Supporting Information

Synthesis, Crystal Structures and, Magnetic and Photoluminescent Properties of Lanthanide-based Metal-organic Frameworks Constructed with 2,5-dihydroxybenzene-1, 4-dicarboxylic acid

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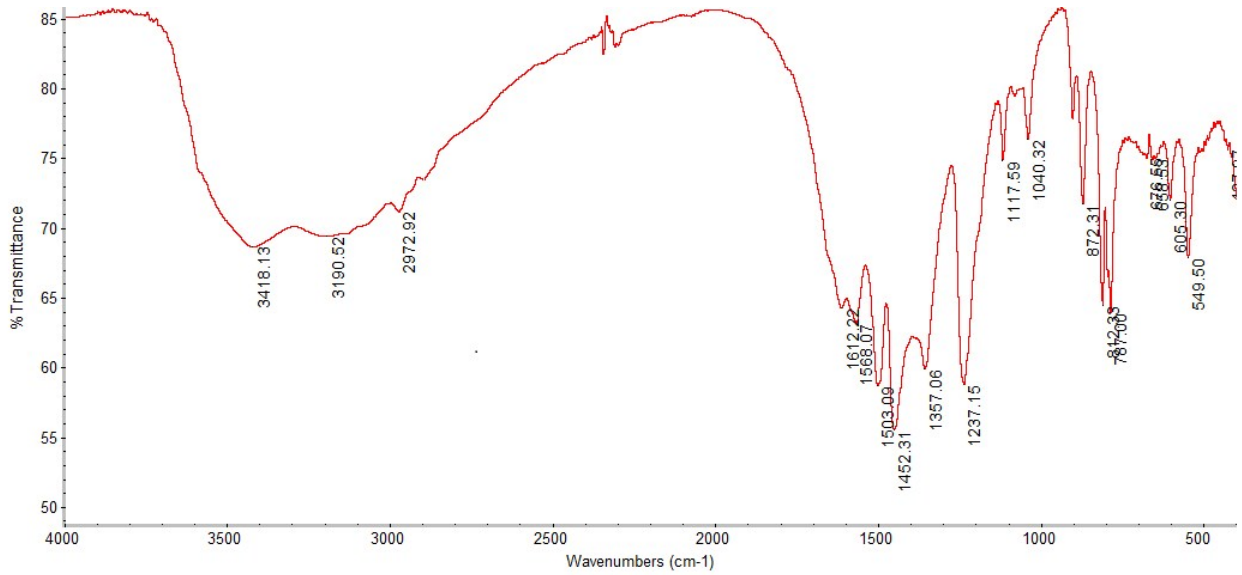

Figure S1. FTIR spectrum of $[Eu(C_8H_4O_6)_{1.5}(H_2O)_2]_n.3n(C_2H_6O).nH_2O$ *n*, **2**

