Supplementary Material (ESI) for Chemical Communications

Supporting materials

A unique tetramer of 4 : 5 β-cyclodextrin–ferrocene in the solid state

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Table 1S Crystal data and structure refinement for **1**.

Empirical formula	$C_{109}H_{194}Fe_{2.50}O_{84.50}$
Formula weight	2996.27
Crystal system	Monoclinic
Space group	C2
Unit cell dimensions (Å,°)	
a	19.378(5)
b	24.094(6)
c	32.776(9)
α	90
β	93.963(5)
γ	90
Volume ($Å^3$)	15266(7)
Z	4
D_{calcd} (g/cm^3)	1.304
μ (mm^{-1})	0.337
F (000)	6356
Range of *h*, *k*, *l*	-23/12, –28/28, –34/38
Reflections collected/unique	38848 / 25259
Max. & min. transmission	1.000000 and 0.564372
Data/restraints/parameters	25259 / 279 / 1842
Goodness-of-fit on F^2	1.052
R & R_w	0.1021 & 0.2424
Largest diff. Peak & hole ($e/Å^3$)	0.800 & -0.555

$^{a}\ R = \Sigma(||F_0|-|F_C||)/\Sigma|F_0|;\ ^{b}\ wR = [\Sigma w(|F_0|^2-|F_C|^2)^2/\Sigma w(F_0^2)]^{1/2}$.

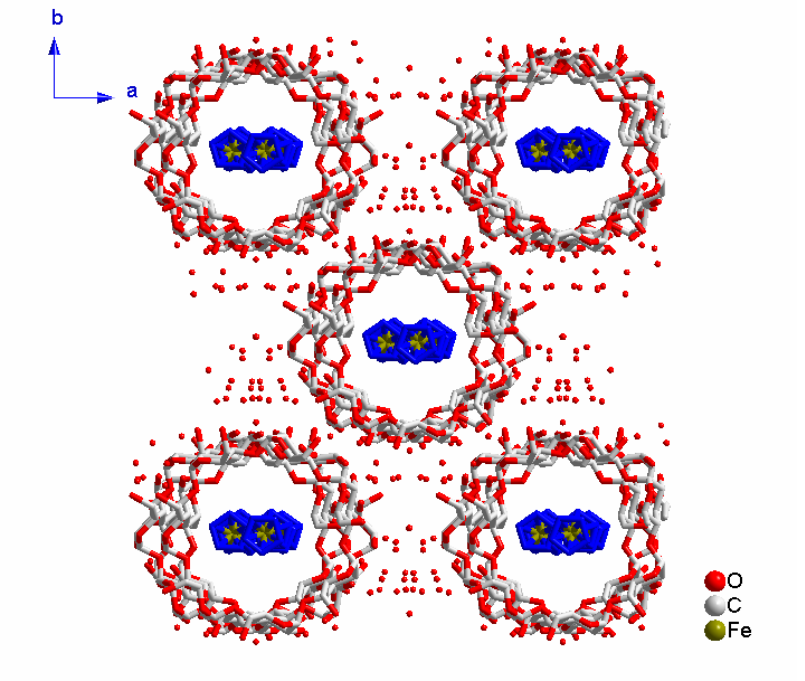

Fig. 1S Crystal structure of **1** viewed down the c axis showing the hexagonal array of CD channels. Water molecules are shown by red circles. Two β-CD molecules are drawn in each channel.

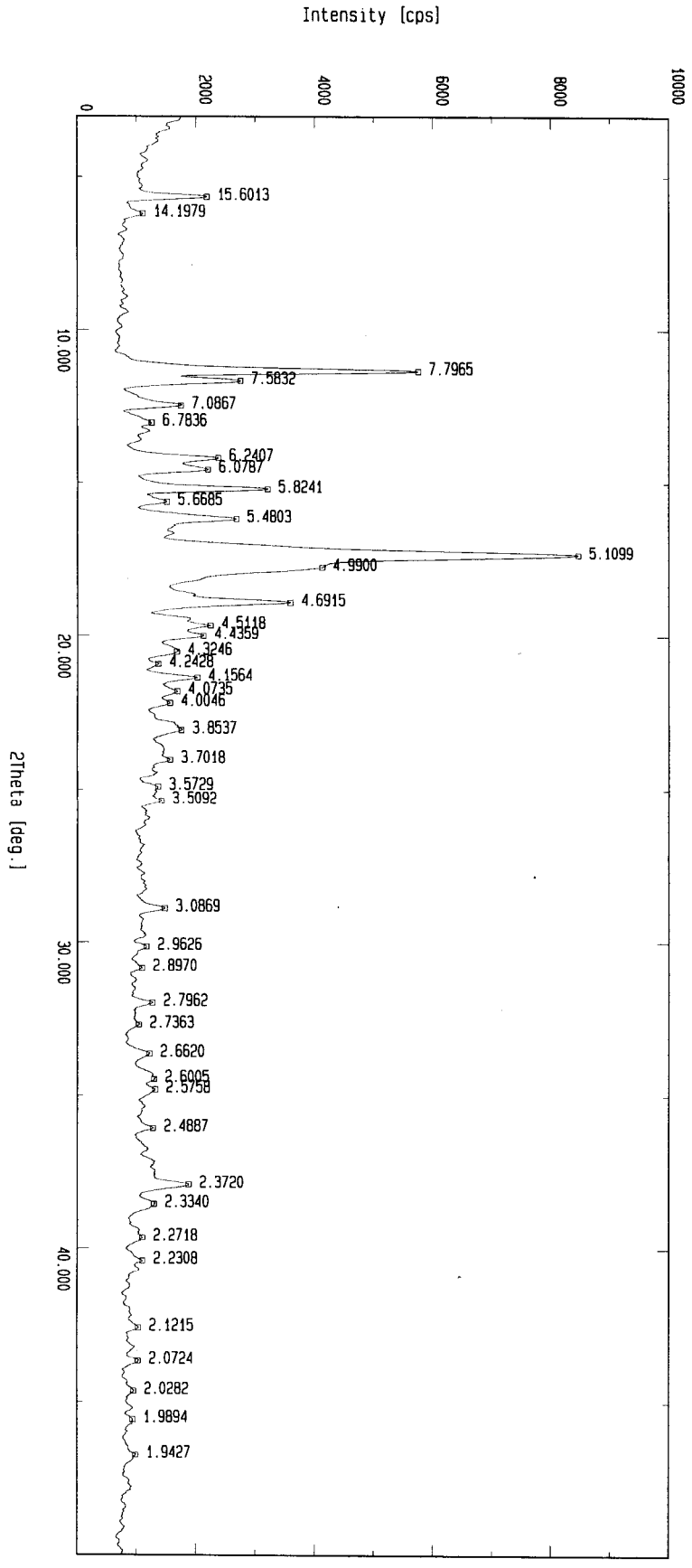

Fig. 2S XRPD pattern for **1**.