

# Supplementary Information

## Additive induced polymorphous behaviour of a conformationally locked hexol

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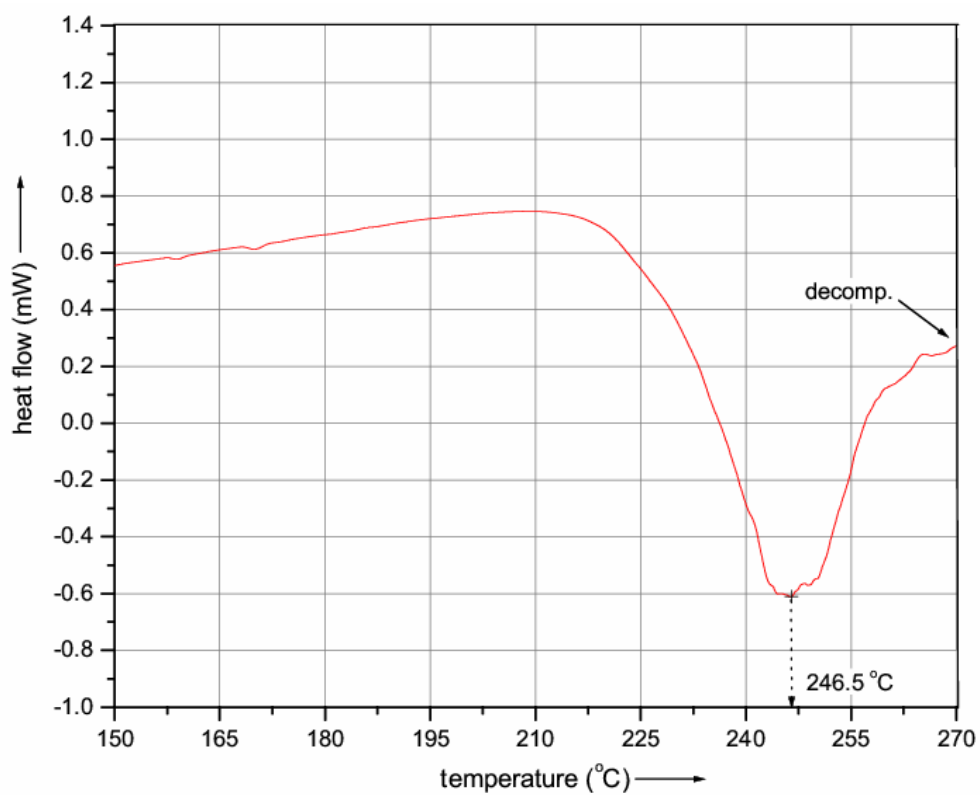
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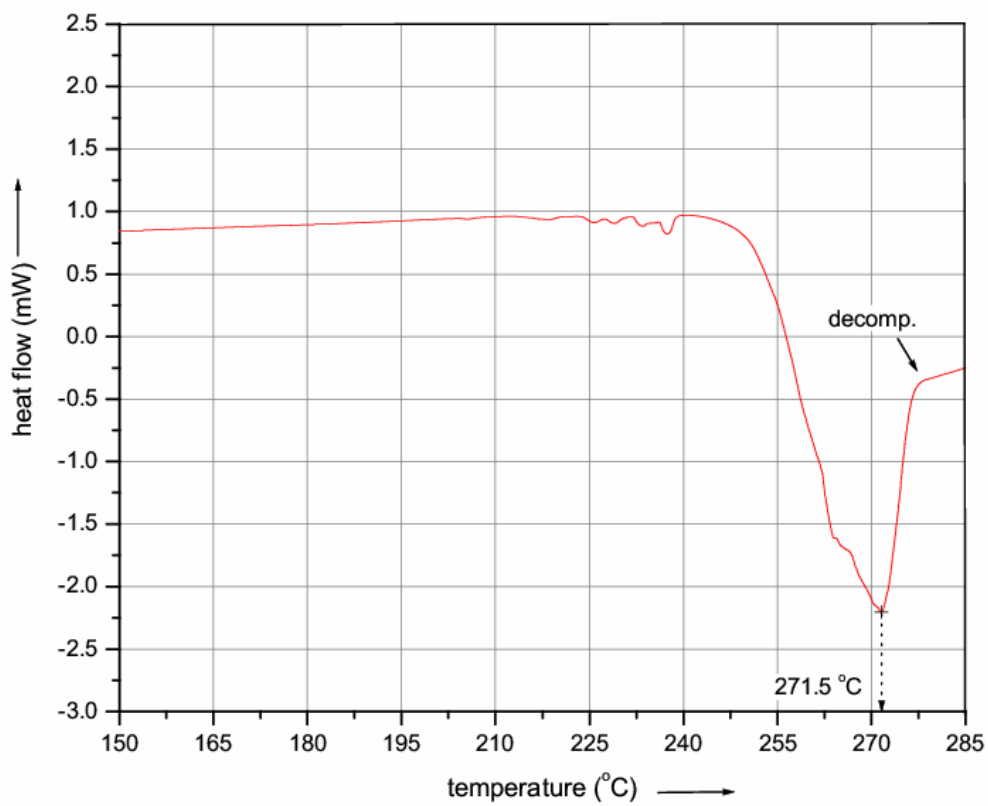
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## DSC plot for the $\alpha$ form of the hexol 2