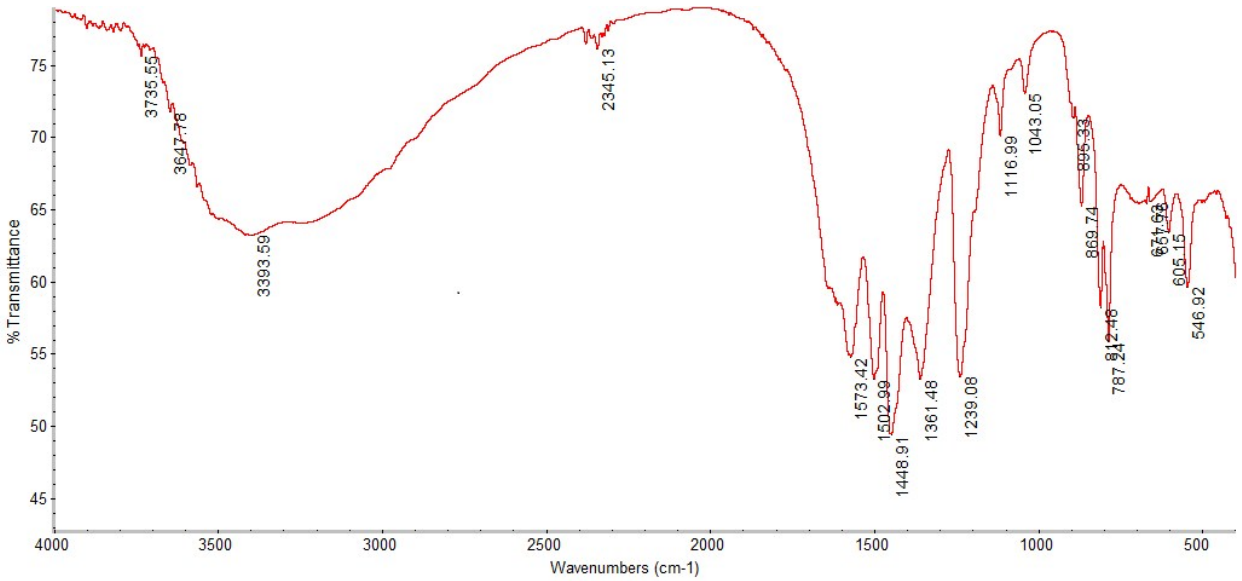

Figure S2. FTIR spectrum of $[Gd(C_8H_4O_6)_{1.5}(H_2O)_2]_n.3n(C_2H_6O).nH_2O$ *n*, **3**

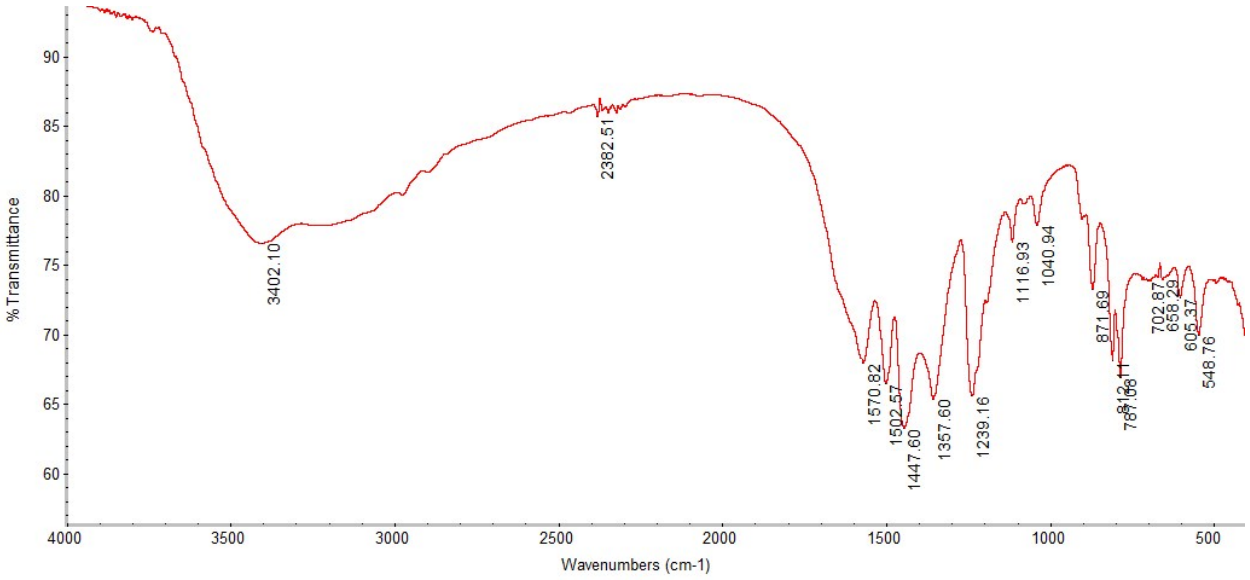

Figure S3. FTIR spectrum of $[Tb(C_8H_4O_6)_{1.5}(H_2O)_2]_n.3n(C_2H_6O).nH_2O_n$, **4**

