Supplementary Information

New Metal-Organic Systems with a Functionalized Oxamate-Type Ligand and Mn^{II}, Fe^{II}, Cu^{II} and Zn^{II}

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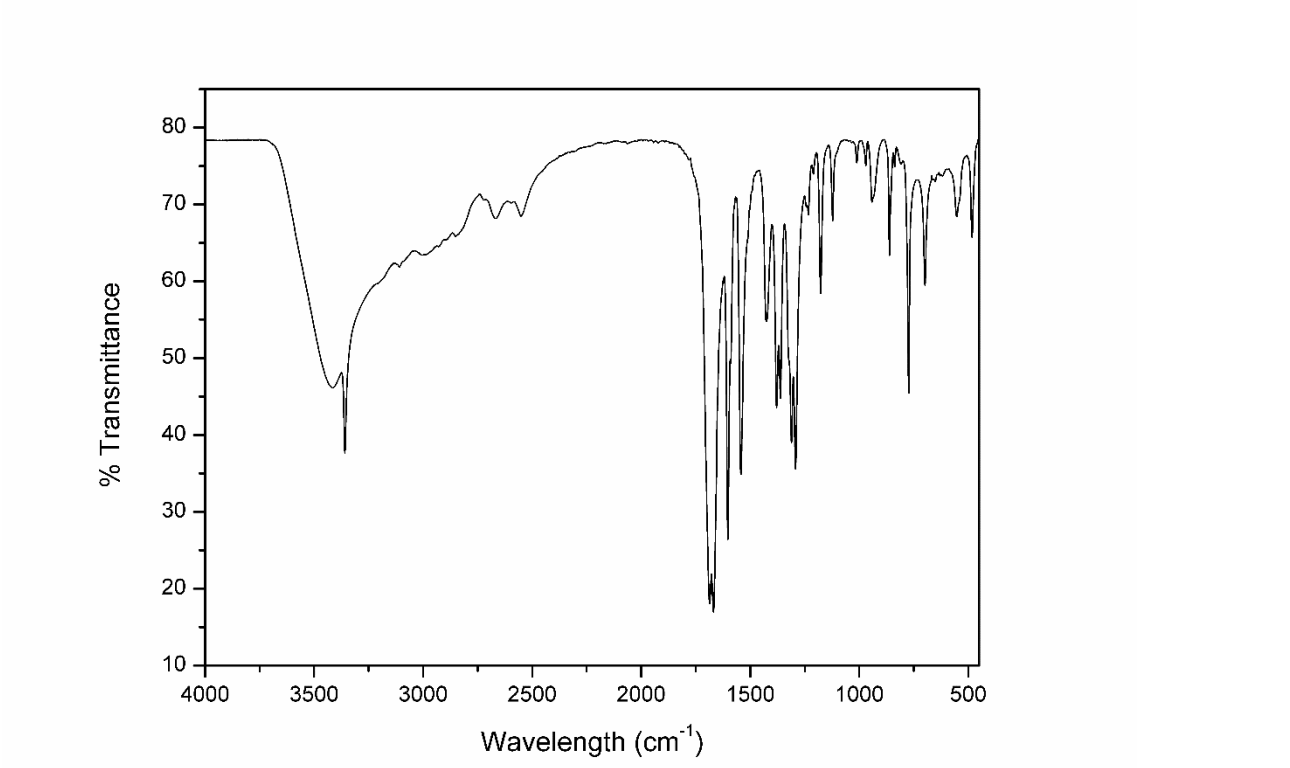

Figure S1. FTIR (KBr) spectrum of compound **1**.

