Supplementary Information

Inclusion compounds of a borneol dumb-bell host with methylcyclohexanones and 2-butanols: Structures and resolutions

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Hirshfeld surface analysis

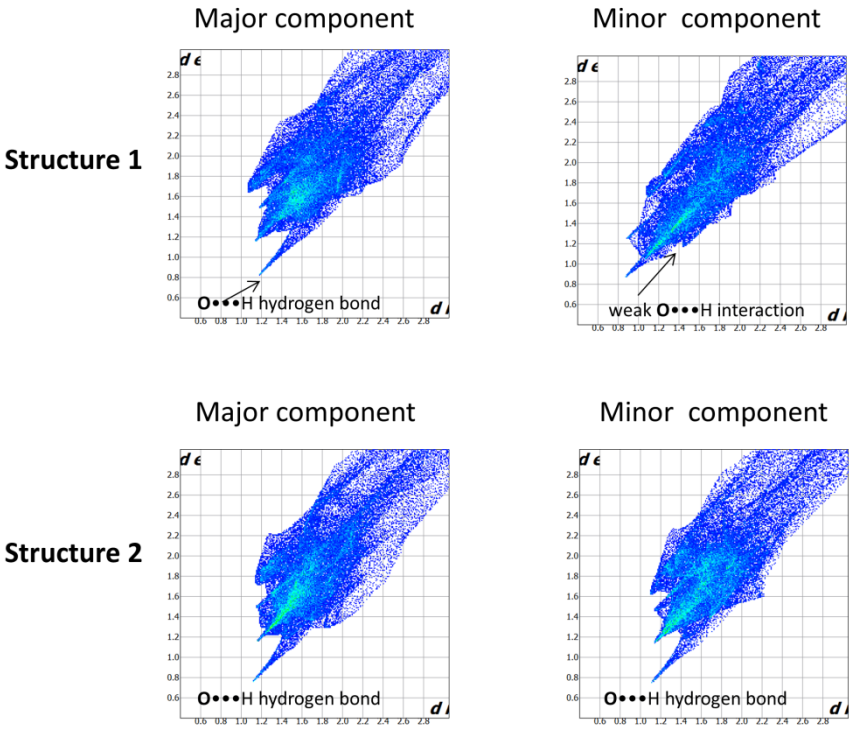

Fig. S1 The 2D plot for the major and minor components of the disordered guest molecules in structures **1** and **2** both for guest B

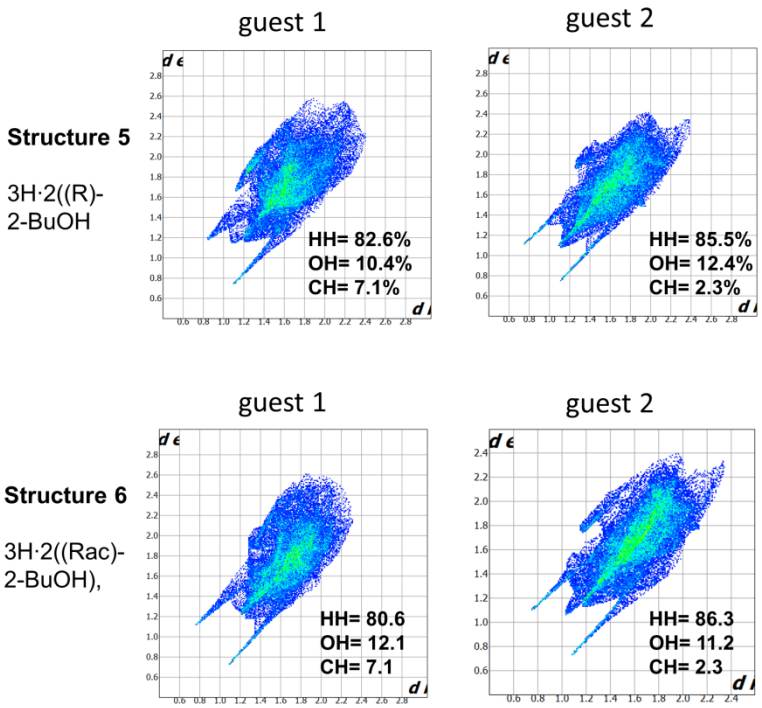

Fig. S2 2D plots of guest 1, guest 2 and host and guest in structures **5** and **6**.

X-ray crystallography

With the exception of structures **2** and **3**, guest molecules were refined isotropically due to disorder. Hydroxyl hydrogen atoms were located in the difference electron density map and O–H distances in structures **4** and **5** were fixed to calculated distances derived from the distance-dependent neutron-normalised method by Lusi and Barbour.[1] The two guest molecules in structure **1** are each disordered over two positions. They were refined isotropically and the C–C and C=O bonds were fixed to appropriate lengths.[2] Hydrogen atoms of the guest and hydroxyl hydrogen atoms of the host were omitted from the final model. In structure **6**, the two guest molecules were each refined as partially populated enantiomers. The C–C and C=O bonds were fixed to appropriate distances. Some of the hydroxyl hydrogen atoms of the disordered guest molecules were omitted from the final model. In structures **4** and **5** the guest molecules are disordered over two positions, the

second positions of the guests could not be modelled to a reasonable geometry, therefore only the highest populated orientations were refined as fully occupied.

Solvent accessible and contact surfaces

In structure **5** the solvent accessible surface as well as the contact surface mapped using the void function in Mercury (probe radius 1.4) is 11.7% (1021.62 $Å^3$) and 2.3% (196.88 $Å^3$) respectively.

In structure **6** the solvent accessible surface as well as the contact surface mapped using the void function in Mercury (probe radius 1.4) is 12.0% (1045.41 $Å^3$) and 2.3% (203.69$Å^3$) respectively.

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[1] M. Lusi and L. J. Barbour*, Cryst. Growth Des.,* 2011, **11**, 5515

[2] F. H. Allen, O. Kennard, D. G. Watson, L. Brammer, A. G. Orpen, and R. Taylor, *J. Chem. Soc., Perkin Trans 2*, 1987, S1-S19