Supporting Information

Ammonium 18-crown-6 complexes with tetrahedral monoanions: X-ray, thermal and comparative analysis of non-covalent interactions

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Contents

Single-crystal X-Ray diffraction (SCXRD)

Table S1. Crystal data and structure refinement for 1-8.

Identification code	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
CCDC number	2402192	2402193	2402214	2402213	2402216	2402217	2402215	2402194
Empirical formula	$C_{24}H_{56}B_2F_8N_2O_{12}$	$C_{24}H_{56}Cr_2F_2N_2O_{18}$	$C_{12}H_{28}ClCrNO_9$	$C_{12}H_{28}NO_9CrBr$	$C_{12}H_{28}NO_{10}Re$	$C_{24}H_{56}N_2O_{21}Tc_2$	$C_{24}H_{58}N_4O_{19}Os_2$	$C_{24}H_{56}Cl_{0.54}N_2O_{20}Re_{1.47}$
Formula weight	738.32	802.70	417.80	462.26	532.55	904.70	1087.14	984.45
Temperature/K	293(2)	293	100(2)	100(2)	100(2)	100(2)	100(2)	293.00
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$
a/Å	21.944(2)	21.8531(9)	12.122(8)	12.5047(16)	11.9350(10)	21.319(3)	21.3399(10)	22.0112(6)
b/Å	8.6178(4)	8.6797(2)	8.382(4)	8.4814(11)	8.4168(7)	8.7279(12)	8.7503(4)	8.6959(2)
c/Å	22.319(2)	22.7358(10)	19.288(9)	18.594(2)	19.2915(16)	22.956(3)	23.0341(10)	22.8383(6)
α/°	90	90	90	90	90	90	90	90
β/°	118.390(13)	118.234(5)	98.899(19)	91.268(5)	100.906(3)	117.557(5)	117.467(2)	117.983(4)
γ/°	90	90	90	90	90	90	90	90
Volume/Å^3	3713.1(7)	3799.4(3)	1936.3(18)	1971.5(4)	1902.9(3)	3786.8(9)	3816.3(3)	3860.3(2)
Z	4	4	4	4	4	4	4	4
ρ_{calc}g/cm^3	1.321	1.403	1.433	1.557	1.859	1.587	1.892	1.694
μ/mm^{-1}	0.126	0.653	0.770	2.647	6.432	0.810	6.730	4.710
F(000)	1568.0	1696.0	880.0	952.0	1048.0	1872.0	2136.0	1972.0
Crystal size/mm^3	0.09 × 0.07 × 0.05	0.09 × 0.07 × 0.05	0.11 × 0.04 × 0.03	0.4 × 0.05 × 0.02	0.4 × 0.28 × 0.2	0.4 × 0.08 × 0.06	0.3 × 0.2 × 0.12	0.07 × 0.04 × 0.03
Radiation	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.382 to 54.998	7.124 to 55	8.346 to 49.992	8.354 to 49.99	8.29 to 59.996	8.512 to 49.998	8.484 to 54.998	7.058 to 50
Index ranges	-28 ≤ h ≤ 28, -11 ≤ k ≤ 10, -	-28 ≤ h ≤ 28, -11 ≤ k ≤ 11, -	-14 ≤ h ≤ 14, -8 ≤ k ≤ 9, -22	-14 ≤ h ≤ 14, -10 ≤ k ≤ 8, -	-16 ≤ h ≤ 16, -10 ≤ k ≤ 11, -	-25 ≤ h ≤ 25, -9 ≤ k ≤ 10, -27	-27 ≤ h ≤ 27, -11 ≤ k ≤ 9, -	-26 ≤ h ≤ 26, -10 ≤ k ≤ 10, -

	28 ≤ l ≤ 28	29 ≤ l ≤ 29	≤ l ≤ 22	22 ≤ l ≤ 22	26 ≤ l ≤ 27	≤ l ≤ 27	29 ≤ l ≤ 29	26 ≤ l ≤ 27
Reflections collected	40197	71415	28215	28086	27752	57659	67667	61670
Independent reflections	8511 [R_{int} = 0.0388, R_{sigma} = 0.0368]	8713 [R_{int} = 0.0482, R_{sigma} = 0.0333]	3385 [R_{int} = 0.2483, R_{sigma} = 0.1696]	3437 [R_{int} = 0.1625, R_{sigma} = 0.1065]	5512 [R_{int} = 0.0594, R_{sigma} = 0.0487]	6656 [R_{int} = 0.1518, R_{sigma} = 0.0938]	8730 [R_{int} = 0.0684, R_{sigma} = 0.0445]	6772 [R_{int} = 0.0455, R_{sigma} = 0.0221]
Data/restraints/parameters	8511/32/465	8713/8/465	3385/4/233	3437/21/229	5512/21/229	6656/94/466	8730/94/466	6772/12/448
Goodness-of-fit on F^2	1.068	1.051	1.001	1.001	1.008	1.016	1.025	1.092
Final R indexes [I>=2σ (I)]	R_1 = 0.0919, wR_2 = 0.2820	R_1 = 0.0501, wR_2 = 0.1465	R_1 = 0.0665, wR_2 = 0.1296	R_1 = 0.0624, wR_2 = 0.1274	R_1 = 0.0288, wR_2 = 0.0547	R_1 = 0.0525, wR_2 = 0.1063	R_1 = 0.0309, wR_2 = 0.0521	R_1 = 0.0636, wR_2 = 0.1829
Final R indexes [all data]	R_1 = 0.1321, wR_2 = 0.3154	R_1 = 0.0736, wR_2 = 0.1618	R_1 = 0.1748, wR_2 = 0.1754	R_1 = 0.1366, wR_2 = 0.1569	R_1 = 0.0445, wR_2 = 0.0593	R_1 = 0.1039, wR_2 = 0.1277	R_1 = 0.0487, wR_2 = 0.0571	R_1 = 0.0681, wR_2 = 0.1870
Largest diff. peak/hole / e $Å^{-3}$	0.78/-0.38	0.74/-0.50	0.46/-0.63	0.64/-0.77	1.56/-1.68	1.01/-0.89	2.01/-1.53	1.71/-0.71

Table S2. Bond Lengths for **1.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
F8	B2	1.376(4)		O10	C21	1.438(7)
O4	C8	1.438(5)		O11	C23	1.431(7)
O4	C9	1.390(5)		O11	C22	1.422(7)
O2	C4	1.450(5)		F3	B1	1.389(5)
O2	C5	1.397(5)		F1	B1	1.357(5)
O3	C7	1.416(5)		F5	B2	1.395(6)
O3	C6	1.430(5)		F6	B2	1.339(5)
O1	C3	1.388(5)		F7	B2	1.327(5)
O1	C2	1.460(5)		F4	B1	1.340(5)
O7	C15	1.428(5)		F2	B1	1.346(6)
O7	C14	1.397(5)		C8	C7	1.456(7)
O5	C10	1.428(5)		C9	C10	1.471(7)
O5	C11	1.403(5)		C15	C16	1.444(7)
O6	C1	1.401(5)		C4	C3	1.479(7)
O6	C12	1.429(5)		C6	C5	1.489(7)
O8	C17	1.429(6)		C2	C1	1.438(6)
O8	C16	1.414(5)		C12	C11	1.460(7)

O12	C13	1.454(6)		C13	C14	1.442(7)
O12	C24	1.403(6)		C17	C18	1.463(8)
O9	C18	1.433(6)		C24	C23	1.490(9)
O9	C19	1.422(6)		C19	C20	1.449(9)
O10	C20	1.421(7)		C21	C22	1.439(9)

Table S3. Bond Angles for **1.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C9	O4	C8	112.3(3)		C14	C13	O12	110.1(4)
C5	O2	C4	113.7(3)		O8	C17	C18	109.7(3)
C7	O3	C6	112.6(3)		O7	C14	C13	109.3(4)
C3	O1	C2	113.4(3)		O9	C18	C17	109.3(4)
C14	O7	C15	112.4(3)		O12	C24	C23	108.7(4)
C11	O5	C10	114.5(3)		O5	C11	C12	109.6(4)
C1	O6	C12	112.5(3)		F1	B1	F3	109.2(4)
C16	O8	C17	111.5(4)		F4	B1	F3	106.9(4)
C24	O12	C13	114.5(4)		F4	B1	F1	110.9(4)
C19	O9	C18	113.7(4)		F4	B1	F2	113.7(5)
C20	O10	C21	113.3(5)		F2	B1	F3	105.1(4)
C22	O11	C23	114.3(5)		F2	B1	F1	110.7(4)
O4	C8	C7	110.6(3)		O11	C23	C24	108.4(4)
O4	C9	C10	109.7(3)		O8	C16	C15	109.6(3)
O3	C7	C8	109.2(3)		F8	B2	F5	109.2(4)
O7	C15	C16	108.8(3)		F6	B2	F8	111.6(3)
O2	C4	C3	109.7(3)		F6	B2	F5	105.0(4)
O5	C10	C9	109.9(3)		F7	B2	F8	108.7(3)
O3	C6	C5	109.3(3)		F7	B2	F5	108.6(4)
O1	C3	C4	109.3(3)		F7	B2	F6	113.6(5)
C1	C2	O1	110.8(3)		O9	C19	C20	109.9(4)
O6	C1	C2	110.1(3)		O10	C20	C19	109.6(4)
O2	C5	C6	108.4(3)		O10	C21	C22	110.6(4)
O6	C12	C11	110.1(4)		O11	C22	C21	109.8(4)

Table S4. Hydrogen Bonds for **1.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C10	H10B	F4	0.97	2.73	3.363(6)	123.5
C17	H17A	F5[1]	0.97	2.68	3.337(6)	125.1
N2	H2C	F8	1.020(10)	2.04(2)	2.994(4)	154(4)
N2	H2C	F7	1.020(10)	2.14(3)	2.985(4)	139(4)
N1	H1C	O1	1.020(10)	1.867(15)	2.878(4)	170(6)
N2	H2D	O9	1.020(10)	1.840(14)	2.848(4)	169(4)
N2	H2E	O7	1.021(10)	1.867(19)	2.861(3)	164(5)
N1	H1D	F6	1.018(10)	2.47(3)	3.383(5)	149(3)

N1	H1D	F7	1.018(10)	2.15(3)	3.010(4)	141(3)
N2	H2F	O11	1.023(10)	1.846(19)	2.837(4)	162(4)
N1	H1E	O3	1.024(10)	1.901(16)	2.912(4)	168(5)
N1	H1F	O5	1.020(10)	1.841(18)	2.827(4)	162(4)

