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
**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. 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. 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 Å³) and 2.3% (196.88 Å³)
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 Å³) and 2.3% (203.69Å³)
respectively.

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