crystals

MDPI

Design and synthesis of multicomponent Re(IV)-containing magnetic materials for optoelectronics

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Table S1. Crystal data and structure refinement for $(C_6H_{14}N)_{10}(ReCl_6)_3 \cdot 4(Cl) \cdot 2(H_2O)$.

Empirical formula	$C_{60}H_{144}Cl_{22}N_{10}O_2Re_3$	
Formula weight	2376.34	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1 (No. 2)	
Unit cell dimensions	a = 11.211(3) Å	α= 80.87(3)°.
	b = 13.4385(3) Å	β= 74.29(3)°.
	c = 16.6585(4) Å	γ = 87.95(3)°.
Volume	2385.4(1) $Å^3$	
Z	1	
Density (calculated)	1.65 Mg/m^3	
Absorption coefficient	4.45 mm^{-1}	
F(000)	1189	
Crystal size	0.10 x 0.10 x 0.05 mm	
Theta range for data collection	2.15 to 30.51°.	
Index ranges	-16<=h<=16, -18<=k<=19, -23<=l<=23	
Reflections collected	66071	
Independent reflections	14487 [R(int) = 0.0321]	
Completeness to theta = 25.000°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	0.989 and 0.526	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14487 / 0 / 541	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R_1 = 0.0202, wR_2 = 0.0395	
R indices (all data)	R_1 = 0.0268, wR_2 = 0.0408	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.56 and -0.98 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $(C_6 H_{14} N)_{10} (ReCl_6)_3 \cdot 4(Cl) \cdot 2(H_2 O)$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Re(1)	0	5000	10000	12(1)
Cl(1)	-797(1)	6659(1)	9973(1)	16(1)
Cl(2)	1372(1)	5476(1)	8656(1)	17(1)
Cl(3)	1493(1)	5459(1)	10643(1)	17(1)
Re(2)	2892(1)	10203(1)	3667(1)	16(1)
Cl(4)	3760(1)	11804(1)	3024(1)	18(1)
Cl(5)	965(1)	10964(1)	4178(1)	17(1)
Cl(6)	4853(1)	9476(1)	3228(1)	23(1)
Cl(7)	3358(1)	10439(1)	4938(1)	24(1)
Cl(8)	2424(1)	10023(1)	2401(1)	28(1)
Cl(11)	1149(1)	8633(1)	7600(1)	23(1)
Cl(12)	4716(1)	6295(1)	8870(1)	19(1)
O(1W)	6838(1)	7792(1)	8872(1)	23(1)
N(1)	9403(2)	9399(1)	3643(1)	22(1)
C(1)	8843(2)	8595(1)	3326(1)	20(1)
C(2)	8812(2)	7604(2)	3918(1)	27(1)
C(3)	8277(2)	6764(2)	3595(1)	34(1)
C(4)	8989(3)	6670(2)	2696(2)	37(1)
C(5)	9013(3)	7677(2)	2115(1)	39(1)
C(6)	9572(2)	8514(2)	2431(1)	27(1)
N(2)	-963(2)	6886(1)	8014(1)	21(1)
C(10)	-1133(2)	6701(1)	7188(1)	16(1)
C(11)	-2119(2)	5901(1)	7321(1)	21(1)
C(12)	-2279(2)	5760(2)	6464(1)	26(1)
C(13)	-1053(2)	5478(2)	5877(1)	29(1)
C(14)	-50(2)	6256(2)	5778(1)	28(1)
C(15)	99(2)	6417(2)	6631(1)	22(1)
N(3)	3862(2)	4046(1)	9647(1)	17(1)
C(30)	4491(2)	3346(1)	9050(1)	16(1)
C(31)	5881(2)	3517(2)	8806(1)	25(1)
C(32)	6532(2)	2806(2)	8194(2)	34(1)
C(33)	6038(2)	2931(2)	7418(1)	32(1)
C(34)	4636(2)	2798(2)	7665(1)	30(1)
C(35)	3987(2)	3502(2)	8282(1)	25(1)

