Inclusion Compounds from a Decomposing Host: a Cautionary Tale

Gaelle Ramon[1,2], Mino R. Caira[2], Anthony W. Coleman[1], Luigi R. Nassimbeni[2], Benjamin Taljaard[3], *[1]IBCP, CNRS-UMR 5086, Lyon, France. [2]Chemistry Dept, UCT, South Africa. [3]Chemistry Dept, UPE, South Africa.* E-mail: ramon@science.uct.ac.za

5-Naphthalen-1-yl-5H-dibenzo[a,d]cyclohepten-5-ol (1) has been synthesised from bromo-naphthalene and 5H-Dibenzo[a,d]cyclohepten-5-one (2). Analysis (IR, NMR, TLC) showed the product to be pure. It was stored in a dark bottle in an inert atmosphere. However, when recrystallised from EtOH, we found that the crystal structure contained 1, 2 and a dimer of 2 (refered as 3). Upon recrystallisation from toluene, we obtained a crystal containing 1 and 2, while from hot DMSO we obtained different crystals of 1·DMSO and 3.

When recrystallised from either pyridine or 1,4-dioxane, we obtained crystals of the respective solvates, and we employed the dioxane solvate in order to purify the mixture of the contaminated host which contains 1 + 2 + 3.

Pure 1 was obtained by desorption of its dioxane inclusion compound, and allowed us to estimate that it is present in 59% quantity in the original mixture.

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