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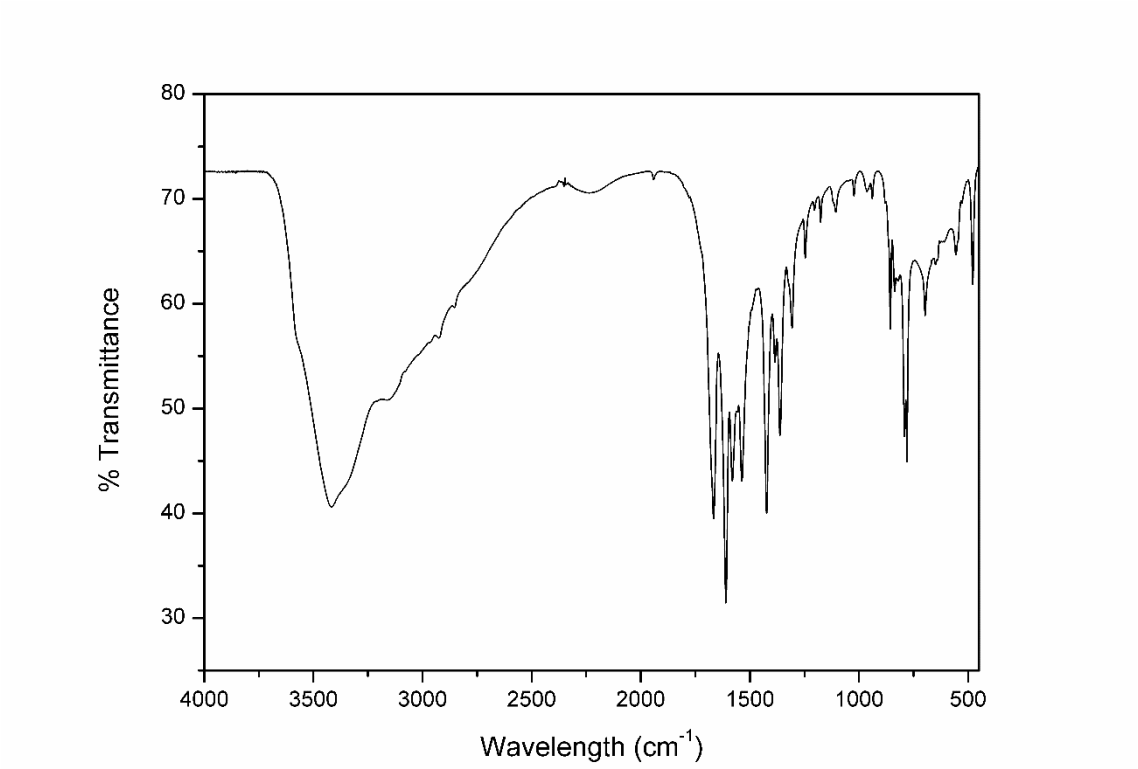

Figure S2. FTIR (KBr) spectrum of compound **2**.