[1]1-X,2-Y,1-Z

Table S5. Torsion Angles for **1.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O4	C8	C7	O3	-69.8(4)		C6	O3	C7	C8	-177.3(3)
O4	C9	C10	O5	62.0(4)		C3	O1	C2	C1	-177.1(3)
O2	C4	C3	O1	-66.6(4)		C2	O1	C3	C4	-177.8(3)
O3	C6	C5	O2	63.0(4)		C1	O6	C12	C11	179.6(4)
O1	C2	C1	O6	68.7(4)		C5	O2	C4	C3	-177.4(3)
O7	C15	C16	O8	-68.5(4)		C12	O6	C1	C2	-175.1(3)
O6	C12	C11	O5	-61.3(5)		C13	O12	C24	C23	-175.8(4)
O8	C17	C18	O9	65.8(5)		C17	O8	C16	C15	177.0(4)
O12	C13	C14	O7	68.0(5)		C14	O7	C15	C16	-179.1(3)
O12	C24	C23	O11	-67.4(5)		C18	O9	C19	C20	-177.5(4)
O9	C19	C20	O10	-63.2(5)		C24	O12	C13	C14	-176.2(4)
O10	C21	C22	O11	68.8(5)		C11	O5	C10	C9	170.5(4)
C8	O4	C9	C10	178.6(3)		C23	O11	C22	C21	173.3(4)
C9	O4	C8	C7	173.8(3)		C16	O8	C17	C18	178.5(4)
C7	O3	C6	C5	-175.5(3)		C19	O9	C18	C17	177.2(4)
C15	O7	C14	C13	177.8(3)		C20	O10	C21	C22	-176.6(4)
C4	O2	C5	C6	173.7(3)		C21	O10	C20	C19	179.1(4)
C10	O5	C11	C12	-170.4(4)		C22	O11	C23	C24	177.2(4)

Table S6. Bond Lengths for **8.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Re1	O14	1.660(7)		O9	C17	1.434(13)
Re1	O15	1.669(9)		O9	C16	1.419(12)
Re1	O13	1.633(7)		O4	C6	1.395(11)
Re1	O16	1.658(8)		O4	C7	1.416(11)
Cl2	O17	1.503(7)		O5	C9	1.369(12)
Cl2	O19	1.516(9)		O5	C8	1.460(11)
Cl2	O20	1.547(8)		O8	C14	1.432(13)
Cl2	O18	1.474(10)		O8	C15	1.443(14)
O11	C21	1.389(10)		O7	C13	1.433(13)
O11	C20	1.443(10)		O7	C24	1.402(12)
O2	C3	1.393(10)		C3	C4	1.482(13)
O2	C2	1.469(10)		C21	C22	1.498(15)
O6	C10	1.450(10)		C2	C1	1.454(15)
O6	C11	1.394(12)		C10	C9	1.491(15)
O10	C18	1.439(11)		C23	C24	1.490(16)
O10	C19	1.434(11)		C18	C17	1.441(15)

O3	C4	1.406(11)		C20	C19	1.398(14)
O3	C5	1.426(11)		C11	C12	1.486(16)
O12	C23	1.403(11)		C14	C13	1.433(15)
O12	C22	1.443(11)		C6	C5	1.465(15)
O1	C12	1.459(11)		C15	C16	1.458(19)
O1	C1	1.403(11)		C8	C7	1.450(16)

Table S7. Bond Angles for **8.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O14	Re1	O15	108.4(5)		O2	C3	C4	109.0(6)
O13	Re1	O14	109.1(4)		O11	C21	C22	107.9(7)
O13	Re1	O15	110.7(5)		C1	C2	O2	109.6(7)
O13	Re1	O16	110.6(4)		O6	C10	C9	109.0(7)
O16	Re1	O14	108.8(4)		O12	C23	C24	108.2(8)
O16	Re1	O15	109.3(6)		O5	C9	C10	109.9(7)
O17	Cl2	O19	109.7(5)		O3	C4	C3	110.5(7)
O17	Cl2	O20	105.4(4)		O10	C18	C17	109.8(8)
O19	Cl2	O20	110.7(7)		C19	C20	O11	110.2(7)
O18	Cl2	O17	112.7(5)		O6	C11	C12	109.2(7)
O18	Cl2	O19	109.5(5)		O12	C22	C21	109.4(7)
O18	Cl2	O20	108.6(5)		C20	C19	O10	111.5(7)
C21	O11	C20	112.7(7)		O8	C14	C13	110.9(9)
C3	O2	C2	112.2(7)		C14	C13	O7	110.8(10)
C11	O6	C10	113.3(7)		O4	C6	C5	110.4(7)
C19	O10	C18	113.4(7)		O3	C5	C6	110.1(7)
C4	O3	C5	114.7(7)		O8	C15	C16	111.0(8)
C23	O12	C22	112.3(7)		O1	C12	C11	109.0(7)
C1	O1	C12	113.1(7)		C7	C8	O5	110.4(7)
C16	O9	C17	113.2(8)		O7	C24	C23	109.9(8)
C6	O4	C7	112.3(7)		O1	C1	C2	109.9(7)
C9	O5	C8	113.6(7)		O9	C17	C18	109.9(8)
C14	O8	C15	114.5(8)		O4	C7	C8	109.6(8)
C24	O7	C13	115.6(8)		O9	C16	C15	108.8(8)

Table S8. Hydrogen Bonds for **8.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2	H2C	O11	1.02	1.91	2.863(7)	152.8
N2	H2D	O7	1.02	1.87	2.871(8)	165.5
N2	H2E	O20	1.02	2.05	3.004(10)	154.2
N2	H2F	O9	1.02	1.83	2.844(8)	172.4
N1	H1D	O5	1.02	1.91	2.891(8)	159.1
N1	H1E	O2	1.02	2.28	3.039(8)	130.0
N1	H1E	O3	1.02	1.98	2.820(8)	137.5
N1	H1F	O6	1.02	2.24	2.950(8)	124.7
N1	H1F	O1	1.02	1.99	2.896(8)	145.7

Table S9. Torsion Angles for **8**.

A	B	C	D	Angle/°		A	B	C	D	Angle/°

O11	C21	C22	O12	68.0(9)		C4	O3	C5	C6	-171.7(8)
O11	C20	C19	O10	-69.3(9)		C18	O10	C19	C20	179.3(7)
O2	C3	C4	O3	61.5(9)		C20	O11	C21	C22	177.5(6)
O2	C2	C1	O1	-69.1(9)		C11	O6	C10	C9	-178.3(7)
O6	C10	C9	O5	-68.1(9)		C22	O12	C23	C24	-175.3(7)
O6	C11	C12	O1	64.1(10)		C19	O10	C18	C17	-178.7(8)
O10	C18	C17	O9	65.9(10)		C14	O8	C15	C16	-178.4(8)
O12	C23	C24	O7	-65.5(10)		C13	O7	C24	C23	176.1(9)
O4	C6	C5	O3	-61.3(10)		C6	O4	C7	C8	-176.2(7)
O5	C8	C7	O4	69.0(9)		C5	O3	C4	C3	172.1(7)
O8	C14	C13	O7	67.0(12)		C15	O8	C14	C13	-175.4(8)
O8	C15	C16	O9	-63.9(9)		C12	O1	C1	C2	-176.2(7)
C3	O2	C2	C1	173.5(7)		C8	O5	C9	C10	-178.7(7)
C21	O11	C20	C19	177.9(7)		C24	O7	C13	C14	172.3(8)
C2	O2	C3	C4	179.1(6)		C1	O1	C12	C11	-175.7(7)
C10	O6	C11	C12	175.5(7)		C17	O9	C16	C15	-179.8(7)
C23	O12	C22	C21	-175.4(7)		C7	O4	C6	C5	180.0(7)
C9	O5	C8	C7	-178.7(7)		C16	O9	C17	C18	176.6(7)

Table S10. Bond Lengths for **2.**

Atom	**Atom**	**Length/Å**		**Atom**	**Atom**	**Length/Å**
Cr1	O16	1.635(2)		O9	C19	1.436(4)
Cr1	O15	1.649(2)		O9	C18	1.406(4)
Cr1	O14	1.617(2)		O8	C16	1.410(4)
Cr1	O13	1.628(3)		O8	C17	1.434(4)
Cr2	F1	1.712(2)		O10	C20	1.394(4)
Cr2	O17	1.605(2)		O10	C21	1.439(4)
Cr2	O18	1.611(2)		O5	C10	1.430(5)
Cr2	O19	1.612(2)		O5	C11	1.418(4)
O2	C5	1.398(4)		O4	C9	1.420(4)
O2	C4	1.426(4)		O4	C8	1.429(4)
O6	C1	1.418(4)		C5	C6	1.474(5)
O6	C12	1.416(4)		C13	C14	1.469(5)
O1	C3	1.414(4)		C16	C15	1.485(5)
O1	C2	1.431(4)		C3	C4	1.465(5)
O3	C6	1.429(4)		C20	C19	1.490(5)
O3	C7	1.414(4)		C1	C2	1.464(5)
O12	C13	1.425(4)		C18	C17	1.482(5)
O12	C24	1.417(4)		C22	C21	1.468(5)
O11	C22	1.409(4)		C7	C8	1.468(6)
O11	C23	1.424(4)		C24	C23	1.479(5)
O7	C14	1.413(3)		C12	C11	1.470(6)
O7	C15	1.428(4)		C10	C9	1.470(6)

Table S11. Bond Angles for **2.**

Atom	**Atom**	**Atom**	**Angle/°**		**Atom**	**Atom**	**Atom**	**Angle/°**
O16	Cr1	O15	110.11(14)		O2	C5	C6	109.1(3)
O14	Cr1	O16	110.09(14)		O12	C13	C14	109.5(2)

O14	Cr1	O15	108.60(15)		O8	C16	C15	109.3(3)
O14	Cr1	O13	110.83(19)		O7	C14	C13	109.9(2)
O13	Cr1	O16	109.76(17)		O1	C3	C4	109.2(2)
O13	Cr1	O15	107.40(15)		O10	C20	C19	109.4(2)
O17	Cr2	F1	108.95(12)		O2	C4	C3	109.6(2)
O17	Cr2	O18	107.90(13)		O7	C15	C16	109.9(2)
O17	Cr2	O19	111.53(14)		O9	C19	C20	109.0(2)
O18	Cr2	F1	110.16(14)		O6	C1	C2	109.9(3)
O18	Cr2	O19	110.25(17)		O1	C2	C1	110.3(2)
O19	Cr2	F1	108.06(13)		O3	C6	C5	109.5(3)
C5	O2	C4	112.8(2)		O9	C18	C17	108.7(3)
C12	O6	C1	113.0(3)		O11	C22	C21	109.3(3)
C3	O1	C2	111.6(2)		O10	C21	C22	110.0(2)
C7	O3	C6	113.8(3)		O3	C7	C8	109.1(3)
C24	O12	C13	113.2(2)		O12	C24	C23	109.1(3)
C22	O11	C23	111.9(3)		O11	C23	C24	109.9(3)
C14	O7	C15	112.3(2)		O8	C17	C18	109.4(3)
C18	O9	C19	113.3(3)		O6	C12	C11	109.2(3)
C16	O8	C17	113.0(3)		O5	C10	C9	110.2(3)
C20	O10	C21	112.9(2)		O4	C9	C10	109.3(3)
C11	O5	C10	112.7(3)		O4	C8	C7	109.2(3)
C9	O4	C8	114.4(3)		O5	C11	C12	110.0(3)