N(4)	2217(2)	7570(1)	9122(1)	19(1)
C(41)	2604(2)	8402(1)	9504(1)	18(1)
C(42)	3597(2)	9046(1)	8837(1)	21(1)
C(43)	4018(2)	9876(2)	9229(1)	30(1)
C(44)	2934(2)	10511(2)	9617(1)	33(1)
C(45)	1907(2)	9863(2)	10260(1)	35(1)
C(46)	1493(2)	9023(2)	9872(1)	28(1)
N(5)	3831(2)	8543(1)	6316(1)	28(1)
C(55)	3613(2)	6701(2)	6730(1)	34(1)
C(53A)	4289(3)	5559(3)	5649(2)	22(1)
C(54A)	3287(3)	5728(3)	6457(2)	19(1)
C(52A)	4387(4)	6452(3)	4934(2)	22(1)
C(50A)	3544(3)	7594(3)	6004(2)	14(1)
C(51A)	4587(3)	7441(3)	5219(2)	18(1)
C(51B)	3579(4)	7552(3)	5327(3)	32(1)
C(50B)	4171(5)	7552(3)	6006(3)	27(1)
C(54B)	3984(5)	5678(4)	6366(3)	36(1)
C(53B)	3373(5)	5654(4)	5685(3)	38(1)
C(52B)	3799(5)	6550(3)	4966(3)	26(1)
Cl(9A)	2083(2)	8614(2)	4369(1)	16(1)
Cl(9B)	1849(2)	8629(2)	4170(1)	19(1)

Table S3. Bond lengths [Å] and angles [°] for $(C_6H_{14}N)_{10}(ReCl_6)_3 \cdot 4(Cl) \cdot 2(H_2O)$.

Re(1)-Cl(2)	2.3537(4)
Re(1)-Cl(2)#1	2.3537(4)
Re(1)-Cl(3)#1	2.3629(4)
Re(1)-Cl(3)	2.3629(4)
Re(1)-Cl(1)#1	2.3704(4)
Re(1)-Cl(1)	2.3704(4)
Re(2)-Cl(9A)	2.350(2)
Re(2)-Cl(6)	2.3510(5)
Re(2)-Cl(8)	2.3555(5)
Re(2)-Cl(5)	2.3579(4)
Re(2)-Cl(4)	2.3625(4)
Re(2)-Cl(9B)	2.371(2)
Re(2)-Cl(7)	2.3842(5)
O(1W)-H(1W)	0.85
O(1W)-H(2W)	0.85
N(1)-C(1)	1.500(2)
N(1)-H(11N)	0.82(3)
N(1)-H(12N)	0.90(3)
N(1)-H(13N)	0.90(3)
C(1)-C(6)	1.512(3)
C(1)-C(2)	1.523(3)
C(1)-H(1)	1.00
C(2)-C(3)	1.530(3)
C(2)-H(2A)	0.99
C(2)-H(2B)	0.99
C(3)-C(4)	1.517(3)
C(3)-H(3A)	0.99
C(3)-H(3B)	0.99
C(4)-C(5)	1.530(3)
C(4)-H(4A)	0.99
C(4)-H(4B)	0.99
C(5)-C(6)	1.534(3)
C(5)-H(5A)	0.99
C(5)-H(5B)	0.99
C(6)-H(6A)	0.99
C(6)-H(6B)	0.99
N(2)-C(10)	1.498(2)
N(2)-H(21N)	0.91(3)