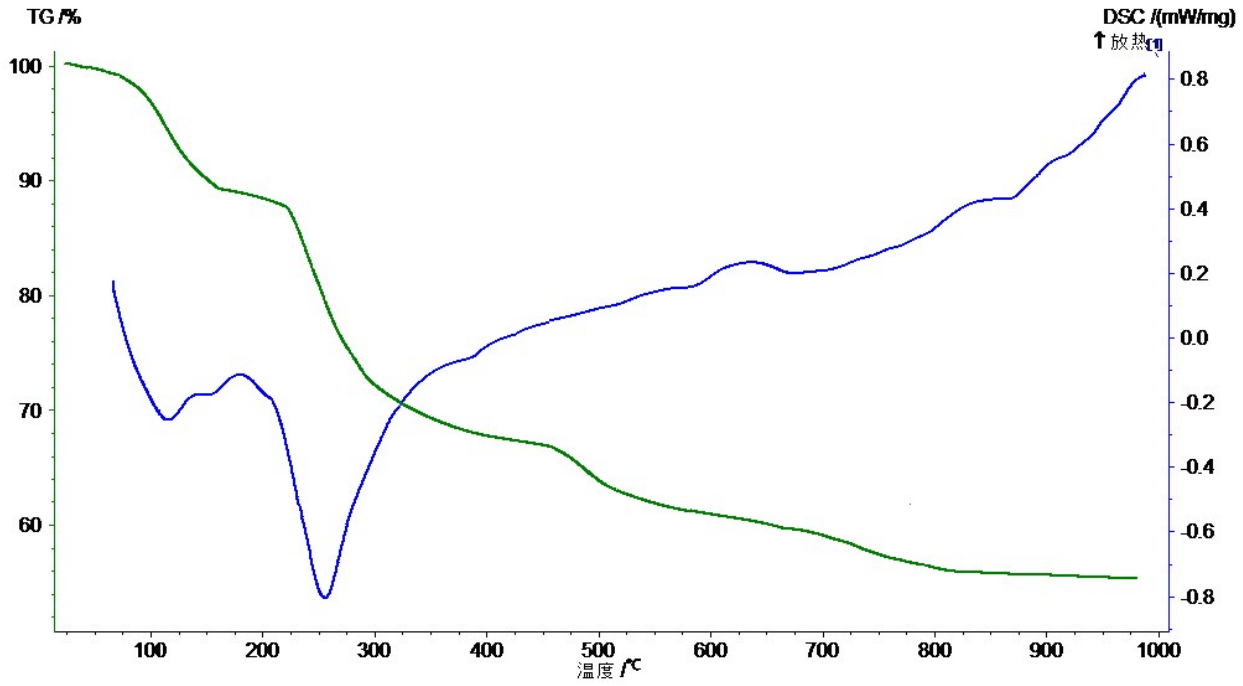

Figure S4. TG-DSC curves of $[Ce(C_8H_4O_6)Cl(H_2O)_3]_n$, **1**

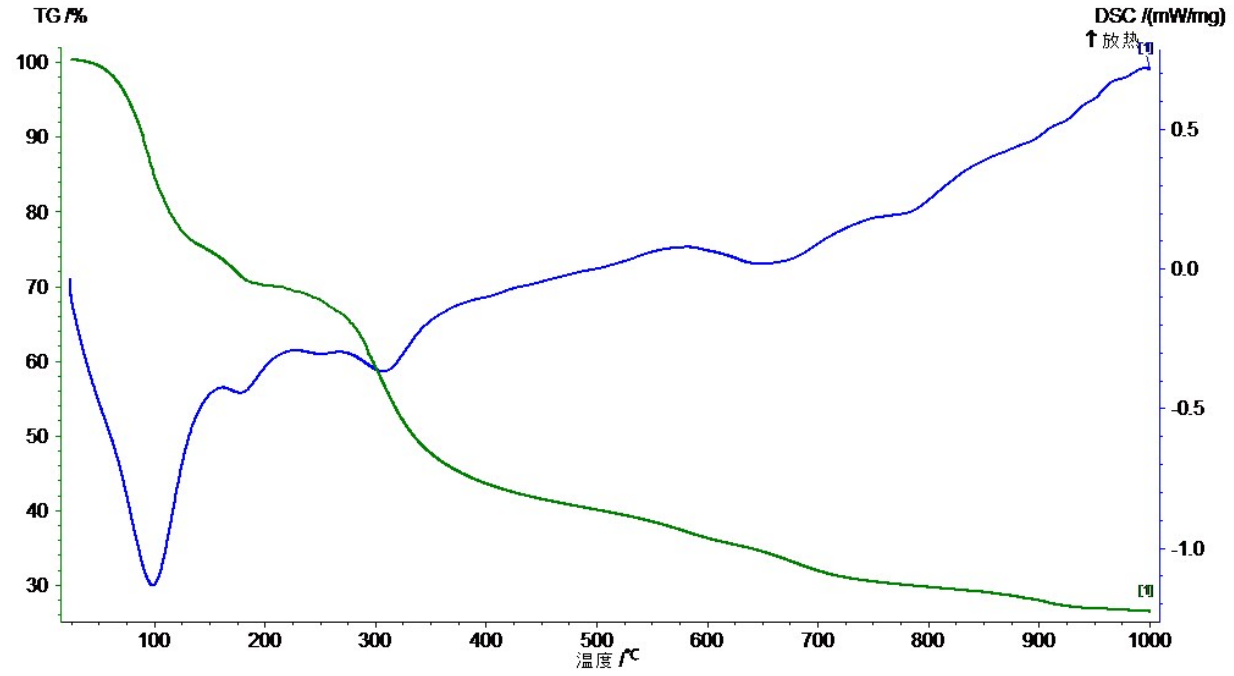

Figure S5. TG-DSC curves of $[Eu(C_8H_4O_6)_{1.5}(H_2O)_2]_n.3n(C_2H_6O).nH_2O_n$, **2**

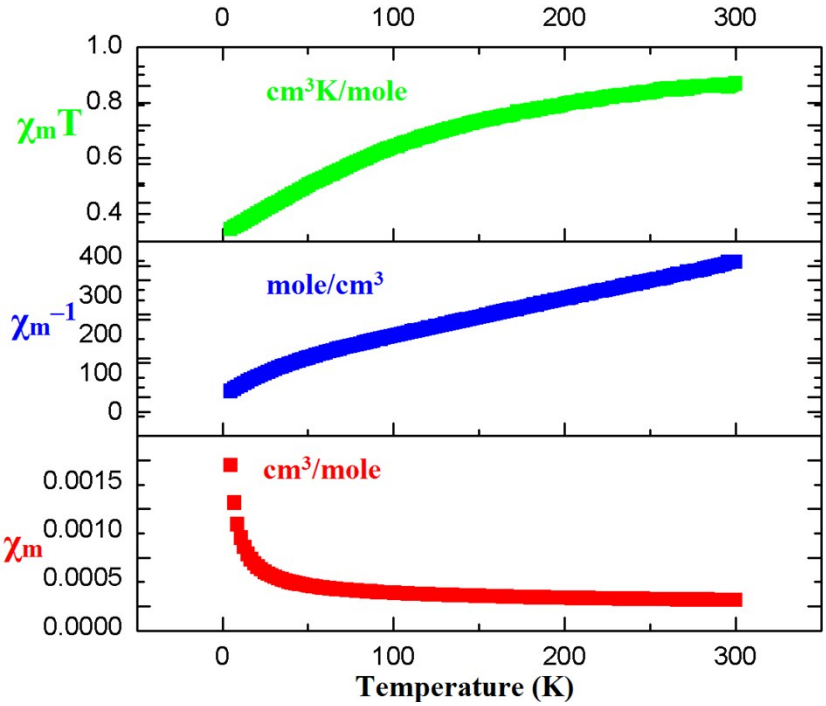

Figure S6 Temperature dependence of χ_m, χ_m^{-1} and $\chi_m T$ for **1** at an applied field of 2 KOe.