Table S12. Hydrogen Bonds for **2.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C13	H13A	O14[1]	0.97	2.73	3.389(4)	125.4
C19	H19A	O14[2]	0.97	2.50	3.390(4)	152.7
C2	H2B	F1[3]	0.97	2.68	3.331(4)	125.3
N2	H2C	O18	1.032(2)	2.21(2)	3.029(3)	135(2)
N2	H2D	O12	1.032(2)	1.841(15)	2.838(3)	161(4)
N1	H1C	O2	1.032(2)	1.832(6)	2.861(3)	175(4)
N2	H2E	O8	1.032(2)	1.856(5)	2.887(3)	176(4)
N2	H2F	O10	1.032(2)	1.849(5)	2.879(3)	176(5)
N1	H1D	O4	1.032(2)	1.814(9)	2.835(3)	169(4)
N1	H1E	O6	1.032(2)	1.832(7)	2.858(3)	172(4)
N1	H1F	O17	1.032(2)	2.25(3)	3.120(3)	141(3)
N1	H1F	O18	1.032(2)	2.07(2)	2.967(3)	143(3)

[1]1/2+X,1/2-Y,1/2+Z; [2]1-X,-Y,1-Z; [3]1-X,-Y,2-Z

Table S13. Torsion Angles for **2.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O2	C5	C6	O3	-68.3(3)		C4	O2	C5	C6	-177.7(2)
O6	C1	C2	O1	-65.0(3)		C15	O7	C14	C13	-179.1(2)
O6	C12	C11	O5	64.1(3)		C19	O9	C18	C17	-175.8(3)
O1	C3	C4	O2	69.0(3)		C1	O6	C12	C11	179.9(3)
O3	C7	C8	O4	66.6(4)		C2	O1	C3	C4	-179.1(2)
O12	C13	C14	O7	-62.7(3)		C6	O3	C7	C8	175.3(3)
O12	C24	C23	O11	61.9(4)		C18	O9	C19	C20	177.9(3)

O11	C22	C21	O10	-68.3(3)		C22	O11	C23	C24	-179.7(3)
O9	C18	C17	O8	-64.3(4)		C21	O10	C20	C19	178.1(2)
O8	C16	C15	O7	69.9(3)		C7	O3	C6	C5	174.8(3)
O10	C20	C19	O9	68.6(3)		C24	O12	C13	C14	-173.8(3)
O5	C10	C9	O4	-68.0(4)		C23	O11	C22	C21	177.2(2)
C5	O2	C4	C3	-178.7(2)		C17	O8	C16	C15	177.3(2)
C13	O12	C24	C23	171.9(3)		C12	O6	C1	C2	-177.1(3)
C16	O8	C17	C18	176.1(3)		C10	O5	C11	C12	179.9(3)
C14	O7	C15	C16	-174.2(2)		C9	O4	C8	C7	-177.3(3)
C3	O1	C2	C1	178.5(3)		C8	O4	C9	C10	-171.9(3)
C20	O10	C21	C22	177.5(3)		C11	O5	C10	C9	175.5(3)

Table S14. Bond Lengths for **3.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Cr1	Cl1	2.201(2)		O7	C12	1.425(7)
Cr1	O1	1.600(5)		O8	C3	1.434(7)
Cr1	O2	1.609(5)		O8	C4	1.420(7)
Cr1	O3	1.583(5)		O9	C7	1.420(8)
O4	C8	1.424(7)		O9	C11	1.418(7)
O4	C9	1.421(6)		C1	C5	1.489(9)
O5	C2	1.420(7)		C2	C8	1.512(8)
O5	C5	1.433(6)		C3	C11	1.495(10)
O6	C1	1.424(7)		C4	C12	1.506(8)
O6	C10	1.419(7)		C6	C10	1.490(8)
O7	C6	1.426(6)		C7	C9	1.481(9)

Table S15. Bond Angles for **3.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Cr1	Cl1	106.9(2)		O6	C1	C5	109.7(5)
O1	Cr1	O2	110.7(3)		O5	C2	C8	108.8(5)
O2	Cr1	Cl1	109.6(2)		O8	C3	C11	108.9(5)
O3	Cr1	Cl1	105.9(2)		O8	C4	C12	108.7(5)
O3	Cr1	O1	110.7(3)		O5	C5	C1	109.4(5)
O3	Cr1	O2	112.8(3)		O7	C6	C10	108.7(5)
C9	O4	C8	113.1(5)		O9	C7	C9	108.3(6)
C2	O5	C5	110.6(5)		O4	C8	C2	107.8(5)
C10	O6	C1	113.0(5)		O4	C9	C7	109.4(5)
C12	O7	C6	112.4(5)		O6	C10	C6	109.5(5)
C4	O8	C3	112.3(5)		O9	C11	C3	109.4(6)
C11	O9	C7	111.9(5)		O7	C12	C4	108.1(5)

Table S16. Hydrogen Bonds for **3.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N10	H10C	O6	0.86(2)	2.04(2)	2.889(7)	170(6)
N10	H10D	O8	0.87(2)	2.00(3)	2.865(8)	169(9)
N10	H10E	O1	0.87(2)	2.18(7)	2.860(9)	134(8)
N10	H10E	O3[1]	0.87(2)	2.24(7)	2.904(8)	133(8)

N10	H10F	O4	0.86(2)	2.03(3)	2.887(8)	170(8)

[1]1-X,1-Y,1-Z

Table S17. Torsion Angles for **3.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O5	C2	C8	O4	65.6(7)		C4	O8	C3	C11	173.4(6)
O6	C1	C5	O5	-72.1(6)		C5	O5	C2	C8	-173.0(5)
O7	C6	C10	O6	67.4(6)		C6	O7	C12	C4	-179.7(5)
O8	C3	C11	O9	69.1(7)		C7	O9	C11	C3	-176.1(5)
O8	C4	C12	O7	-64.1(7)		C8	O4	C9	C7	-177.7(6)
O9	C7	C9	O4	-67.4(7)		C9	O4	C8	C2	174.7(5)
C1	O6	C10	C6	177.6(4)		C10	O6	C1	C5	179.6(5)
C2	O5	C5	C1	179.5(5)		C11	O9	C7	C9	-178.0(5)
C3	O8	C4	C12	-179.5(5)		C12	O7	C6	C10	-178.6(5)

Table S18. Bond Lengths for **4.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Br1	Cr1	2.3508(14)		O7	C9	1.419(8)
Cr1	O1	1.607(5)		O8	C10	1.439(7)
Cr1	O2	1.603(5)		O8	C11	1.414(8)
Cr1	O3	1.603(4)		O9	C1	1.427(6)
O4	C2	1.416(7)		O9	C12	1.423(7)
O4	C3	1.436(7)		C1	C2	1.480(8)
O5	C4	1.429(6)		C3	C4	1.487(8)
O5	C5	1.426(7)		C5	C6	1.490(8)
O6	C6	1.447(8)		C7	C8	1.494(10)
O6	C7	1.442(7)		C9	C10	1.487(10)
O7	C8	1.412(8)		C11	C12	1.493(8)

Table S19. Bond Angles for **4.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Cr1	Br1	108.55(17)		O9	C1	C2	108.8(5)
O2	Cr1	Br1	108.14(19)		O4	C2	C1	110.3(5)
O2	Cr1	O1	110.0(3)		O4	C3	C4	108.7(5)
O2	Cr1	O3	111.5(3)		O5	C4	C3	109.7(4)
O3	Cr1	Br1	106.81(19)		O5	C5	C6	109.6(5)
O3	Cr1	O1	111.7(2)		O6	C6	C5	108.6(5)
C2	O4	C3	112.7(4)		O6	C7	C8	108.0(6)
C5	O5	C4	111.2(4)		O7	C8	C7	110.9(6)
C7	O6	C6	111.9(5)		O7	C9	C10	110.3(6)
C8	O7	C9	111.8(5)		O8	C10	C9	109.9(6)
C11	O8	C10	112.5(5)		O8	C11	C12	109.1(5)
C12	O9	C1	112.9(5)		O9	C12	C11	109.0(5)

Table S20. Hydrogen Bonds for **4.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1C	O1	0.74(3)	2.27(3)	2.968(7)	156(5)
N1	H1D	O8	0.75(3)	2.15(3)	2.898(7)	174(5)
N1	H1E	O4	0.74(3)	2.15(3)	2.883(6)	167(5)
N1	H1F	O6	0.75(3)	2.13(3)	2.870(7)	172(6)

Table S21. Torsion Angles for **4.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O4	C3	C4	O5	69.2(6)		C4	O5	C5	C6	177.9(5)
O5	C5	C6	O6	-63.1(7)		C5	O5	C4	C3	179.1(5)
O6	C7	C8	O7	63.4(7)		C6	O6	C7	C8	179.6(5)
O7	C9	C10	O8	-68.6(7)		C7	O6	C6	C5	-175.9(5)
O8	C11	C12	O9	67.2(7)		C8	O7	C9	C10	174.5(5)
O9	C1	C2	O4	-64.9(6)		C9	O7	C8	C7	178.3(5)
C1	O9	C12	C11	175.0(5)		C10	O8	C11	C12	-174.9(5)
C2	O4	C3	C4	-179.5(4)		C11	O8	C10	C9	-177.3(6)
C3	O4	C2	C1	-177.9(4)		C12	O9	C1	C2	176.5(6)

Table S22. Bond Lengths for **5.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Re1	O1	1.725(3)		O8	C9	1.436(4)
Re1	O2	1.724(3)		O9	C10	1.429(4)
Re1	O3	1.727(2)		O9	C11	1.434(4)
Re1	O4	1.723(2)		O10	C1	1.417(4)
O5	C2	1.415(4)		O10	C12	1.432(3)
O5	C3	1.434(4)		C1	C2	1.504(4)
O6	C4	1.430(4)		C3	C4	1.499(5)
O6	C5	1.436(4)		C5	C6	1.499(4)
O7	C6	1.436(4)		C7	C8	1.512(4)
O7	C7	1.426(4)		C9	C10	1.504(5)
O8	C8	1.417(4)		C11	C12	1.502(5)

Table S23. Bond Angles for **5.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Re1	O3	111.04(13)		O10	C1	C2	109.1(3)
O2	Re1	O1	108.19(14)		O5	C2	C1	108.9(3)
O2	Re1	O3	109.67(13)		O5	C3	C4	108.7(3)
O4	Re1	O1	109.40(13)		O6	C4	C3	109.0(3)
O4	Re1	O2	109.70(13)		O6	C5	C6	109.1(3)
O4	Re1	O3	108.83(12)		O7	C6	C5	108.8(3)
C2	O5	C3	112.1(2)		O7	C7	C8	109.0(2)
C4	O6	C5	112.0(2)		O8	C8	C7	108.7(3)
C7	O7	C6	110.7(2)		O8	C9	C10	108.6(3)
C8	O8	C9	112.4(3)		O9	C10	C9	109.3(3)
C10	O9	C11	110.9(2)		O9	C11	C12	108.4(3)
C1	O10	C12	112.2(2)		O10	C12	C11	109.2(3)