N(2)-H(22N)	0.88(3)
N(2)-H(23N)	0.84(3)
C(10)-C(15)	1.514(3)
C(10)-C(11)	1.518(2)
C(10)-H(10)	1.00
C(11)-C(12)	1.528(3)
C(11)-H(11A)	0.99
C(11)-H(11B)	0.99
C(12)-C(13)	1.531(3)
C(12)-H(12A)	0.99
C(12)-H(12B)	0.99
C(13)-C(14)	1.522(3)
C(13)-H(13A)	0.99
C(13)-H(13B)	0.99
C(14)-C(15)	1.524(3)
C(14)-H(14A)	0.99
C(14)-H(14B)	0.99
C(15)-H(15A)	0.99
C(15)-H(15B)	0.99
N(3)-C(30)	1.497(2)
N(3)-H(31N)	0.88(3)
N(3)-H(32N)	0.86(2)
N(3)-H(33N)	0.87(2)
C(30)-C(35)	1.515(3)
C(30)-C(31)	1.516(2)
C(30)-H(30)	1.0000
C(31)-C(32)	1.531(3)
C(31)-H(31A)	0.99
C(31)-H(31B)	0.99
C(32)-C(33)	1.522(3)
C(32)-H(32A)	0.99
C(32)-H(32B)	0.99
C(33)-C(34)	1.523(3)
C(33)-H(33A)	0.99
C(33)-H(33B)	0.99
C(34)-C(35)	1.528(3)
C(34)-H(34A)	0.99
C(34)-H(34B)	0.99
C(35)-H(35A)	0.99
C(35)-H(35B)	0.99

N(4)-C(41)	1.500(2)
N(4)-H(41N)	0.86(3)
N(4)-H(42N)	0.89(3)
N(4)-H(43N)	0.85(3)
C(41)-C(46)	1.516(3)
C(41)-C(42)	1.523(3)
C(41)-H(41)	1.0000
C(42)-C(43)	1.525(3)
C(42)-H(42A)	0.99
C(42)-H(42B)	0.99
C(43)-C(44)	1.516(3)
C(43)-H(43A)	0.99
C(43)-H(43B)	0.99
C(44)-C(45)	1.531(3)
C(44)-H(44A)	0.99
C(44)-H(44B)	0.99
C(45)-C(46)	1.529(3)
C(45)-H(45A)	0.99
C(45)-H(45B)	0.99
C(46)-H(46A)	0.99
C(46)-H(46B)	0.99
N(5)-C(50B)	1.504(5)
N(5)-C(50A)	1.527(4)
N(5)-H(51N)	0.82(3)
N(5)-H(52N)	0.84(3)
N(5)-H(53N)	0.97(3)
C(55)-C(50B)	1.536(5)
C(55)-C(54A)	1.536(5)
C(55)-C(50A)	1.579(4)
C(55)-C(54B)	1.586(5)
C(55)-H(55A)	0.99
C(55)-H(55B)	0.99
C(55)-H(55C)	0.99
C(55)-H(55D)	0.99
C(53A)-C(54A)	1.544(5)
C(53A)-C(52B)	1.783(6)
C(53A)-H(53A)	0.99
C(53A)-H(53B)	0.99
C(54A)-H(54A)	0.99
C(54A)-H(54B)	0.99

C(52A)-C(51A)	1.523(6)
C(52A)-C(53B)	1.702(6)
C(52A)-H(52A)	0.9900
C(52A)-H(52B)	0.9900
C(50A)-C(51A)	1.537(5)
C(50A)-H(50A)	1.00
C(51A)-H(51A)	0.99
C(51A)-H(51B)	0.99
C(51B)-C(50B)	1.458(6)
C(51B)-C(52B)	1.545(6)
C(51B)-H(51C)	0.99
C(51B)-H(51D)	0.99
C(50B)-H(50B)	1.00
C(54B)-C(53B)	1.480(7)
C(54B)-H(54C)	0.99
C(54B)-H(54D)	0.99
C(53B)-H(53C)	0.99
C(53B)-H(53D)	0.99
C(52B)-H(52C)	0.99
C(52B)-H(52D)	0.99
Cl(2)-Re(1)-Cl(2)#1	180.0
Cl(2)-Re(1)-Cl(3)#1	89.662(15)
Cl(2)#1-Re(1)-Cl(3)#1	90.339(15)
Cl(2)-Re(1)-Cl(3)	90.339(15)
Cl(2)#1-Re(1)-Cl(3)	89.660(15)
Cl(3)#1-Re(1)-Cl(3)	180.0
Cl(2)-Re(1)-Cl(1)#1	89.813(15)
Cl(2)#1-Re(1)-Cl(1)#1	90.187(15)
Cl(3)#1-Re(1)-Cl(1)#1	89.622(15)
Cl(3)-Re(1)-Cl(1)#1	90.379(15)
Cl(2)-Re(1)-Cl(1)	90.188(15)
Cl(2)#1-Re(1)-Cl(1)	89.812(15)
Cl(3)#1-Re(1)-Cl(1)	90.378(15)
Cl(3)-Re(1)-Cl(1)	89.621(15)
Cl(1)#1-Re(1)-Cl(1)	180.0
Cl(9A)-Re(2)-Cl(6)	89.56(5)
Cl(9A)-Re(2)-Cl(8)	94.20(4)
Cl(6)-Re(2)-Cl(8)	91.790(18)
Cl(9A)-Re(2)-Cl(5)	90.92(5)
Cl(6)-Re(2)-Cl(5)	176.348(16)

