

A Hydrogen-bonded and π - π Assembled 3D Supramolecular Network, [Co(en)₃] \cdot 1.5(C₅O₅), with 1D Microporous Hydrophilic Channels Showing Reversible Water ad/de-sorption Property

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Supplementary Materials :

STable 1. The N–H...O and O–H...O hydrogen bonds for **1**.

SFigure 1. TG measurements of cyclic ethanol (EtOH) de- and re-solvation processes were repeated three times.

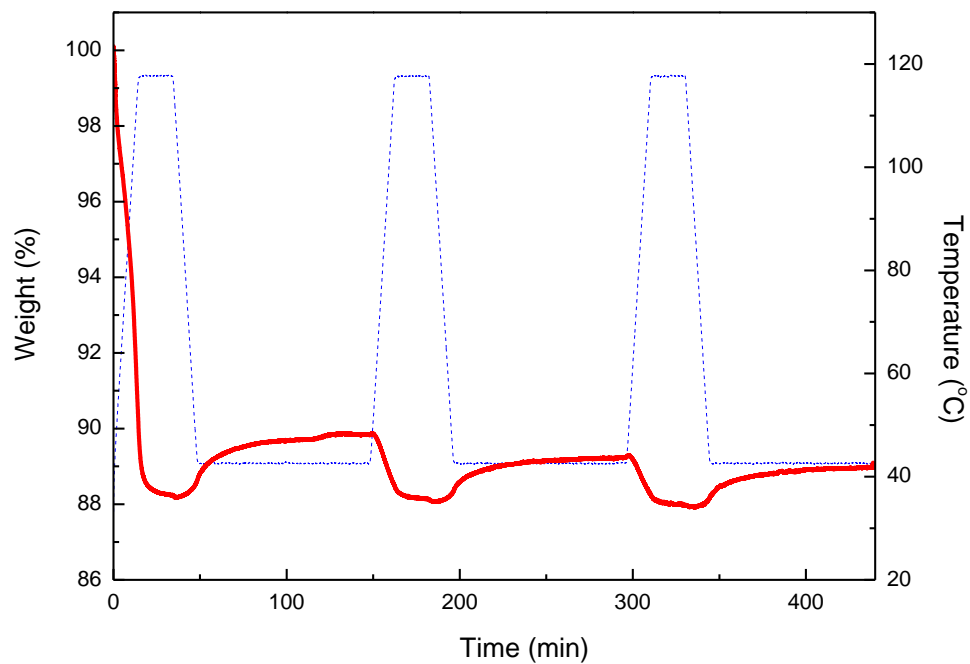
SFigure 2. Simulated PXRD pattern of **1** from single-crystal x-ray diffraction data and *in-situ* temperature-dependent powder XRD of **1** at various temperatures.

SFigure 3. N₂ Gas adsorption-desorption isotherms for **1** at 77 K.

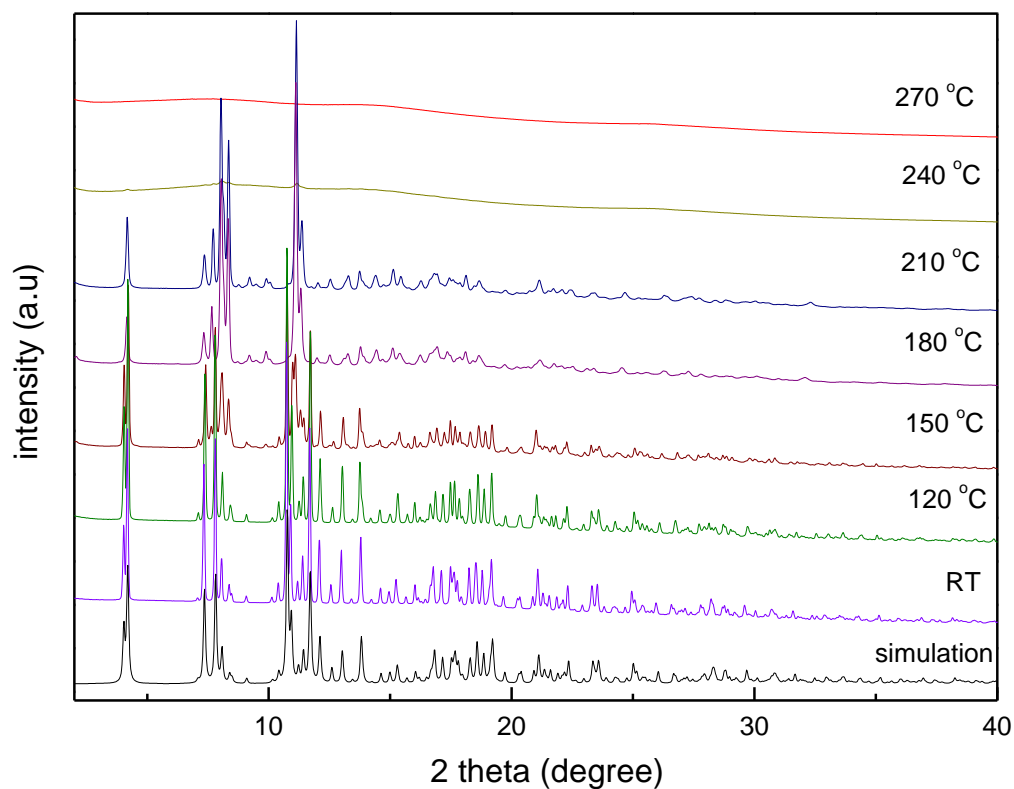
Table 1. The N–H...O and O–H...O hydrogen bonds for **1**^a.

