohost crystals are formed instead in the monoclinic space group $P2_1/c$. Finally, resolved **1** crystallises solvent-free in the tetragonal space group $P4_122$ (or its enantiomorph). All of these five very different crystal forms utilise different hydrogen-bonded supramolecular synthons to create their structures. These arrangements will be described and contrasted. In particular, it will be argued that the most common cubic crystal form is a supramolecular cousin of the well-known host Dianin's compound, despite the very different molecular structures of the two compounds.



Keywords: hydrates and clathrates, hydrogen bonding in organic crystals, inclusion compounds polymorphism

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¹H NMR application to inclusion chemistry: Selectivity profiles of a xanthenol-related host

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10,11-Dihydro-5-(1-naphthyl)-5H-dibenzo[a,d]cyclohepten-5-ol (H) is a derivative from the xanthenol family. We obtained its alpha-structure by recrystallisation at room temperature in ethanol. Subsequently, we crystallised it at room temperature from pyridine (Pyr), 1,4-dioxane (Diox) and DMSO. In all cases, we obtained 1:1 host:guest inclusion compounds displaying hydrogen bonding between the host and the guest molecules. The three structures belong to very different space groups ($C2/c$, $P-1$ and $P2_1/c$ respectively for pyridine, 1,4-dioxane and DMSO) which was interesting to consider when carrying out competition experiments between the solvents with H. We characterized the selectivity profile of our host H with the three solvents using ¹H NMR. We have carried out competition experiments between pairs of guest molecules and characterized the ensuing inclusion compounds formed. We rationalise the structural results with the molecular properties of the guests in terms of their donor/acceptor capacities.

Keywords: inclusion compound, host-guest chemistry, crystal structure