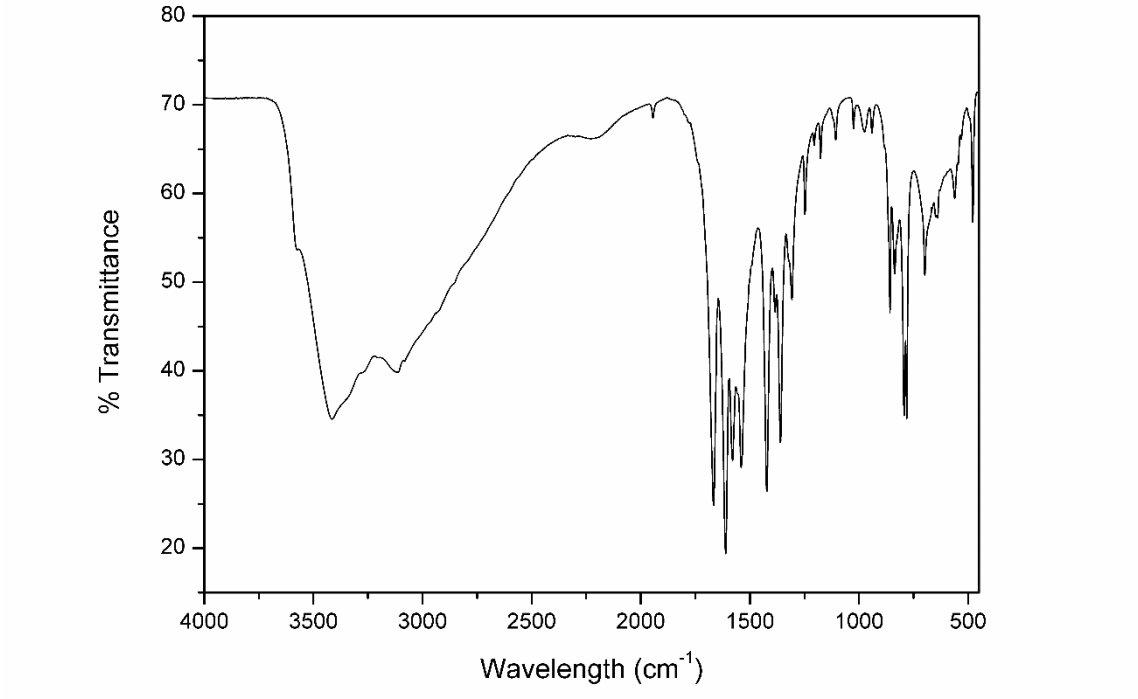

Figure S3. FTIR (KBr) spectrum of compound **3**.

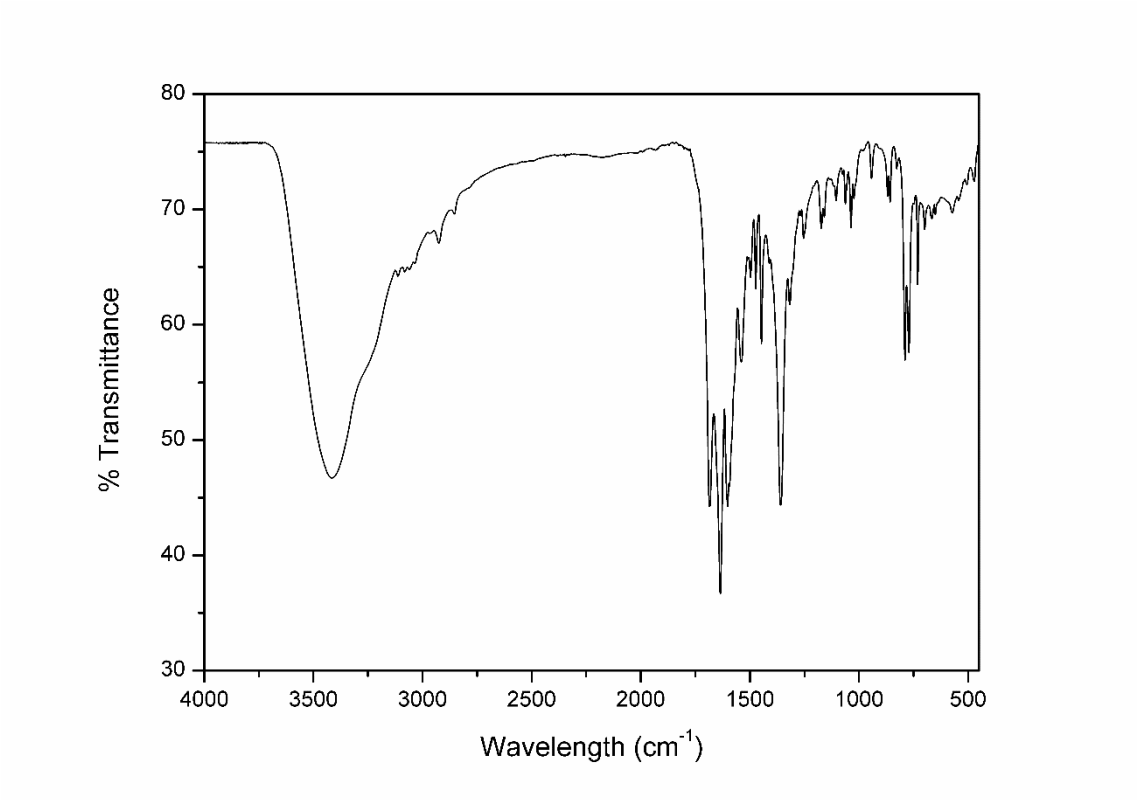

Figure S4. FTIR (KBr) spectrum of compound **4**.