D–H...A (°)	D–H (Å)	H...A (Å)	D...A (Å)	∠ D–H...A (°)
N(1)–H(1A)...O(4) _(ii)	0.92	2.15	2.9854	151
N(1)–H(1B)...O(2)	0.92	2.10	2.9697	156
N(2)–H(2A)...O(9)	0.92	2.10	2.9892	163
N(2)–H(3B)...O(8) _(iii)	0.92	2.20	3.0594	155
N(3)–H(3A)...O(7) _(iv)	0.92	2.17	2.9987	149
N(3)–H(3B)...O(7)	0.92	2.08	2.9486	158
N(4)–H(4A)...O(1) _(v)	0.92	2.13	2.9305	144
N(4)–H(4B)...O(1)	0.92	2.38	3.0364	128
N(4)–H(4B)...O(4) _(ii)	0.92	2.21	2.9464	136°
N(5)–H(5A)...O(11)	0.92	2.24	3.0812	153
N(5)–H(5B)...O(1)	0.92	2.10	2.9858	161
N(5)–H(5B)...O(2)	0.92	2.53	2.9778	110°
N(6)–H(6A)...O(5) _(v)	0.92	1.98	2.8277	152
N(6)–H(6B)...O(6)	0.92	1.93	2.8289	165
O(9)–H(9C)...O(11)	0.87	2.39	3.1840	152
O(9)–H(9D)...O(12)	0.87	2.10	2.7581	132
O(10)–H(10D)...O(6)	0.85	2.47	3.0261	124
O(10)–H(10D)...O(6) _(i)	0.85	2.37	3.0261	134°
O(11)–H(11C)...O(12)	1.00	1.78	2.4475	121
O(11)–H(11D)...O(12) _(vii)	0.95	1.82	2.6407	142
C(9)–H(9B)...O(7) _(iv)	0.99	2.55	3.5168	165
C(11)–H(11B)...O(4) _(ii)	0.99	2.42	3.1495	130
C(13)–H(13B)...O(3) _(vi)	0.99	2.51	3.0624	115
C(14)–H(14A)...O(9)	0.99	2.54	3.4788	159

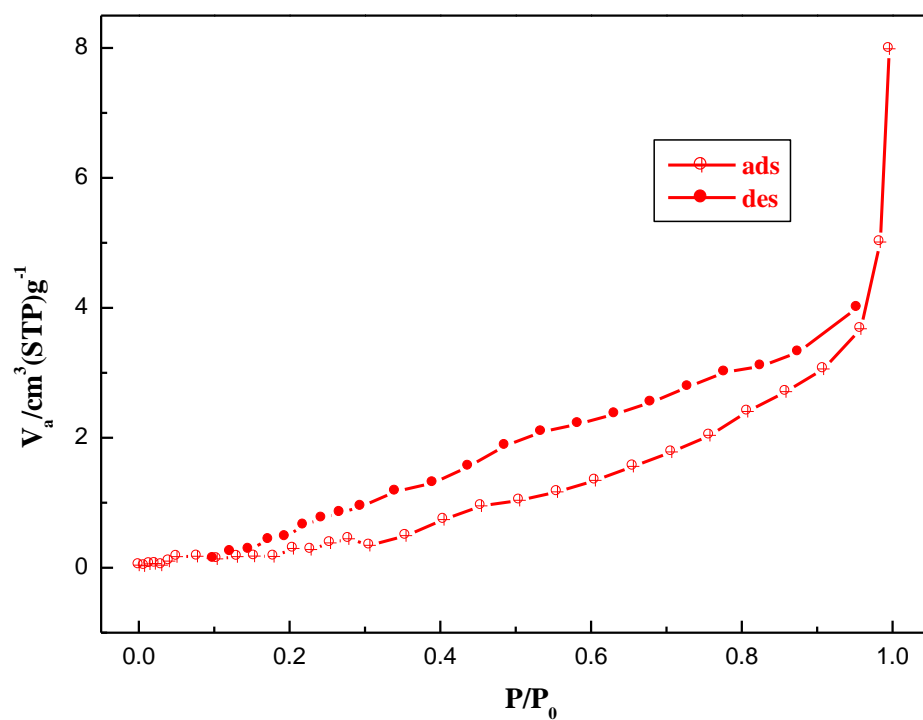
^aSymmetry operations used to generate equivalent atoms: (i) -x, y, 3/2-z (ii) 1/2-x, 1/2-y, -z (iii) -x, -y, 1-z (iv) x, -y, -1/2+z (v) 1/2-x, 1/2-y, 1-z (vi) x, y, 1+z (vii) x, 1-y, -1/2+z



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SFigure 2. Simulated PXRD pattern of **1** from single-crystal x-ray diffraction data and *in-situ* temperature-dependent powder XRD of **1** at various temperatures.



SFigure 3. N_2 Gas adsorption-desorption isotherms for 1 at 77 K.