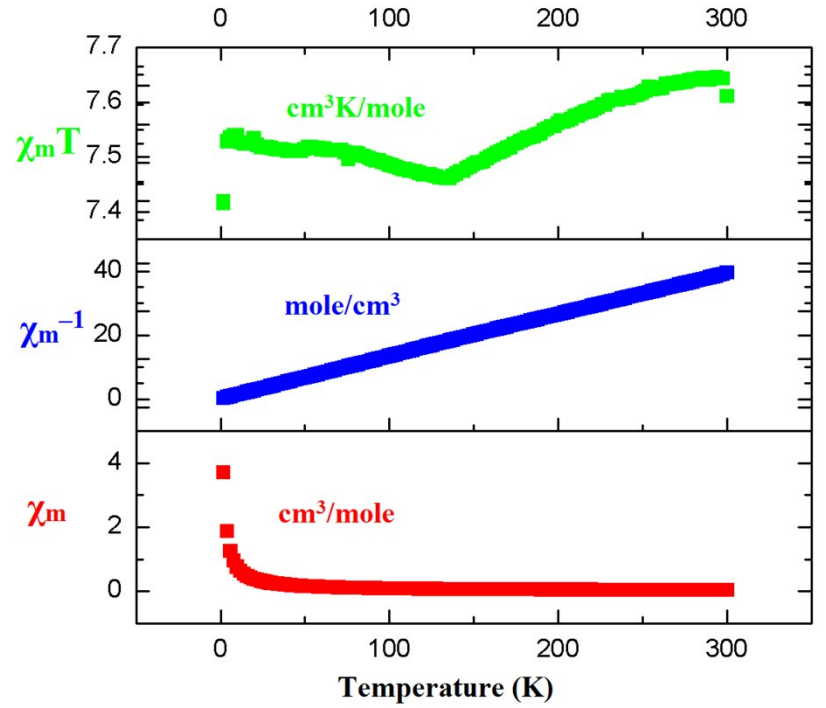

Figure S7 Temperature dependence of χ_m, χ_m^{-1} and $\chi_m T$ for **3** at an applied field of 2 KOe.