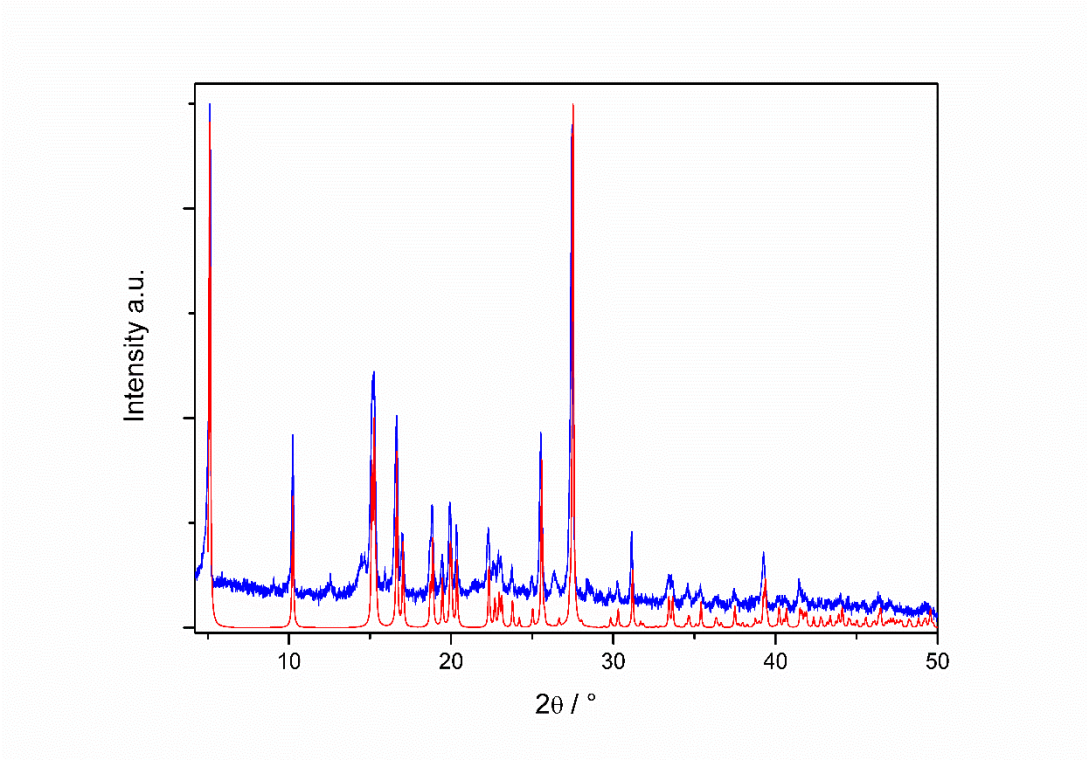

Figure S5. Calculated (solid red line) and experimental (solid blue line) PXRD pattern for compound **1**.

