

Supramolecular reactivity of naphthalene-1,4,5,8-tetracarboxylic acid towards transition metal ions: coordination polymers and discrete complexes with Cu^{II}, Ni^{II} and Co^{II}

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SUPPLEMENTARY MATERIAL

Table S1 . Hydrogen-bonding parameters

OH(donor)	O(acceptor)	O-H (Å)	H...A (Å)	O...A (Å)	O-H...A (°)
1 (labels 13-15 and 16-18 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)					
OH13	O18(x+1,y+1,z)	0.99	2.01	2.993(5)	169
OH13	O2(2-x,1-y,1-z)	1.01	2.27	3.167(4)	148
OH14	O11(1-x,1-y,z)	1.05	2.05	3.086(4)	170
OH14	O17	1.03	2.19	3.194(4)	166
OH15	O16(x+1,y,z)	1.02	2.10	3.080(4)	162
OH15	O17	1.02	2.06	2.974(4)	148
OH16	O4(1-x,1-y,z)	0.94	1.89	2.823(3)	174
OH16	O17	0.94	1.86	2.751(4)	158
OH17	O12(1-x,2-y,z)	0.97	1.82	2.779(3)	167
OH17	O17(1-x,2-y,z)	1.01	1.76	2.774(5)	174
OH18	O4(x-1,y,z)	0.97	1.78	2.719(4)	162
2 (labels 20-21 and 22 refer to coordinated and non-coordinated water, respectively; labels 2,4,12 and 13 represent carboxylate O-atoms)					
OH20	O12(-x,y-1,1/2-z)	0.91	2.17	2.939(4)	142
OH20	O4(-x,y,1/2-z)	0.91	1.98	2.869(4)	165
OH21	O22(1/2-x,1/2-y,-z)	0.89	1.96	2.797(3)	155
OH21	O4(x,1-y,z-1/2)	0.90	1.95	2.797(3)	156
OH22	O12(1/2-x,y-1/2,1/2-z)	0.90	2.06	2.914(3)	160
OH22	O13(1/2-x,1/2-y,-z)	0.90	1.94	2.788(3)	157
3 (labels 13-15 and 16-17 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)					
OH13	O17(x+1,y,z)	0.95	2.08	2.992(4)	161
OH13	O12(x,y+1,z-1)	0.95	2.08	2.971(4)	155
OH14	O11(1-x,-y,2-z)	0.95	2.12	3.066(4)	173
OH14	O11(x+1,y,z-1)	0.95	2.63	3.373(4)	136
OH15	O12(-x,-y,2-z)	0.95	2.11	3.001(4)	155
OH15	O12(x,y+1,z-1)	0.95	2.51	3.302(4)	141
OH16	O17	0.95	1.83	2.691(4)	150
OH16	O11(x,y,z-1)	0.95	1.78	2.723(4)	171
OH17	O4(-x,1-y,1-z)	0.95	1.83	2.768(4)	170
OH17	O16(-x,1-y,-z)	0.95	1.79	2.709(4)	162
4 (labels 13-16 and 17-18 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)					
OH13	O18(x-1,y,z)	0.95	1.68	2.608(3)	164
OH13	O12(-x,-y,2-z)	0.95	1.71	2.658(3)	175
OH14	O18	0.95	2.21	3.149(3)	169
OH14	O4(x,1/2-y,z-1/2)	0.95	2.35	3.199(3)	148
OH15	O11(-x,y+1/2,1/2-z)	0.95	2.09	2.987(3)	156
OH15	O4	0.95	2.53	3.230(3)	131
OH16	O4(x,1/2-y,z-1/2)	0.95	2.53	3.042(3)	114
OH16	O2(-x,-y,1-z)	0.95	2.15	2.994(3)	147
OH17	O11(x,-1/2-y,z-1/2)	0.95	1.81	2.749(3)	173
OH17	O4(1-x,y-1/2,1/2-z)	0.95	1.87	2.791(3)	163
OH18	O12(x,y,z-1)	0.95	1.79	2.711(3)	163
OH18	O17(1-x,-y,1-z)	0.95	1.74	2.680(3)	174

5 (labels 14-18 and 19 refer to coordinated and non-coordinated water, respectively; labels 3,5,12 and 13 represent carboxylate O-atoms)