Table S24. Hydrogen Bonds for **5.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1C	O8	0.849(17)	2.045(18)	2.892(4)	175(3)
N1	H1D	O1	0.860(18)	2.10(2)	2.818(4)	140(2)
N1	H1D	O4[1]	0.860(18)	2.51(3)	3.046(4)	122(2)
N1	H1E	O6	0.859(17)	2.033(18)	2.878(3)	168(3)
N1	H1F	O10	0.849(17)	2.045(18)	2.884(3)	169(3)

[1]1-X,1-Y,1-Z

Table S25. Torsion Angles for **5.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O5	C3	C4	O6	-65.6(3)		C4	O6	C5	C6	-178.7(3)
O6	C5	C6	O7	71.8(3)		C5	O6	C4	C3	-176.0(3)
O7	C7	C8	O8	-67.2(3)		C6	O7	C7	C8	172.0(3)
O8	C9	C10	O9	67.5(3)		C7	O7	C6	C5	-179.4(3)
O9	C11	C12	O10	-67.8(4)		C8	O8	C9	C10	178.3(3)
O10	C1	C2	O5	63.7(4)		C9	O8	C8	C7	-176.8(2)
C1	O10	C12	C11	-176.0(3)		C10	O9	C11	C12	177.8(3)
C2	O5	C3	C4	178.7(3)		C11	O9	C10	C9	-179.9(3)
C3	O5	C2	C1	178.0(3)		C12	O10	C1	C2	179.0(3)

Table S26. Bond Lengths for **6.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Tc1	O1	1.703(4)		C4	C7	1.506(9)
Tc1	O2	1.701(5)		C6	C8	1.496(9)
Tc1	O3	1.717(5)		C9	C12	1.486(9)
Tc1	O4	1.694(4)		C10	C11	1.498(8)
Tc2	O5	1.705(4)		O15	C13	1.420(7)
Tc2	O6	1.716(5)		O15	C16	1.433(7)
Tc2	O7	1.702(4)		O16	C15	1.436(6)
Tc2	O8	1.709(4)		O16	C19	1.429(7)
O9	C1	1.438(7)		O17	C17	1.434(6)
O9	C3	1.428(7)		O17	C18	1.427(7)
O10	C2	1.443(6)		O18	C14	1.426(6)
O10	C10	1.438(7)		O18	C21	1.427(7)
O11	C5	1.437(7)		O19	C22	1.412(7)
O11	C8	1.436(8)		O19	C24	1.425(7)
O12	C7	1.430(8)		O20	C20	1.423(8)
O12	C9	1.442(7)		O20	C23	1.447(6)
O13	C4	1.435(7)		C13	C14	1.512(8)
O13	C6	1.429(7)		C15	C22	1.500(9)
O14	C11	1.438(7)		C16	C17	1.489(8)

O14	C12	1.435(6)		C18	C19	1.488(8)
C1	C5	1.486(9)		C20	C21	1.506(8)
C2	C3	1.499(8)		C23	C24	1.494(9)

Table S27. Bond Angles for **6.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
O1	Tc1	O3	106.9(2)		O12	C7	C4	108.8(5)
O2	Tc1	O1	110.7(2)		O11	C8	C6	108.9(5)
O2	Tc1	O3	110.3(3)		O12	C9	C12	108.4(5)
O4	Tc1	O1	110.4(2)		O10	C10	C11	109.0(5)
O4	Tc1	O2	109.6(2)		O14	C11	C10	109.0(5)
O4	Tc1	O3	108.9(3)		O14	C12	C9	109.2(5)
O5	Tc2	O6	110.0(2)		C13	O15	C16	112.0(4)
O5	Tc2	O8	109.5(2)		C19	O16	C15	112.6(5)
O7	Tc2	O5	109.5(2)		C18	O17	C17	110.4(4)
O7	Tc2	O6	109.5(2)		C14	O18	C21	111.8(4)
O7	Tc2	O8	109.7(2)		C22	O19	C24	111.7(5)
O8	Tc2	O6	108.6(2)		C20	O20	C23	112.2(5)
C3	O9	C1	112.0(5)		O15	C13	C14	108.6(5)
C10	O10	C2	112.1(4)		O18	C14	C13	108.0(5)
C8	O11	C5	112.5(5)		O16	C15	C22	109.2(5)
C7	O12	C9	111.6(4)		O15	C16	C17	109.6(5)
C6	O13	C4	111.7(5)		O17	C17	C16	109.2(5)
C12	O14	C11	111.0(4)		O17	C18	C19	109.9(5)
O9	C1	C5	109.6(5)		O16	C19	C18	109.8(5)
O10	C2	C3	108.6(5)		O20	C20	C21	108.5(5)
O9	C3	C2	109.8(5)		O18	C21	C20	108.5(5)
O13	C4	C7	108.2(5)		O19	C22	C15	109.1(5)
O11	C5	C1	109.4(5)		O20	C23	C24	108.0(5)
O13	C6	C8	108.6(5)		O19	C24	C23	110.1(5)

Table S28. Hydrogen Bonds for **6.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O6	0.870(10)	1.798(5)	2.642(10)	162.5(6)
O1W	H1WB	O4	0.869(10)	2.198(5)	2.907(11)	138.7(6)
N1	H1A	O1W	0.89(2)	1.98(3)	2.793(10)	153(4)
N1	H1B	O10	0.88(2)	1.97(2)	2.840(6)	173(4)
N1	H1C	O11	0.88(2)	2.03(2)	2.869(6)	161(4)
N1	H1D	O12	0.88(2)	1.99(2)	2.868(6)	175(4)
N1	H1D	O14	0.88(2)	2.66(4)	3.076(6)	110(3)
N2	H2C	O16	0.88(2)	2.01(2)	2.883(6)	169(4)
N2	H2D	O15	0.87(2)	2.04(2)	2.877(6)	162(4)
N2	H2E	O3	0.89(2)	1.99(2)	2.853(7)	164(4)
N2	H2F	O20	0.88(2)	1.96(2)	2.818(6)	163(4)

Table S29. Torsion Angles for **6.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°
O9	C1	C5	O11	70.3(6)		O15	C13	C14	O18	-68.2(6)
O10	C2	C3	O9	-64.4(6)		O15	C16	C17	O17	68.4(6)
O10	C10	C11	O14	62.4(7)		O16	C15	C22	O19	66.1(6)
O12	C9	C12	O14	-69.3(6)		O17	C18	C19	O16	-64.5(6)
O13	C4	C7	O12	70.0(6)		O20	C20	C21	O18	66.1(6)
O13	C6	C8	O11	-64.6(7)		O20	C23	C24	O19	-67.7(6)
C1	O9	C3	C2	-178.8(5)		C13	O15	C16	C17	-176.0(4)
C2	O10	C10	C11	171.7(5)		C14	O18	C21	C20	174.0(5)
C3	O9	C1	C5	-172.3(5)		C15	O16	C19	C18	-177.0(5)
C4	O13	C6	C8	-178.1(5)		C16	O15	C13	C14	-176.7(4)
C5	O11	C8	C6	175.7(5)		C17	O17	C18	C19	175.7(5)
C6	O13	C4	C7	179.7(5)		C18	O17	C17	C16	178.6(5)
C7	O12	C9	C12	177.6(4)		C19	O16	C15	C22	-176.2(5)
C8	O11	C5	C1	175.4(5)		C20	O20	C23	C24	-169.1(5)
C9	O12	C7	C4	177.0(4)		C21	O18	C14	C13	172.6(5)
C10	O10	C2	C3	-175.8(5)		C22	O19	C24	C23	172.1(5)
C11	O14	C12	C9	178.4(5)		C23	O20	C20	C21	-175.3(5)
C12	O14	C11	C10	-176.5(5)		C24	O19	C22	C15	177.5(5)

Table S30. Bond Lengths for **7.**

Atom	Atom	Length/Å		Atom	Atom	Length/Å
Os1	N1	1.685(4)		C4	C7	1.504(7)
Os1	O2	1.728(4)		C6	C8	1.508(6)
Os1	O3	1.757(4)		C9	C12	1.500(7)
Os1	O4	1.724(3)		C10	C11	1.499(6)
Os2	O6	1.748(4)		O15	C13	1.430(5)
Os2	N5	1.715(4)		O15	C16	1.432(5)
Os2	N7	1.728(3)		O16	C15	1.431(5)
Os2	N8	1.729(4)		O16	C19	1.428(5)
O9	C1	1.429(5)		O17	C17	1.435(5)
O9	C3	1.425(5)		O17	C18	1.427(5)
O10	C2	1.429(5)		O18	C14	1.432(5)
O10	C10	1.429(5)		O18	C21	1.430(5)
O11	C5	1.427(5)		O19	C22	1.431(6)
O11	C8	1.431(6)		O19	C24	1.434(6)
O12	C7	1.434(5)		O20	C20	1.428(6)
O12	C9	1.432(5)		O20	C23	1.442(5)
O13	C4	1.433(5)		C13	C14	1.503(6)
O13	C6	1.422(5)		C15	C22	1.494(7)
O14	C11	1.428(5)		C16	C17	1.499(6)
O14	C12	1.433(5)		C18	C19	1.502(6)
C1	C5	1.504(7)		C20	C21	1.501(6)
C2	C3	1.502(6)		C23	C24	1.486(7)

Table S31. Bond Angles for **7.**

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
N1	Os1	O2	108.8(2)		O12	C7	C4	108.6(4)

N1	Os1	O3	106.42(19)		O11	C8	C6	108.8(4)
N1	Os1	O4	108.67(19)		O12	C9	C12	108.9(4)
O2	Os1	O3	111.53(19)		O10	C10	C11	109.8(4)
O4	Os1	O2	111.10(17)		O14	C11	C10	109.4(4)
O4	Os1	O3	110.2(2)		O14	C12	C9	109.0(3)
N5	Os2	O6	110.3(2)		C13	O15	C16	111.9(3)
N5	Os2	N7	108.92(18)		C19	O16	C15	112.3(4)
N5	Os2	N8	109.06(19)		C18	O17	C17	110.0(3)
N7	Os2	O6	110.08(17)		C21	O18	C14	112.1(3)
N7	Os2	N8	109.60(19)		C22	O19	C24	111.9(4)
N8	Os2	O6	108.85(18)		C20	O20	C23	112.8(3)
C3	O9	C1	111.7(3)		O15	C13	C14	108.9(4)
C10	O10	C2	112.6(3)		O18	C14	C13	108.5(4)
C5	O11	C8	112.6(3)		O16	C15	C22	109.6(4)
C9	O12	C7	112.0(3)		O15	C16	C17	109.3(3)
C6	O13	C4	111.8(3)		O17	C17	C16	108.9(3)
C11	O14	C12	110.7(3)		O17	C18	C19	110.0(4)
O9	C1	C5	109.5(4)		O16	C19	C18	109.5(4)
O10	C2	C3	109.3(4)		O20	C20	C21	108.8(4)
O9	C3	C2	109.7(4)		O18	C21	C20	108.7(4)
O13	C4	C7	108.9(4)		O19	C22	C15	108.8(4)
O11	C5	C1	109.4(4)		O20	C23	C24	108.7(4)
O13	C6	C8	108.5(4)		O19	C24	C23	110.3(4)