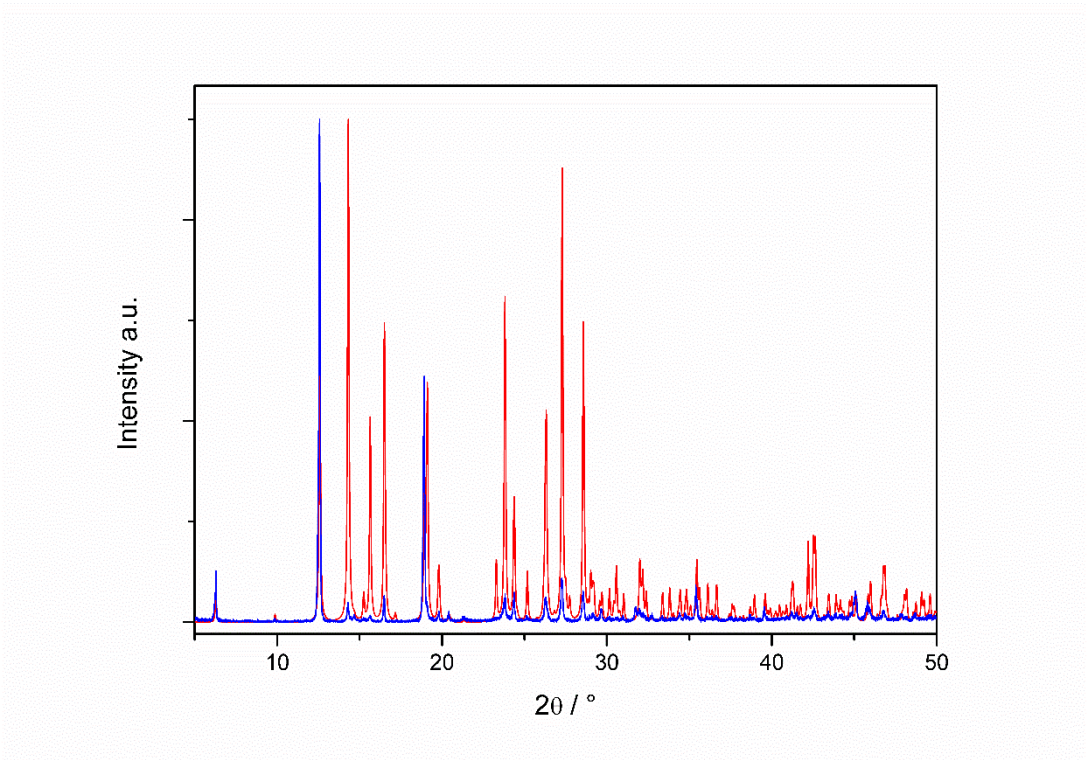

Figure S6. Calculated (solid red line) and experimental (solid blue line) PXRD pattern for compound **2**.

