

**Table S1 Crystal data and structure refinement for  $\alpha$ -CD·CH<sub>4</sub>·4.98H<sub>2</sub>O**

<b>CCDC deposition number</b>	CCDC_2247021
<b>Empirical formula</b>	C <sub>37</sub> H <sub>73.7</sub> O <sub>34.85</sub>
<b>Formula weight</b>	1068.49
<b>T/K</b>	100(2)
<b>Crystal system</b>	orthorhombic
<b>Space group</b>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
<b>a/Å</b>	9.3540(11)
<b>b/Å</b>	14.3606(18)
<b>c/Å</b>	37.141(5)
<b><math>\alpha</math>/°</b>	90
<b><math>\beta</math>/°</b>	90
<b><math>\gamma</math>/°</b>	90
<b>Volume/Å<sup>3</sup></b>	4989.1(11)
<b>Z</b>	4
<b><math>\rho_{\text{calc}}/\text{cm}^3</math></b>	1.423
<b><math>\mu/\text{mm}^{-1}</math></b>	0.128
<b>F(000)</b>	2271.0
<b>Crystal size/mm<sup>3</sup></b>	0.29 × 0.22 × 0.13
<b>Radiation</b>	MoK $\alpha$ ( $\lambda$ = 0.71073)
<b>2<math>\theta</math> range for data collection/°</b>	4.386 to 66.282
<b>Index ranges</b>	-12 ≤ h ≤ 14, -20 ≤ k ≤ 22, -51 ≤ l ≤ 57
<b>Reflections collected</b>	57921
<b>Independent reflections</b>	18978 [ $R_{\text{int}}$ = 0.0424, $R_{\text{sigma}}$ = 0.0507]
<b>Data/restraints/parameters</b>	18978/2/705
<b>Goodness-of-fit on F<sup>2</sup></b>	1.043
<b>Final R indexes [<math>I \geq 2\sigma(I)</math>]</b>	$R_1$ = 0.0511, $wR_2$ = 0.1326
<b>Final R indexes [all data]</b>	$R_1$ = 0.0644, $wR_2$ = 0.1408
<b>Largest diff. peak/hole / e Å<sup>-3</sup></b>	1.86/-0.40
<b>Flack parameter</b>	-0.1(2)