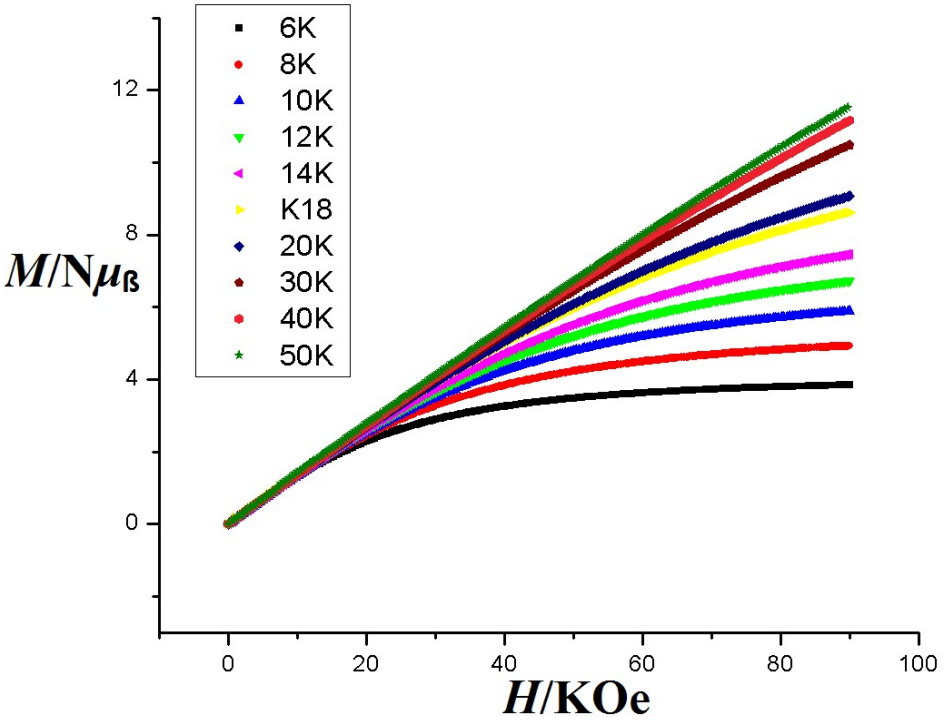

Figure S8 Magnetization *M* versus field *H* of **4** in the range 0-90 kOe.

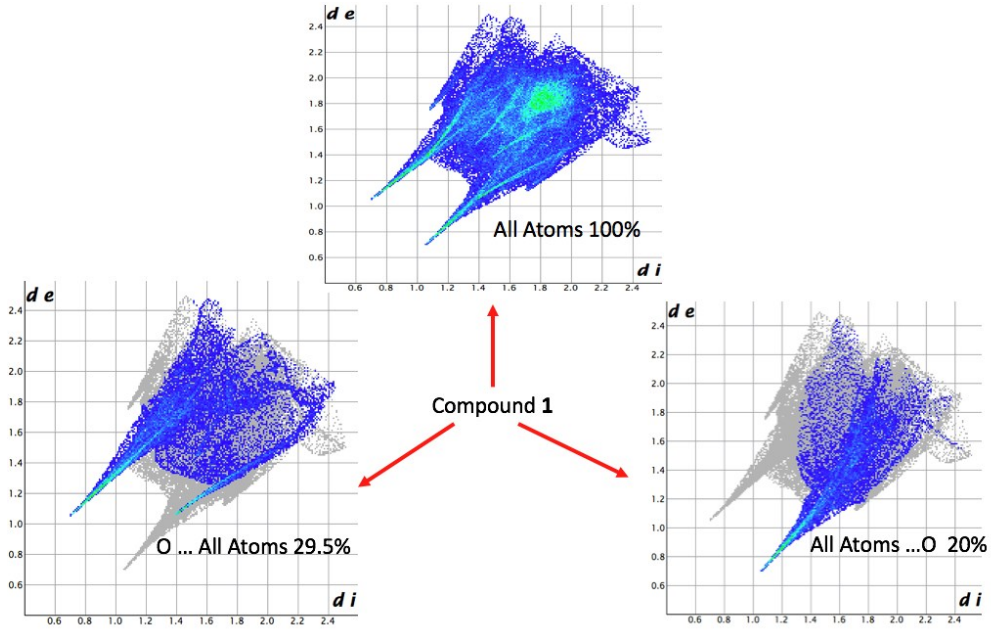

Figure S9. Fingerprint plots of total specific pairs of intermolecular interactions for **1**

Table S1: key crystal data for complexes **1**–**4**.