rate of heating = 5  $^{\circ}\text{C}/\text{min}$ , sample decomposes upon melting

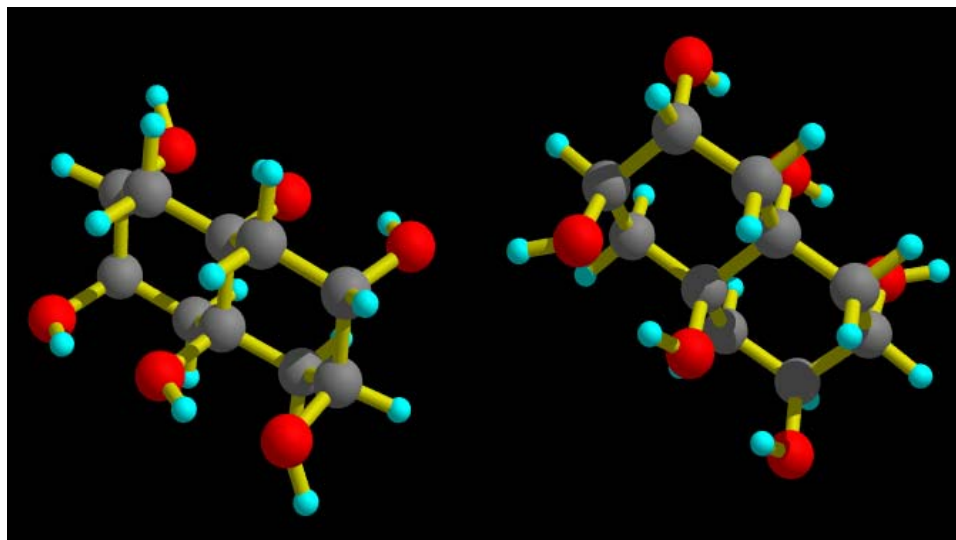
## DSC plot for the $\beta$ form of the hexol 2



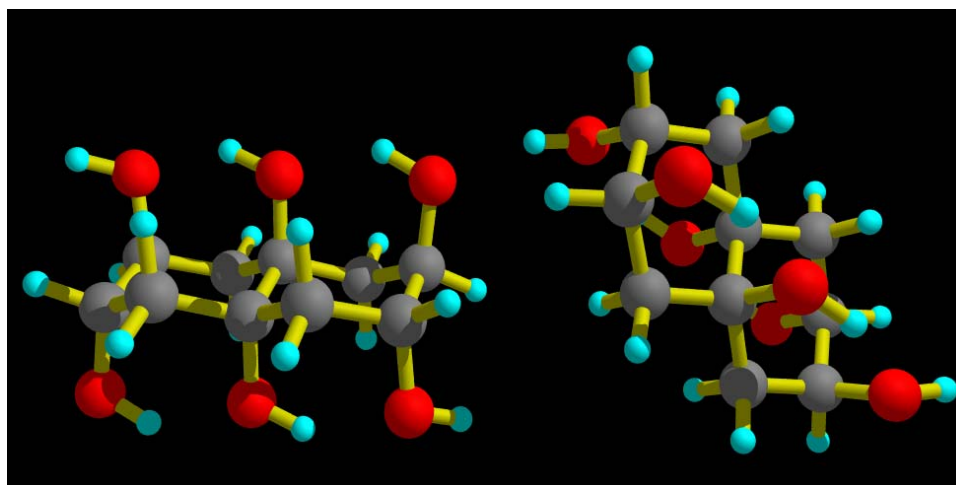
rate of heating = 5 °C/min, sample decomposes upon melting