Cl(8)-Re(2)-Cl(5)	91.785(17)
Cl(9A)-Re(2)-Cl(4)	176.70(3)
Cl(6)-Re(2)-Cl(4)	89.552(16)
Cl(8)-Re(2)-Cl(4)	89.008(17)
Cl(5)-Re(2)-Cl(4)	89.761(15)
Cl(6)-Re(2)-Cl(9B)	94.09(5)
Cl(8)-Re(2)-Cl(9B)	83.51(4)
Cl(5)-Re(2)-Cl(9B)	87.06(5)
Cl(4)-Re(2)-Cl(9B)	171.77(4)
Cl(9A)-Re(2)-Cl(7)	87.33(4)
Cl(6)-Re(2)-Cl(7)	89.077(17)
Cl(8)-Re(2)-Cl(7)	178.251(18)
Cl(5)-Re(2)-Cl(7)	87.330(16)
Cl(4)-Re(2)-Cl(7)	89.480(17)
Cl(9B)-Re(2)-Cl(7)	97.94(4)
H(1W)-O(1W)-H(2W)	104.7(10)
C(1)-N(1)-H(11N)	112.2(18)
C(1)-N(1)-H(12N)	112.7(15)
H(11N)-N(1)-H(12N)	105(2)
C(1)-N(1)-H(13N)	111.8(16)
H(11N)-N(1)-H(13N)	108(2)
H(12N)-N(1)-H(13N)	107(2)
N(1)-C(1)-C(6)	109.71(16)
N(1)-C(1)-C(2)	109.18(15)
C(6)-C(1)-C(2)	112.02(17)
N(1)-C(1)-H(1)	108.6
C(6)-C(1)-H(1)	108.6
C(2)-C(1)-H(1)	108.6
C(1)-C(2)-C(3)	110.18(16)
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2B)	109.6
C(3)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(2)	111.39(18)
C(4)-C(3)-H(3A)	109.3
C(2)-C(3)-H(3A)	109.3
C(4)-C(3)-H(3B)	109.3
C(2)-C(3)-H(3B)	109.3
H(3A)-C(3)-H(3B)	108.0