Table S32. Hydrogen Bonds for **7.**

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1W	H1WA	O6	0.866(7)	1.805(4)	2.632(8)	158.7(5)
O1W	H1WB	O4	0.867(8)	2.176(4)	2.925(9)	144.3(5)
N3	H3C	O1W	0.876(17)	2.00(2)	2.788(8)	149(3)
N3	H3D	O10	0.865(17)	1.989(19)	2.842(5)	169(3)
N3	H3D	O14	0.865(17)	2.64(3)	3.073(5)	112(3)
N3	H3E	O11	0.862(17)	2.028(19)	2.875(5)	167(3)
N3	H3F	O12	0.866(17)	2.025(18)	2.889(4)	175(3)
N2	H2C	O16	0.874(17)	2.015(18)	2.887(5)	177(3)
N2	H2D	O15	0.865(17)	2.029(18)	2.885(4)	170(3)
N2	H2E	O3	0.863(17)	1.971(18)	2.828(5)	172(3)
N2	H2F	O20	0.868(17)	2.01(2)	2.834(5)	157(3)

Table S33. Torsion Angles for **7.**

A	B	C	D	Angle/°		A	B	C	D	Angle/°

O9	C1	C5	O11	69.6(5)		O15	C13	C14	O18	-68.5(4)
O10	C2	C3	O9	-64.4(4)		O15	C16	C17	O17	68.4(4)
O10	C10	C11	O14	62.3(5)		O16	C15	C22	O19	66.5(5)
O12	C9	C12	O14	-68.2(4)		O17	C18	C19	O16	-64.9(5)
O13	C4	C7	O12	70.2(4)		O20	C20	C21	O18	65.8(5)
O13	C6	C8	O11	-65.0(5)		O20	C23	C24	O19	-66.6(5)
C1	O9	C3	C2	-179.2(3)		C13	O15	C16	C17	-176.2(3)
C2	O10	C10	C11	173.1(4)		C14	O18	C21	C20	174.6(4)
C3	O9	C1	C5	-172.4(3)		C15	O16	C19	C18	-177.6(4)
C4	O13	C6	C8	-177.6(4)		C16	O15	C13	C14	-177.4(3)
C5	O11	C8	C6	175.8(4)		C17	O17	C18	C19	175.8(4)
C6	O13	C4	C7	180.0(4)		C18	O17	C17	C16	179.1(4)
C7	O12	C9	C12	177.2(3)		C19	O16	C15	C22	-176.3(4)
C8	O11	C5	C1	175.3(4)		C20	O20	C23	C24	-169.1(4)
C9	O12	C7	C4	177.2(3)		C21	O18	C14	C13	172.7(4)
C10	O10	C2	C3	-176.6(4)		C22	O19	C24	C23	171.6(4)
C11	O14	C12	C9	178.1(4)		C23	O20	C20	C21	-176.2(4)
C12	O14	C11	C10	-176.7(4)		C24	O19	C22	C15	177.7(4)

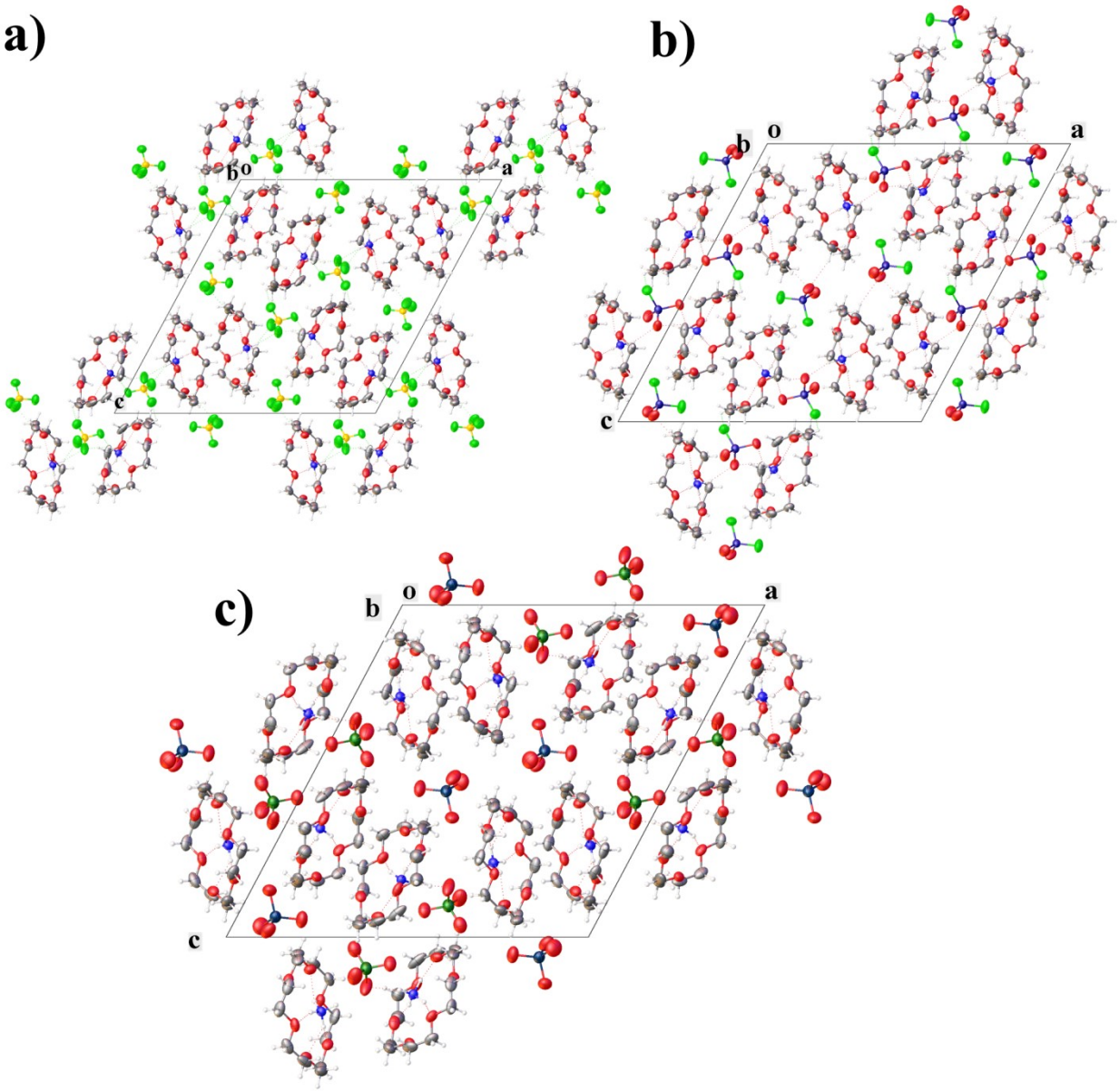

Fig S1. Crystal packing in structures **1**-**2** (a-b) and **8** (c) of the first comparison group.

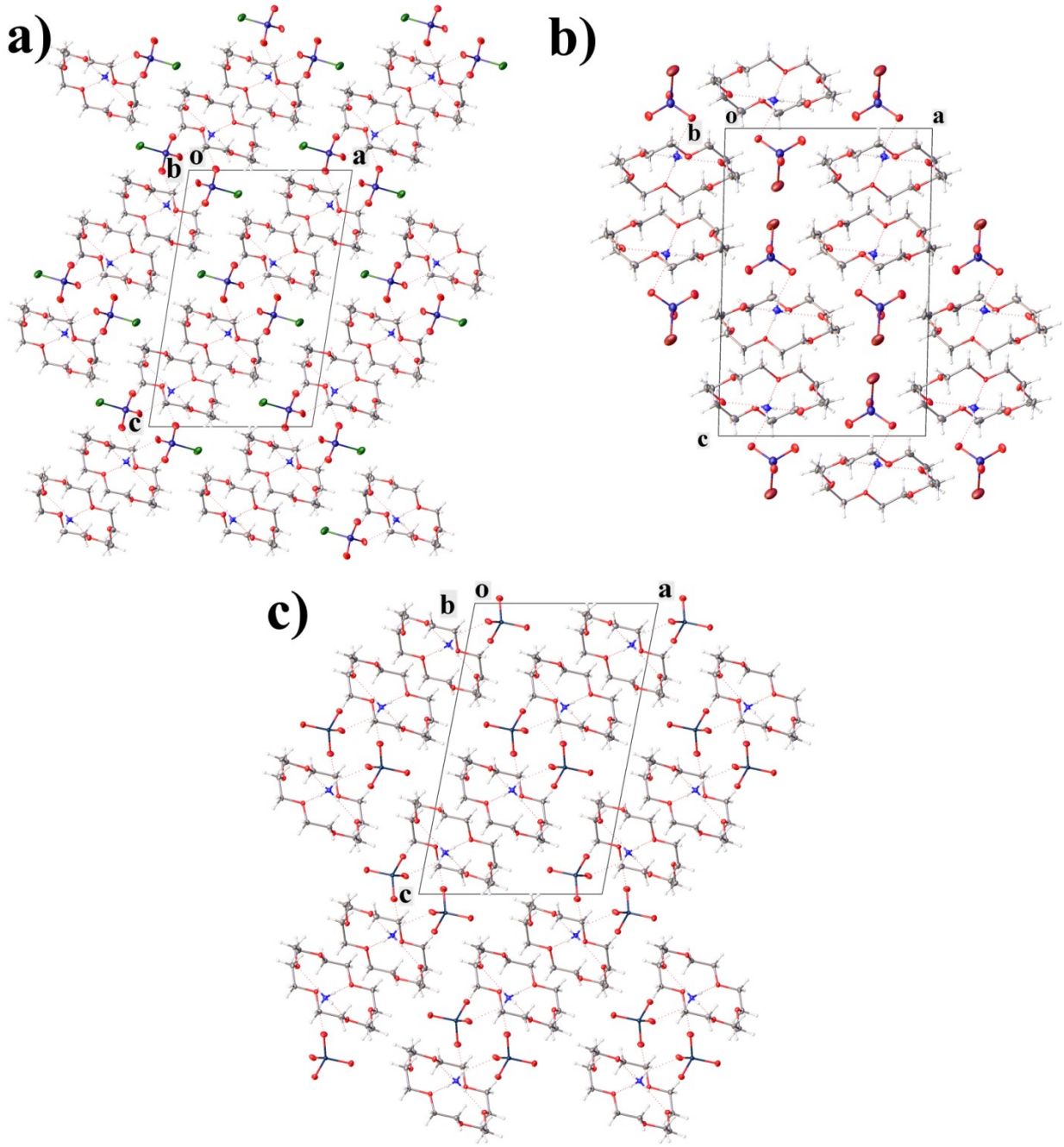

Fig S2. Crystal packing in structures **3-5** of the second comparison group.