	1	**2**	**3**	**4**
Emp. formula	$C_8H_{10}CeClO_9$	$C_{18}H_{30}EuO_{15}$	$C_{18}H_{30}GdO_{15}$	$C_{18}H_{30}O_{15}Tb$
M_r	425.73	638.38	643.67	645.34
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$ (No. 2)	$P2_1/n$ (No. 14)	$P2_1/n$ (No. 14)	$P2_1/n$ (No. 14)
a (Å)	6.9439 (3)	12.5345 (2)	12.53408 (13)	12.52570 (12)
b (Å)	9.7400 (4)	14.4309 (2)	14.43816 (18)	14.44759 (14)
c (Å)	10.3973 (4)	14.2786 (2)	14.25451 (16)	14.23151 (13)
α (°)	63.431 (4)	90	90	90
β (°)	77.659 (4)	106.3480 (10)	106.5332 (12)	106.7894 (10)
γ (°)	73.969 (4)	90	90	90
V (Å^3)	601.15 (5)	2478.35 (6)	2472.97 (5)	2465.64 (4)
Z	2	4	4	4
Data scanned	6012	14122	20744	17599
Unique data	2291	4720	4756	4797
R_{Int}	0.056	0.034	0.037	0.031
$R(F)$	0.029	0.033	0.025	0.029
$wR(F^2)$	0.065	0.088	0.059	0.074
CCDC dep. No.	1937367	1937368	1937369	1937370

Table S2: Geometric parameters of hydrogen bonds for **1**.

O5–H5...O4	0.82	1.88	2.593 (4)	145
O6–H6...O1	0.82	1.84	2.551 (4)	144
O7–H1w...O5^{iii}	0.93	1.81	2.735 (4)	173
O7–H2w...O6^{iv}	0.94	1.93	2.843 (5)	164
O8–H3w...O6^{v}	0.91	2.07	2.923 (4)	156
O8–H4w...O1^{vi}	0.85	2.03	2.825 (5)	156
O9–H5w...O1^{vii}	0.90	1.88	2.774 (4)	172
O9–H6w...O3^{viii}	0.88	2.07	2.842 (4)	147
C5–H5A...Cl1^{ix}	0.93	2.98	3.851 (4)	156

Symmetry codes: (i) –*x*, 1–*y*, 1–*z*; (ii) *x*, *y*–1, *z*+1; (iii) –*x*, 1–*y*, 2–*z*; (iv) *x*, *y*, *z*+1; (v) *x*–1, *y*, *z*+1; (vi) –*x*, –*y*, 2–*z*; (vii) 1–*x*, –*y*, 2–*z*; (viii) 1–*x*, 1–*y*, 1–*z*; (ix) *x*, *y*, *z*–1.

Table S3: Geometric parameters of hydrogen bonds for **2.**

O5–H5...O3	0.82	1.85	2.576 (4)	147
O6–H6...O2	0.82	1.82	2.548 (4)	146
O9–H9...O7^{i}	0.82	1.78	2.516 (4)	147
O10–H10a...O14	0.93	1.85	2.753 (5)	164
O10–H10b...O12	0.85	1.90	2.742 (4)	170
O11–H11a...O13	0.84	1.85	2.682 (5)	169
O11–H11b...O15	0.91	1.92	2.734 (7)	148
O11–H11b...O15a	0.91	1.87	2.749 (15)	162
O12–H12a...O9^{ii}	0.90	1.93	2.825 (4)	170
O12–H12b...O6^{iii}	0.87	1.95	2.777 (4)	159
O13–H13...O9^{ii}	0.84	1.99	2.824 (5)	173
O14–H14...O12^{iv}	0.84	2.01	2.812 (5)	159
O15–H15...O14^{ii}	0.84	2.10	2.910 (8)	163
O15a–H15a...O14^{ii}	0.84	2.17	2.775 (17)	129
C2–H2...O7	0.95	2.51	3.323 (4)	144
C16–H16a...O5^{v}	0.99	2.62	3.235 (8)	121
C17–H17a...O6^{vi}	0.98	2.60	3.533 (12)	160
C18–H18a...O8^{ii}	0.99	2.54	3.327 (10)	136
C17a–H17e...O2^{vi}	0.98	2.37	3.35 (2)	175

Symmetry codes: (i) 1–*x*, 1–*y*, –*z*; (ii) 1½–*x*, *y*–½, ½–*z*; (iii) *x*+1, *y*, *z*; (iv) 2–*x*, 1–*y*, 1–*z*; (v) 1½–*x*, ½+*y*, ½–*z*; (vi) ½+*x*, ½–*y*, *z*–½.