OH14	O19(-x,-y,1-z)	0.89	1.82	2.699(2)	169
OH14	O5(-x,-y,2-z)	0.89	1.79	2.640(2)	158
OH15	O12(-x,-y,2-z)	0.90	1.82	2.698(2)	167
OH15	O16(-x,-y,2-z)	0.90	1.84	2.707(2)	161
OH16	O5(x,y,1-z)	0.89	2.01	2.897(2)	176
OH16	O13(-x,-y,2-z)	0.89	1.88	2.759(2)	169
OH17	O18(-x,-y,1-z)	0.89	2.01	2.866(2)	160
OH17	O13(x,y,1-z)	0.89	1.87	2.754(2)	173
OH18	O3(x,1,y,z)	0.90	2.05	2.867(2)	151
OH18	O19(-x,-y,1-z)	0.89	2.03	2.853(2)	152
OH19	O12(1-x,-y,1-z)	0.89	1.89	2.779(2)	171
OH19	O17(1-x,-y,1-z)	0.86	2.06	2.834(2)	149

6 (labels 25-27 and 28-32 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)

OH25	O4	0.90	1.77	2.645(3)	165
OH25	O11(1-x,1-y,2-z)	0.90	1.84	2.733(3)	174
OH26	O12(1-x,1-y,2-z)	0.90	1.71	2.586(3)	166
OH26	O11	0.89	1.91	2.748(3)	155
OH27	O28(-x,1-y,1-z)	0.90	1.82	2.728(4)	177
OH27	O12(1-x,1-y,2-z)	0.90	2.57	3.298(4)	138
OH28	O26(x,y,z-1)	0.90	1.93	2.824(3)	172
OH28	O31	0.90	1.89	2.777(4)	168
OH29	O31(x,y,1-z)	0.90	2.14	2.940(4)	147
OH29	O32	0.90	1.89	2.776(4)	167
OH30	O11(x,y,z-1)	0.90	1.86	2.751(4)	172
OH30	O28	0.90	2.07	2.857(4)	146
OH31	O4(1-x,1-y,1-z)	0.90	1.85	2.746(4)	173
OH31	O29(1-x,1-y,1-z)	0.90	1.87	2.763(4)	172
OH32	O30(1-x,1-y,1-z)	0.90	1.91	2.808(4)	173
OH32	O30	0.90	2.00	2.815(4)	151

7 (labels 13-17 and 18-21 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)

OH13	O4	0.85	1.78	2.603(3)	163
OH13	O12(x,y,1,z-1)	0.85	2.02	2.860(3)	172
OH14	O12(1-x,1-y,-z)	0.85	1.90	2.752(3)	177
OH14	O11(x,y,1,z-1)	0.85	1.75	2.594(3)	174
OH15	O18(2-x,-y,-z)	0.85	1.89	2.729(3)	167
OH15	O18	0.85	1.90	2.739(3)	168
OH16	O20	0.85	1.87	2.713(5)	174
OH16	O14(2-x,-y,-z-1)	0.85	1.97	2.814(3)	177
OH17	O11(2-x,1-y,-z)	0.85	1.90	2.739(3)	169
OH17	O21(x+1,y,z)	0.84	2.02	2.784(8)	150
OH18	O19	0.85	1.96	2.807(4)	176
OH18	O4(1-x,-y,-z)	0.85	1.87	2.719(3)	179
OH19	O12(x+1,y,z)	0.86	1.99	2.842(4)	180
OH19	O20(x,y+1,z+1)	0.86	2.16	2.854(6)	138
OH20	O19(2-x,-y,-z)	0.89	2.72	3.520(8)	150
OH20	O13(1-x,-y-1,-z-1)	0.85	2.56	3.379(5)	162

8 (labels 19-22 and 23-28 refer to coordinated and non-coordinated water, respectively; labels 2,4,11 and 12 represent carboxylate O-atoms)

OH19	O11	0.90	1.86	2.749(2)	171
OH19	O12(1-x,-y,-z)	0.90	1.74	2.633(2)	170
OH20	O11(1-x,-y,-z)	0.90	1.87	2.756(2)	172
OH20	O4	0.90	1.81	2.667(2)	158
OH21	O23	0.89	1.88	2.772(2)	177
OH21	O24	0.89	2.00	2.824(2)	153
OH22	O27(x+1,y,z)	0.89	1.92	2.804(2)	170
OH22	O26(x+1,y,z)	0.89	1.96	2.842(2)	170
OH23	O25(1-z,1-y,1-z)	0.89	1.89	2.772(2)	173
OH24	O28	0.89	1.86	2.739(3)	167
OH24	O2	0.89	1.89	2.735(3)	157
OH25	O12(1-x,-y,1-z)	0.90	1.87	2.765(2)	173
OH25	O27	0.89	1.99	2.868(2)	169
OH26	O11	0.90	1.91	2.803(2)	176
OH26	O23	0.90	2.00	2.897(2)	176
OH27	O4(1-x,-y,-z)	0.90	1.90	2.788(2)	166
OH27	O24(x-1,y,z)	0.90	1.95	2.802(3)	157
OH28	O25	0.89	1.92	2.803(2)	172
OH28	O26	0.89	1.99	2.855(2)	162