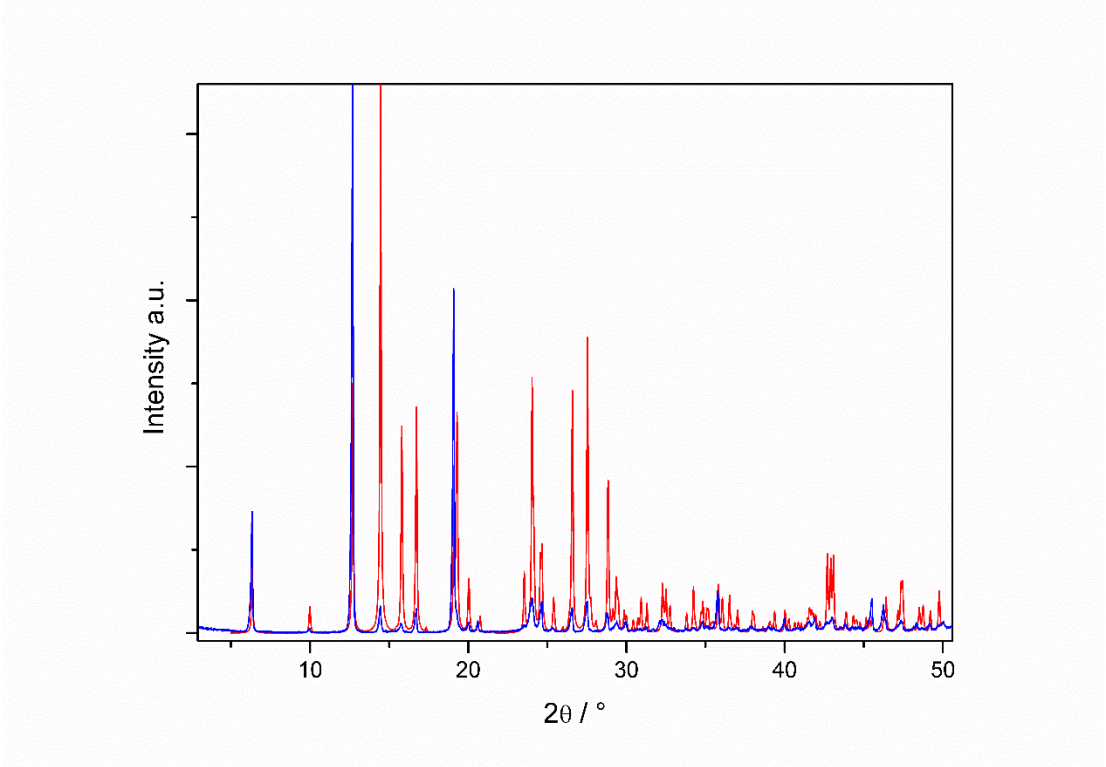

Figure S7. Calculated (solid red line) and experimental (solid blue line) PXRD pattern for compound **3**.

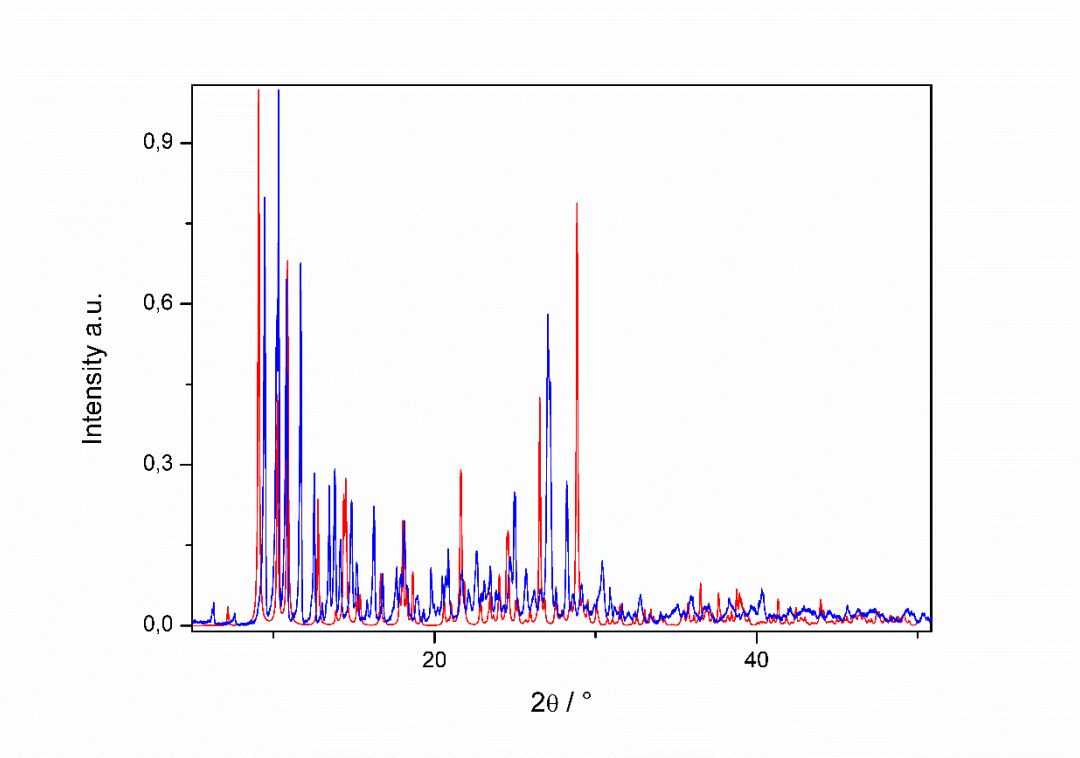

Figure S8. Calculated (solid red line) and experimental (solid blue line) PXRD pattern for compound **4**.