Table S4: Geometric parameters of hydrogen bonds for **3**

O5–H5...O3	0.82	1.86	2.578 (3)	146
O6–H6...O2	0.82	1.82	2.548 (3)	146
O9–H9...O7^{iv}	0.82	1.78	2.513 (3)	147
O10–H10a...O14	0.93	1.85	2.754 (4)	164
O10–H10b...O12	0.85	1.90	2.747 (3)	170
O11–H11a...O13	0.84	1.85	2.679 (3)	168
O11–H11b...O15	0.91	1.92	2.729 (5)	148
O11–H11b...O15a	0.91	1.85	2.732 (12)	163
O12–H12a...O9^{v}	0.90	1.93	2.820 (3)	170
O12–H12b...O6^{vi}	0.87	1.95	2.782 (3)	159
O13–H13...O9^{v}	0.84	1.99	2.824 (4)	173
O14–H14...O12^{vii}	0.84	1.99	2.801 (4)	162
O15–H15...O14^{v}	0.84	2.08	2.899 (6)	163
O15a–H15a...O14^{v}	0.84	2.23	2.808 (12)	126
C2–H2...O7	0.95	2.51	3.320 (3)	143
C18–H18a...O8^{v}	0.99	2.53	3.326 (7)	137
C17a–H17e...O2^{viii}	0.98	2.42	3.399 (19)	176

Symmetry codes: (i) ½–*x*, ½+*y*, ½–*z*; (ii) ½+*x*, ½–*y*, ½ +*z*; (iii) 1–*x*, 1–*y*, 1–*z*; (iv) 1–*x*, 1–*y*, –*z*; (v) 1½–*x*, *y*–½, ½–*z*; (vi) *x*+1, *y*, *z*; (vii) 2–*x*, 1–*y*, 1–*z*; (viii) *x*+½ , ½–*y*, *z*–½.

Table S5: Geometric parameters of hydrogen bonds for **4**

O5–H5...O3	0.82	1.86	2.577 (3)	146
O6–H6...O2	0.82	1.83	2.553 (3)	146
O9–H9...O7^{iv}	0.82	1.79	2.516 (3)	147
O10–H10a...O14	0.93	1.85	2.752 (4)	163
O10–H10b...O12	0.85	1.91	2.754 (3)	171
O11–H11a...O13	0.84	1.86	2.686 (4)	168
O11–H11b...O15	0.91	1.92	2.728 (6)	148
O11–H11b...O15a	0.91	1.85	2.732 (13)	162
O12–H12a...O9^{v}	0.90	1.93	2.829 (3)	170
O12–H12b...O6^{vi}	0.87	1.95	2.786 (3)	159
O13–H13...O9^{v}	0.84	1.99	2.827 (4)	173
O14–H14...O12^{vii}	0.84	1.99	2.802 (4)	164
O15–H15...O14^{v}	0.84	2.05	2.891 (6)	175
O15a–H15a...O14^{v}	0.84	2.23	2.803 (14)	126
C2–H2...O7	0.95	2.51	3.319 (4)	143
C17–H17a...O6^{viii}	0.98	2.57	3.498 (10)	158
C18–H18a...O8^{v}	0.99	2.51	3.317 (8)	138
C17a–H17e...O2^{viii}	0.98	2.42	3.403 (18)	177

Symmetry codes: (i) ½–*x*, ½+*y*, ½–*z*; (ii) ½+*x*, ½–*y*, ½ +*z*; (iii) 1–*x*, 1–*y*, 1–*z*; (iv) 1–*x*, 1–*y*, –*z*; (v) 1½–*x*, *y*–½, ½–*z*; (vi) *x*+1, *y*, *z*; (vii) 2–*x*, 1–*y*, 1–*z*; (viii) *x*+½ , ½–*y*, *z*–½.