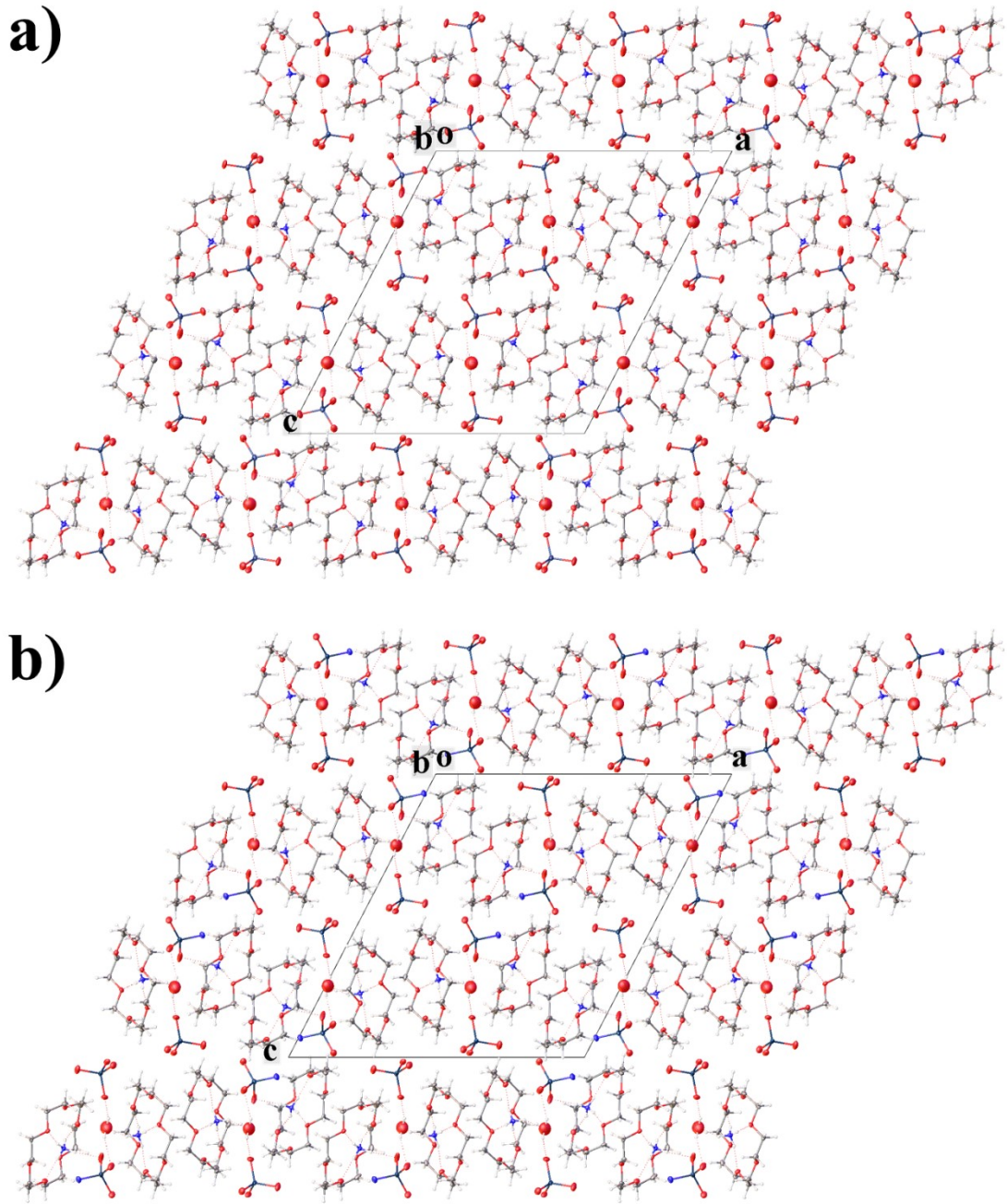

Fig S3. Crystal packing in structures **6**-**7** of the third comparison group.