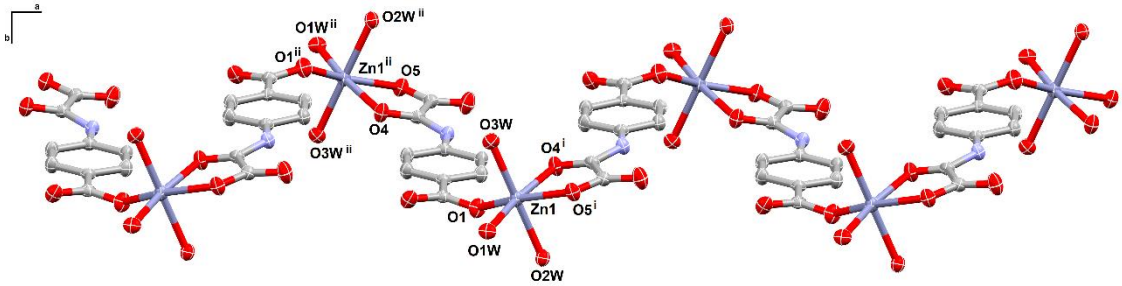

Figure S9. View of a fragment of the neutral zigzag chain of compound **3** running parallel to the crystallographic *a* axis (symmetry code: (i) = ½ + *x*, ½ – *y*,1 – *z*; (ii) = –½ + *x*, ½ – *y*, 1 – *z*).

Table S1. Hydrogen bonds and C–H···O type interactions in **1-4**[a-d]

	D–H···A	D–H / Å	H···A / Å	D···A / Å	D–H···A / degree
1	$N_1–H_{1N}···O_3$	0.86	2.28	2.689(6)	109
	$O_1–H_{1C}···O_2^{i}$	0.82	1.83	2.645(5)	170
	$O_{1W}–H_{1WA}···O_5^{ii}$	0.99	2.05	2.783(6)	129
	$O_{1W}–H_{1WB}···O_3^{iii}$	0.99	1.76	2.744(6)	174
	$O_{1W}–H_{1WB}···O_5^{iii}$	0.99	2.54	3.214(7)	125
2	$N_1–H_{1N}···O_{2W}^{i}$	0.86	2.13	2.981(7)	173
	$O_{1W}–H_{1WA}···O_{4W}^{ii}$	0.99	2.31	3.290(9)	172
	$O_{1W}–H_{1WB}···O_5^{iii}$	1.00	1.73	2.697(6)	162
	$O_{2W}–H_{2WA}···O_2^{iv}$	1.00	1.73	2.661(7)	155
	$O_{2W}–H_{2WB}···O_3^{v}$	0.99	1.99	2.733(7)	130
	$O_{3W}–H_{3WA}···O_2^{vi}$	0.99	1.67	2.650(7)	170
	$O_{3W}–H_{3WB}···O_{1W}^{vi}$	0.99	2.04	2.937(7)	149
	$O_{4W}–H_{4WA}···O_{3W}$	0.99	1.95	2.820(7)	144
	$O_{4W}–H_{4WB}···O_3^{vii}$	0.85	2.22	3.051(5)	164
3	$N_1–H_{1N}···O_{2W}^{i}$	0.86	2.09	2.945(3)	171
	$O_{1W}–H_{1WA}···O_{4W}^{ii}$	0.82	2.52	3.271(5)	157
	$O_{1W}–H_{1WB}···O_5^{iii}$	1.00	1.70	2.696(4)	174
	$O_{2W}–H_{2WA}···O_2^{iv}$	0.99	1.74	2.668(4)	154
	$O_{2W}–H_{2WB}···O_3^{v}$	0.99	1.96	2.770(4)	138
	$O_{3W}–H_{3WA}···O_2^{vi}$	1.00	1.65	2.642(4)	173
	$O_{3W}–H_{3WB}···O_{1W}^{vi}$	0.99	2.06	2.936(3)	146
	$O_{4W}–H_{4WA}···O_{3W}$	0.99	1.92	2.829(4)	152
	$O_{4W}–H_{4WB}···O_3^{vii}$	0.99	2.37	3.055(3)	126

Table S1. Hydrogen bonds and C–H···O type interactions in **1**-**4**[a-d] (cont.)

