Electronic Supplementary Information

Hydrogen-bonded 1D nanotubes and 2D layers of group 12 metal complexes with a pyridylurea ligand

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Table S1. Selected π−stacking interactions and torsion angles of the ligand molecules in **1**−**6**.

compound	parameters of π−π stacking			torsion angles of two **L** arms (°) ($C3-C2_{py}-N2-C6_{urea}$, $C8-C7_{naphthyl}-N3-C6_{urea}$; $C19-C18_{py}-N5-C22_{urea}$, $C24-C23_{naphthyl}-N6-C22_{urea}$)
	centroid−centroid separation (Å)	dihedral angle (°)	vertical displacements between ring centroids (Å)	
$[ZnCl_2L_2]\cdot H_2O$ (**1**)	3.483	2.24	0.456, 0.546	146.20, 67.63; −13.88, 28.78
	3.885	2.24	1.580, 1.707	
$[ZnBr_2L_2]\cdot 0.75EtOH$ (**2a**)	3.569	3.25	0.891, 1.104	30.32, −63.85; −33.83, 60.23
	3.799	5.98	1.337, 1.674	
	3.675	7.20	0.719, 1.148	
$[ZnBr_2L_2]\cdot 0.8H_2O$ (**2b**)	3.665	7.06	0.703, 1.128	−30.64, 64.95; 29.66, −57.74
	3.743	6.00	1.376, 1.727	
$[ZnI_2L_2]$ (**3**)	3.733	5.66	1.476, 1.178	131.32, 46.60; 18.73, −68.55
$[HgCl_2L_2]$ (**4**)	3.754	4.58	0.706, 0.852	−141.53, 47.80; 173.00, −87.53
	3.819	3.14	1.370, 1.208	
$[HgBr_2L_2]$ (**5**)	3.755	2.76	1.258, 1.133	−142.60, 51.17; 177.75, −81.36
	3.710	3.03	0.601, 0.757	
$[HgI_2L]$ (**6**)	3.694	1.34	1.632, 1.514	134.70, 35.83

Table S2. Selected hydrogen bond parameters (Å, °) for **1**−**6**.

Compound	D–H···A	H···A	D···A	∠D−H···A
1	N5−H5B···O3	2.08	2.889(6)	157
	N6−H6A···O3	2.12	2.930(5)	157
	O3−H3D···O1	1.87 (2)	2.701(6)	175
	O3−H3C···O2	1.95 (3)	2.775(6)	166
	N2−H2A···Cl2	2.53	3.320(4)	154
	N3−H3B···Cl2	2.50	3.317(5)	159
2a	N2−H2A···O3	2.51	3.187(12)	136
	N3−H3B···O2	1.95	2.810(8)	178
	N5−H5B···O1	2.15	2.954(6)	154
	N6−H6A···O1	2.27	3.018(7)	145
2b	N3−H3B···O2	1.94	2.797(13)	176
	N5−H5B···O1	2.11	2.920(10)	156
	N6−H6A···O1	2.19	2.955(11)	148
3	N2−H2A···O1	1.95	2.743(6)	153
	N3−H3B···O1	1.97	2.770(6)	154
	N5−H5B···O2	2.09	2.887(6)	155
	N6−H6A···O2	2.31	3.044(6)	144
4	N2−H2B···O2	1.98	2.841(5)	166
	N3−H3B···O2	2.61	3.340(5)	142
	N5−H5B···O1	2.37	3.120(5)	145
	N6−H6B···O1	2.10	2.907(4)	153
5	N2−H2B···O2	1.99	2.831(4)	166
	N3−H3B···O2	2.56	3.275(4)	142
	N5−H5B···O1	2.36	3.105(4)	145
	N6−H6B···O1	2.11	2.902(4)	153
6	N2−H2B···O	2.07	2.863(5)	154
	N3−H3B···O	2.08	2.866(5)	152

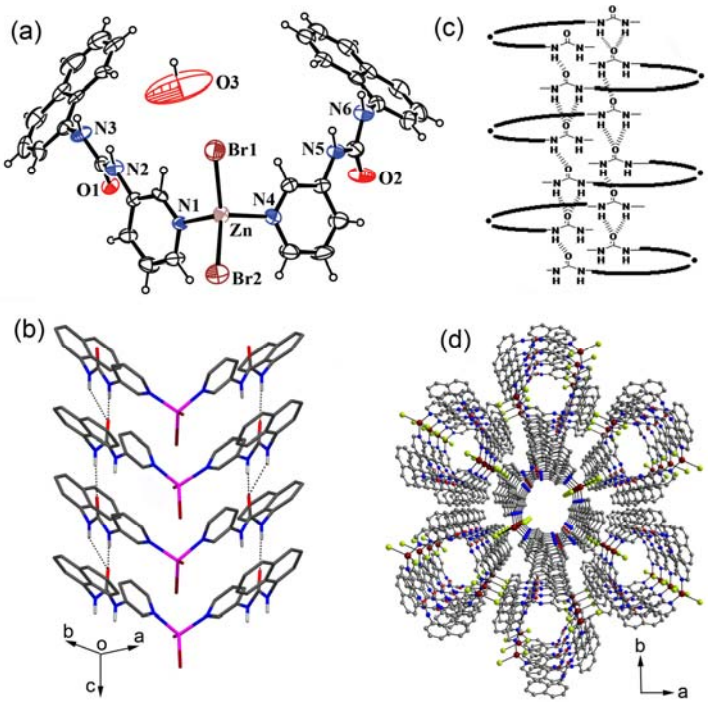

Fig. S1 (a) Molecular structure of $[ZnBr_2L_2]\cdot 0.8H_2O$ (**2b**); (b) The urea self-association in **2b**; (c) Schematic representation of the self-assembly of the semi-macrocyclic $[ZnBr_2L_2]$ synthons into a nanotube; (d) Packing diagram of the 1D H-bonded nanotubes viewed down the *c* axis. Guest solvent molecules and non-urea hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°): Zn−N1, 2.056(8); Zn−N4, 2.038(8); Zn−Br1, 2.325(2); Zn−Br2, 2.3361(16); N1−Zn−Br1, 109.3(2); Br1−Zn−Br2, 124.05(8).