Electronic Supplementary Information for:

An Interesting Molecular-assembly of β-Cyclodextrin Pipelines with Hydrophilic Nickel Maleonitriledithiolate Embedded

Xian Cheng[a], Zhenda Lu[b], Yizhi Li[a], Qi Wang[a], Changsheng Lu[a,]*, Qingjin Meng[a,]*

[a] *State Key Laboratory of Coordination Chemistry, Nanjing National Laboratory of Microstructures, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093 (P. R. China)*

[b] *Department of Chemistry, University of California, Riverside, CA 92521*

*Corresponding author. Tel: +86-25-83596775; Fax: +86-25-83314502.

E-mail address: luchsh@nju.edu.cn

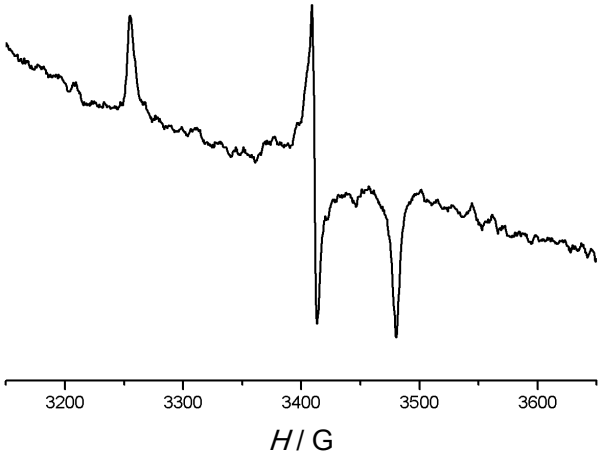

Figure **S1** ESR spectra of inclusion complex **1**

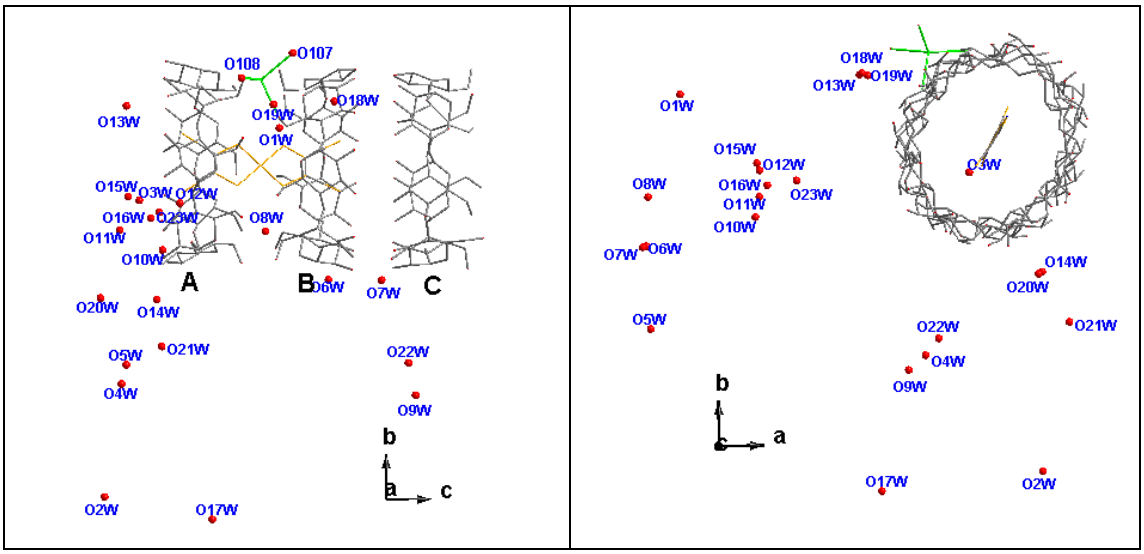

Figure **S2** All the solvent water molecules discovered in the crystal of inclusion complex **1**

Atom label	occupancy	Atom label	occupancy
O1W	0.4	O12W	0.4
O2W	0.4	O13W	0.4
O3W	0.4	O14W	0.4
O4W	0.4	O15W	0.4
O5W	0.4	O16W	0.4
06W	0.4	O17W	0.5
O7W	0.4	O18W	0.3
O8W	0.4	O19W	0.4
O9W	0.4	O20W	0.4
O10W	0.4	O21W	0.3
O11W	0.4	O22W	0.3
		O23W	0.4

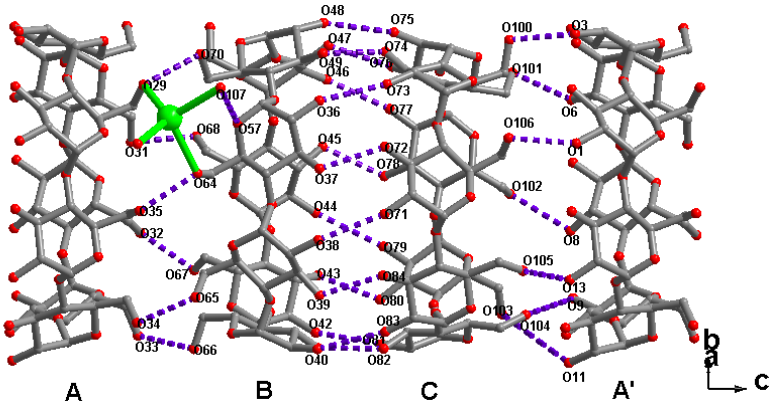

Figure **S3** Hydrogen-bonding networks discovered in the host trimer channels of inclusion complex **1**

	Bond length		
O(31)-O(68)	2.820	O(34)-O(65)	2.813
O(33)-O(66)	2.800	O(35)-O(64)	2.828
O(32)-O(67)	2.743	O(57)-O(107)	3.568
O(29)-O(70)	2.820	O(49)-O(74)	2.965
O(36)-O(73)	2.776	O(37)-O(72)	2.963
O(38)-O(71)	2.965	O(39)-O(84)	2.791
O(40)-O(83)	3.006	O(41)-O(82)	2.880
O(42)-O(81)	2.961	O(43)-O(80)	2.805
O(44)-O(79)	3.122	O(45)-O(78)	2.833
O(46)-O(77)	2.928	O(47)-O(76)	2.906
O(3)-O(100)	2.777	O(6)-O(101)	2.898
O(13)-O(105)	2.969	O(8)-O(102)	2.988
O(11)-O(104)	2.816	O(9)-O(103)	3.009
O(106)-O(1)	2.786		

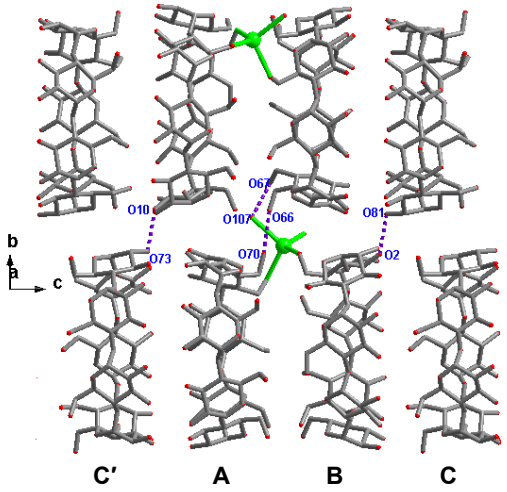

Figure **S4** Hydrogen-bonding networks discovered between the host trimer channels of inclusion complex **1**

	Bond length		
O(10)-O(73)	2.805	O(67)-O(107)	2.757
O(66)-O(70)	2.901	O(2)-O(81)	2.689