	D–H···A	D–H / Å	H···A / Å	D···A / Å	D–H···A / degree
	N_1–H_{1N}···O_{1W}^{i}	0.86	2.08	2.912(12)	163
	O_{1W}–H_{1WA}···O_3^{ii}	0.96	2.66	3.099(12)	107
	O_{1W}–H_{1WA}···O_3^{iii}	0.96	2.10	2.805(11)	126
4	O_{1W}–H_{1WB}···O_{2W}	0.99	1.96	2.930(17)	164
	O_{2W}–H_{2WA}···O_{3W}^{iv}	0.99	2.00	2.901(19)	153
	O_{2W}–H_{2WB}···O_2^{v}	1.00	1.89	2.844(14)	160
	O_{3W}–H_{3WB}···O_1^{vi}	0.99	2.07	2.877(12)	136
	O_{3W}–H_{3WB}···O_2^{vi}	0.99	2.52	3.175(17)	122
	O_{4W}–H_{4WA}···O_{1W}^{i}	0.99	2.54	2.89(2)	100
	C_4–H_4···O_{1W}^{i}	0.93	2.54	3.305(12)	140
	C_7–H_7···$O4_W^{vi}$	0.93	2.68	3.54(2)	156
	C_{11}–H_{11}···O_{4W}^{vii}	0.93	2.53	3.42(2)	159
	C_{13}–H_{13}···O_{3W}^{iv}	0.93	2.46	3.144(19)	130
	C_{19}–H_{19}···O_{3W}^{viii}	0.93	2.57	3.124(15)	118

D: donor; A: acceptor; [a]symmetry code for **1**: (i) = 1 – *x*, –*y*, –*z*; (ii) = –1 + *x*, *y*, *z*; (iii) = 1 – *x*, 1 –*y*, 1 – *z*; [b]symmetry code for **2** and **3**: (i) = ½ – *x*, –½ – *y*, *z*; (ii) = *x*, –1 – *y*, *z*; (iii) = ½ – *x*, ½ – *y*, ½ + *z*; (iv) = ½ – *x*, –½ + *y*, *z*; (v) = –*x*, –*y*, 1 – *z*; (vi) = ½ – *x*, ½ + *y*, *z*; (vii) = –*x*, 1 – *y*, 1 – *z*; [c]symmetry code for **4**: (i) = 1 + *x*, *y*, *z*; (ii) = 1 – *x*, 1 – *y*, 2 – *z*; (iii) = *x*, –1 + *y*, *z*; (iv) = 1 – *x*, 1 – *y*, 1 – *z*; (v) = 1 – *x*, –*y*, 2 – *z*; (vi) = 2 – *x*, 1 – *y*, 2 – *z*; (vii) = *x*, –1 + *y*, *z*; (viii) = 1 – *x*, 2 – *y*, 1 – *z*.

Table S2. Energy of all calculated excited states and their contributions to the *D* and *E* values for **1** obtained from CASSCF/NEVPT2 calculations

Energy[a]	S	D / cm^{-1}	E / cm^{-1}
1097.2	2	–9.657	–0.444
2238.5	2	1.582	–0.918
10195.4	2	-0.619	0.123
12377.9	2	–0.108	0.134
14887.7	1	–0.046	0.306
15388.6	1	–0.026	–0.019
15436.1	1	–0.912	–0.257
18826.1	1	–0.153	0.092
20563.8	1	0.152	0.030
21515.6	1	0.024	–0.002
23688.3	1	–0.003	0.005
24080.3	1	–0.102	–0.017
24421.4	1	0.113	0.015
24786.0	1	–0.024	–0.005
26030.6	1	0.022	0.001
26158.4	1	–0.004	–0.001
26479.3	1	–0.018	–0.011
26615.9	1	–0.171	–0.008
26658.8	1	0.128	0.000
26798.9	1	–0.122	0.084
28571.2	1	0.029	–0.043
30279.8	1	0.012	–0.015
30922.7	1	–0.314	–0.023
31499.0	1	0.160	–0.296

S: spin values; *D*: axial zero-field splitting; *E*: rhombic zero-field splitting.