## DFT single point energy of the packing motifs in the two polymorphs of **2**

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Packing motif in the  $\alpha$  form of the hexol **2**, projected in the standard orientation.  
 $E_1 = -1686.5360632$  Hartrees =  $-1058316.558$  kcal/mol

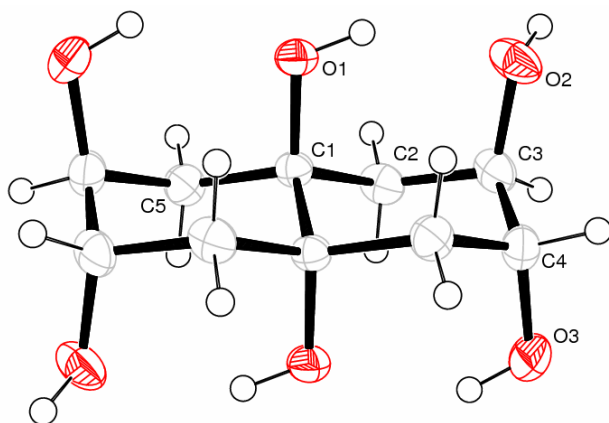


Packing motif in the  $\beta$  form of the hexol **2**, projected in the standard orientation.  
 $E_2 = -1686.5408879$  Hartrees =  $-1058319.586$  kcal/mol

$$\Delta E = E_2 - E_1 \approx -3 \text{ kcal/mol}$$

**CRYSTAL DATA FOR THE  $\alpha$  FORM OF THE HEXOL 2:**  $C_{10}H_{18}O_6$ ,  $M = 234.24$ , monoclinic, space group  $P2_1/n$ ,  $a = 5.7859(12) \text{ \AA}$ ,  $b = 14.326(3) \text{ \AA}$ ,  $c = 6.5982(14) \text{ \AA}$ ,  $\beta = 106.683(3)^\circ$ ,  $V = 523.90(19) \text{ \AA}^3$ ,  $Z = 2$ ,  $\rho_{\text{calcd}} = 1.485 \text{ gcm}^{-3}$ ,  $F(000) = 252$ ,  $\mu = 0.123 \text{ mm}^{-1}$ ,  $R = 0.0379$ ,  $wR = 0.1160$ ,  $\text{GOF} = 1.023$  for 960 reflections with  $I > 2\sigma(I)$ , CCDC-273132 contains the supplementary crystallographic data for this polymorph.

**ORTEP PLOT FOR THE  $\alpha$  FORM OF THE HEXOL 2**



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A view of the hexol **2** in the  $\alpha$  form showing the atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level and hydrogen atoms are shown as small spheres of arbitrary radii. Unlabelled atoms are related to the labeled atoms by the symmetry code (1-x, 1-y, 1-z).

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**HYDROGEN BOND GEOMETRY IN THE**  
 **$\alpha$  FORM OF THE HEXOL 2 (Å, °)**

<b>D-H...A</b>	<b>D-H</b>	<b>H...A</b>	<b>D...A</b>	<b>D-H...A</b>
O1-H1O...O2 <sup>i</sup>	0.82	2.00	2.730 (1)	149
O2-H2O...O3 <sup>ii</sup>	0.82	1.95	2.756 (2)	169
O3-H3O...O1 <sup>iii</sup>	0.82	2.04	2.718 (1)	140

symmetry codes: (i) x, y, z ; (ii)  $\frac{1}{2} + x$ ,  $\frac{1}{2} - y$ ,  $\frac{1}{2} + z$ ; (iii)  $1 - x$ ,  $1 - y$ ,  $1 - z$ .