PXRD part

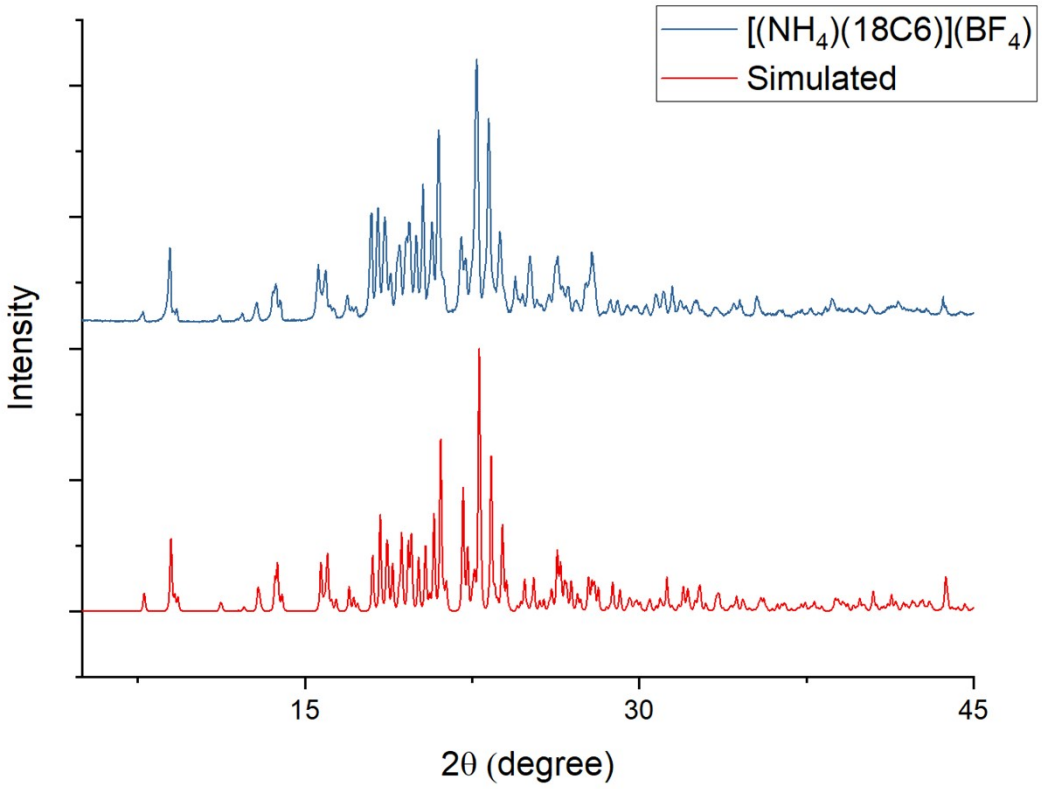

Fig S4. Experimental and theoretical diffraction patterns of compound **1**

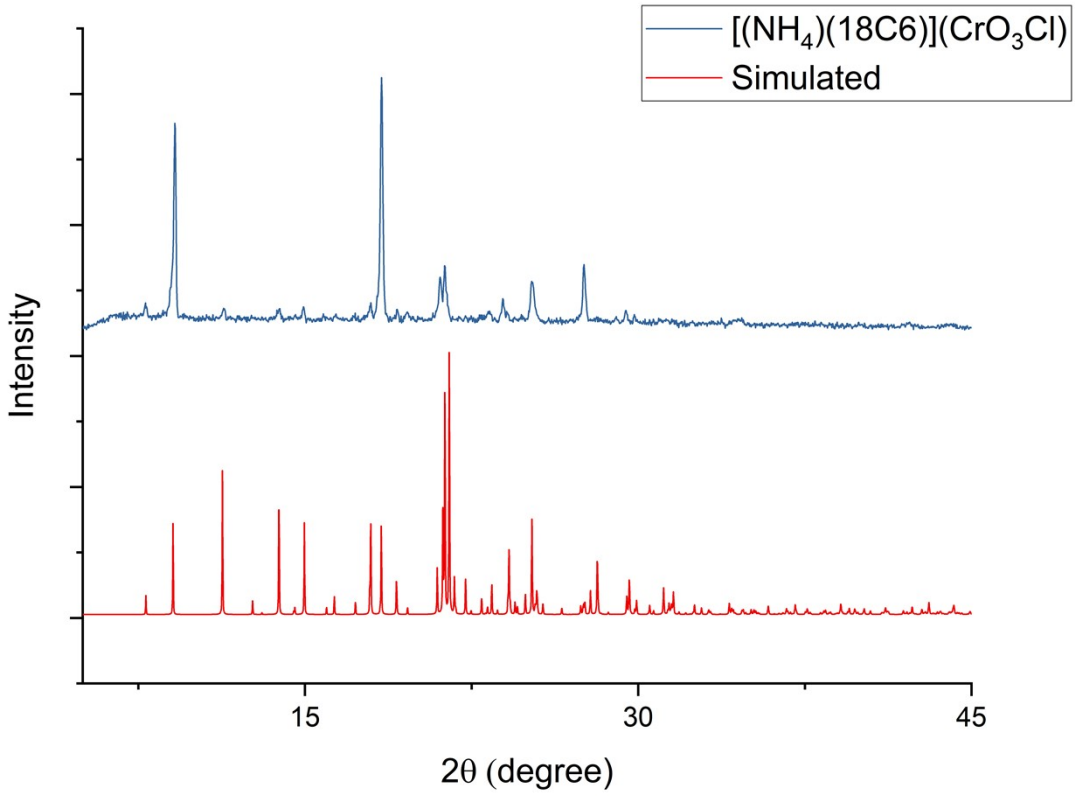

Fig S5. Experimental and theoretical diffraction patterns of compound **3**

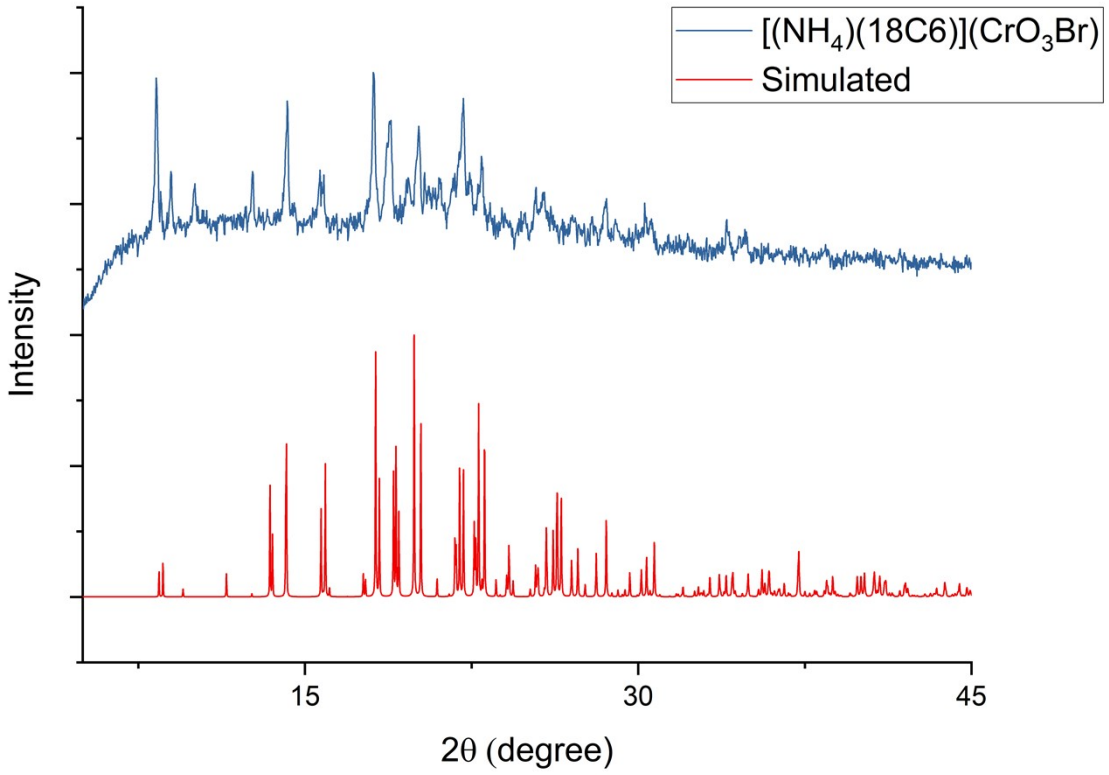

Fig S6. Experimental and theoretical diffraction patterns of compound **4**

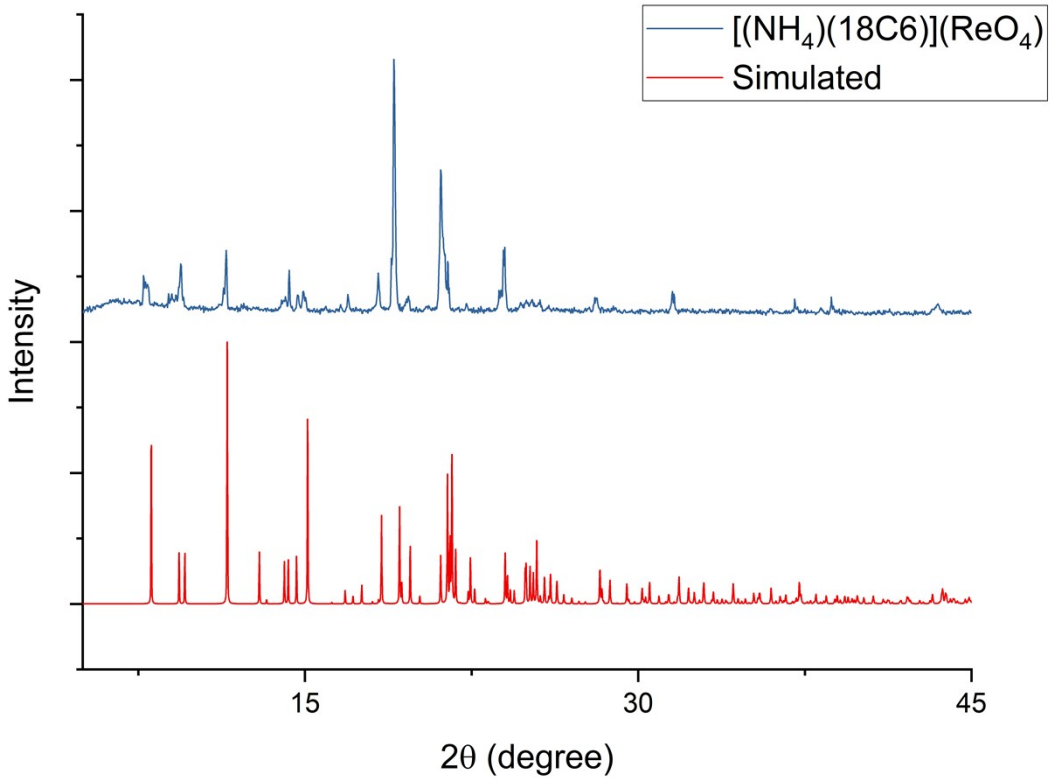

Fig S7. Experimental and theoretical diffraction patterns of compound **5**

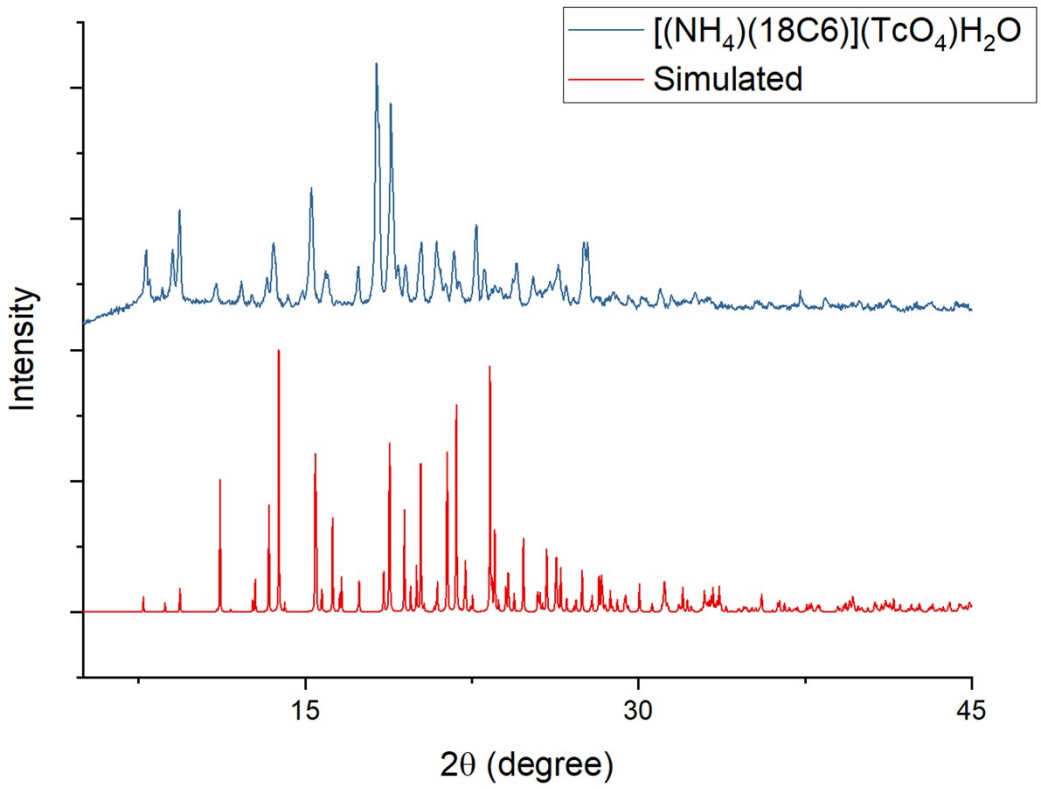

Fig S8. Experimental and theoretical diffraction patterns of compound **6**

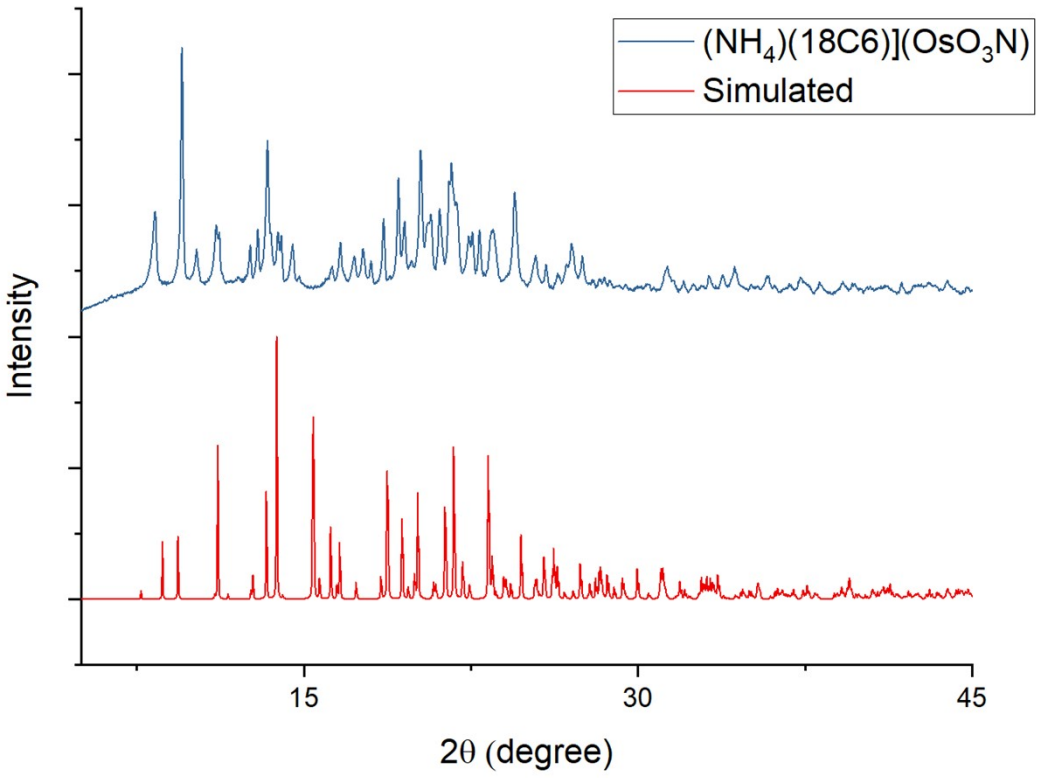

Fig S9. Experimental and theoretical diffraction patterns of compound **7**

Thermal analysis

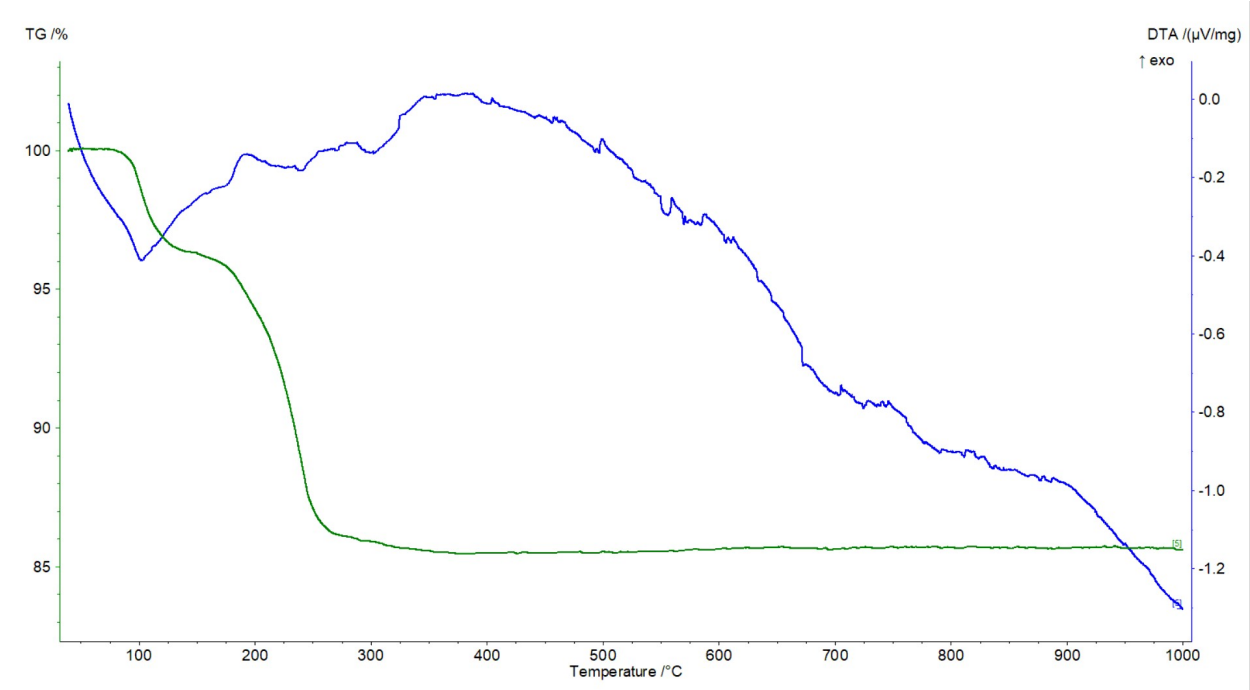

Fig S10. TG and DTA curves compound **7**

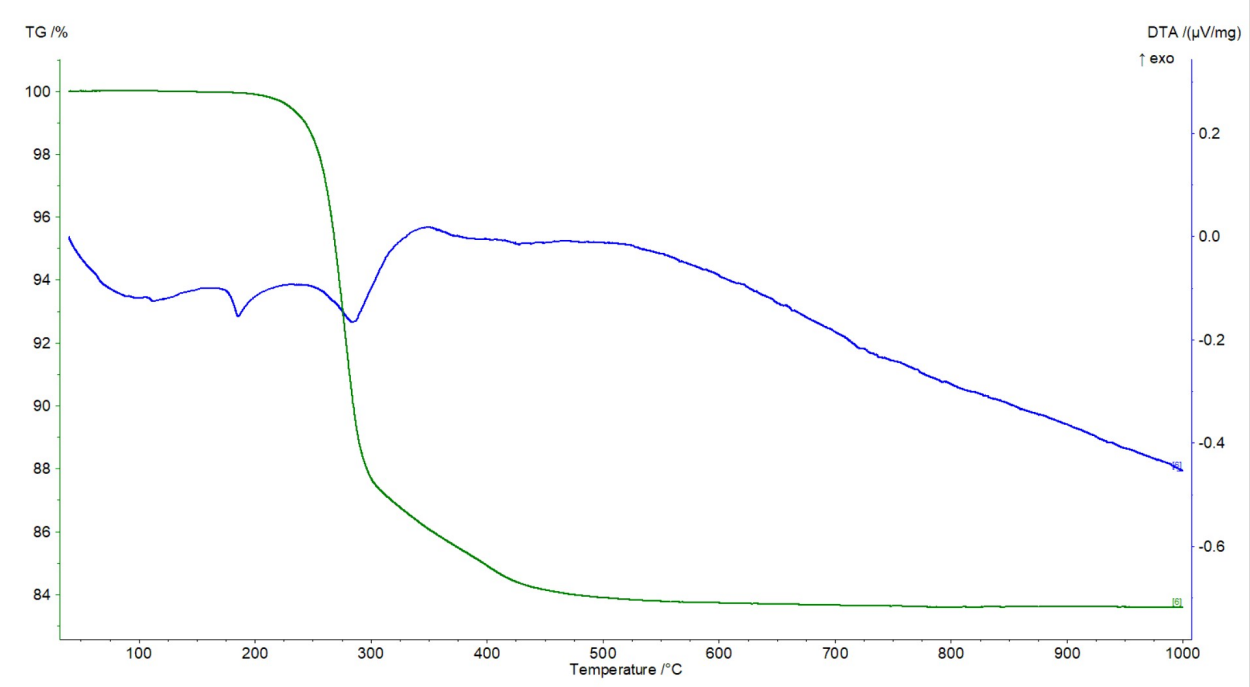

Fig S11. TG and DTA curves compound **5**

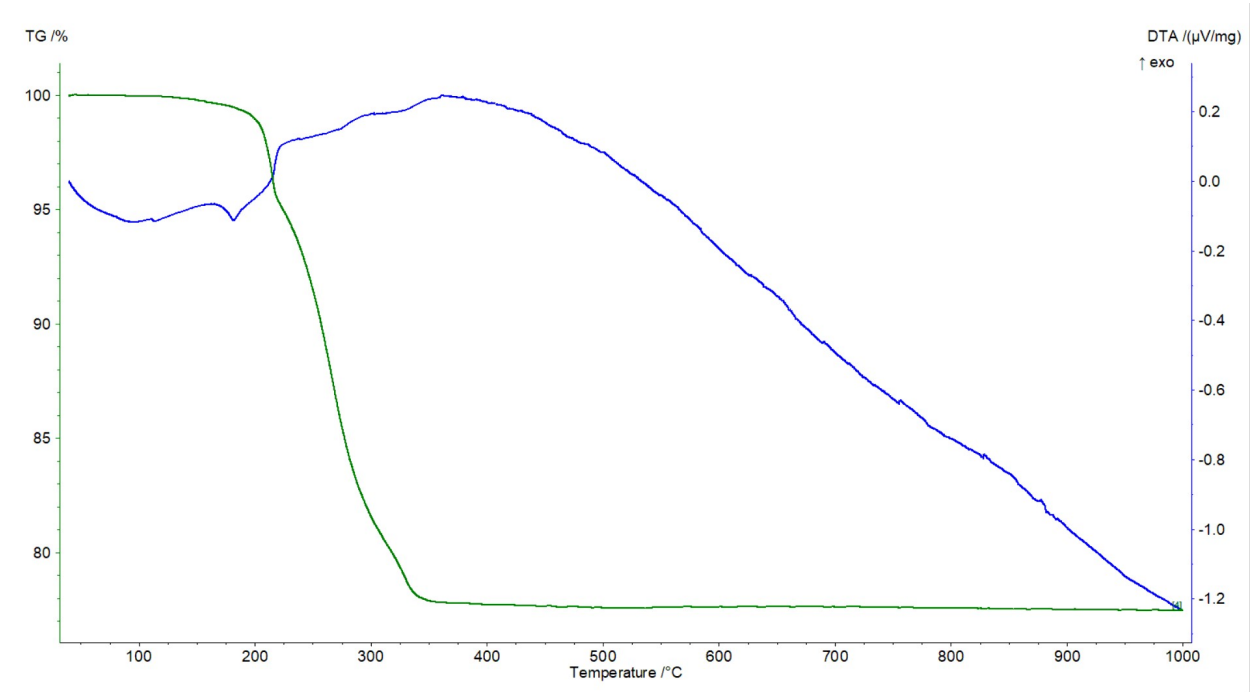

Fig S12. TG and DTA curves compound **6**

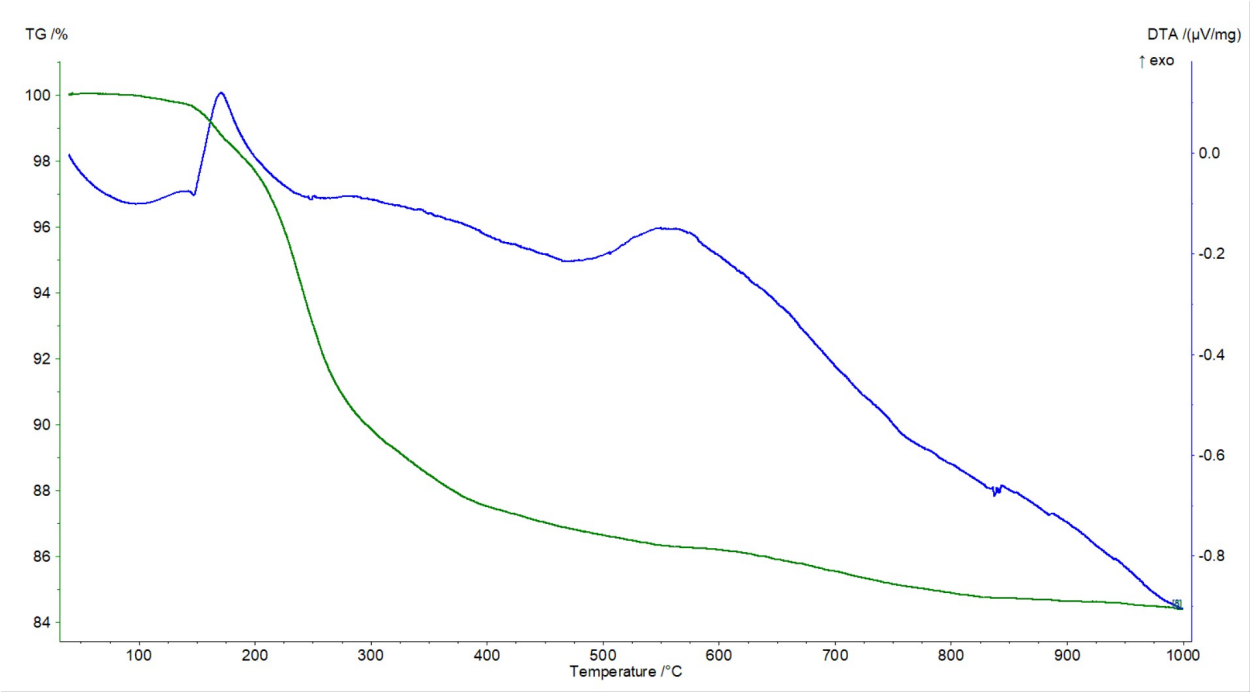

Fig S13. TG and DTA curves compound **3**