C(3)-C(4)-C(5)	110.6(2)
C(3)-C(4)-H(4A)	109.5
C(5)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
C(5)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	108.1
C(4)-C(5)-C(6)	110.98(18)
C(4)-C(5)-H(5A)	109.4
C(6)-C(5)-H(5A)	109.4
C(4)-C(5)-H(5B)	109.4
C(6)-C(5)-H(5B)	109.4
H(5A)-C(5)-H(5B)	108.0
C(1)-C(6)-C(5)	109.57(17)
C(1)-C(6)-H(6A)	109.8
C(5)-C(6)-H(6A)	109.8
C(1)-C(6)-H(6B)	109.8
C(5)-C(6)-H(6B)	109.8
H(6A)-C(6)-H(6B)	108.2
C(10)-N(2)-H(21N)	110.0(14)
C(10)-N(2)-H(22N)	110.7(17)
H(21N)-N(2)-H(22N)	107(2)
C(10)-N(2)-H(23N)	113.0(17)
H(21N)-N(2)-H(23N)	107(2)
H(22N)-N(2)-H(23N)	108(2)
N(2)-C(10)-C(15)	109.29(15)
N(2)-C(10)-C(11)	110.98(15)
C(15)-C(10)-C(11)	111.80(16)
N(2)-C(10)-H(10)	108.2
C(15)-C(10)-H(10)	108.2
C(11)-C(10)-H(10)	108.2
C(10)-C(11)-C(12)	108.92(15)
C(10)-C(11)-H(11A)	109.9
C(12)-C(11)-H(11A)	109.9
C(10)-C(11)-H(11B)	109.9
C(12)-C(11)-H(11B)	109.9
H(11A)-C(11)-H(11B)	108.3
C(11)-C(12)-C(13)	111.21(16)
C(11)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12A)	109.4
C(11)-C(12)-H(12B)	109.4

C(13)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0
C(14)-C(13)-C(12)	110.99(17)
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13B)	109.4
C(12)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(13)-C(14)-C(15)	111.50(17)
C(13)-C(14)-H(14A)	109.3
C(15)-C(14)-H(14A)	109.3
C(13)-C(14)-H(14B)	109.3
C(15)-C(14)-H(14B)	109.3
H(14A)-C(14)-H(14B)	108.0
C(10)-C(15)-C(14)	110.01(16)
C(10)-C(15)-H(15A)	109.7
C(14)-C(15)-H(15A)	109.7
C(10)-C(15)-H(15B)	109.7
C(14)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
C(30)-N(3)-H(31N)	110.9(16)
C(30)-N(3)-H(32N)	109.6(15)
H(31N)-N(3)-H(32N)	109(2)
C(30)-N(3)-H(33N)	111.9(16)
H(31N)-N(3)-H(33N)	104(2)
H(32N)-N(3)-H(33N)	111(2)
N(3)-C(30)-C(35)	109.77(15)
N(3)-C(30)-C(31)	109.77(15)
C(35)-C(30)-C(31)	111.56(16)
N(3)-C(30)-H(30)	108.6
C(35)-C(30)-H(30)	108.6
C(31)-C(30)-H(30)	108.6
C(30)-C(31)-C(32)	110.12(16)
C(30)-C(31)-H(31A)	109.6
C(32)-C(31)-H(31A)	109.6
C(30)-C(31)-H(31B)	109.6
C(32)-C(31)-H(31B)	109.6
H(31A)-C(31)-H(31B)	108.1
C(33)-C(32)-C(31)	111.25(18)
C(33)-C(32)-H(32A)	109.4

C(31)-C(32)-H(32A)	109.4
C(33)-C(32)-H(32B)	109.4
C(31)-C(32)-H(32B)	109.4
H(32A)-C(32)-H(32B)	108.0
C(32)-C(33)-C(34)	111.25(18)
C(32)-C(33)-H(33A)	109.4
C(34)-C(33)-H(33A)	109.4
C(32)-C(33)-H(33B)	109.4
C(34)-C(33)-H(33B)	109.4
H(33A)-C(33)-H(33B)	108.0
C(33)-C(34)-C(35)	111.75(17)
C(33)-C(34)-H(34A)	109.3
C(35)-C(34)-H(34A)	109.3
C(33)-C(34)-H(34B)	109.3
C(35)-C(34)-H(34B)	109.3
H(34A)-C(34)-H(34B)	107.9
C(30)-C(35)-C(34)	110.06(16)
C(30)-C(35)-H(35A)	109.6
C(34)-C(35)-H(35A)	109.6
C(30)-C(35)-H(35B)	109.6
C(34)-C(35)-H(35B)	109.6
H(35A)-C(35)-H(35B)	108.2
C(41)-N(4)-H(41N)	111.6(16)
C(41)-N(4)-H(42N)	111.6(15)
H(41N)-N(4)-H(42N)	107(2)
C(41)-N(4)-H(43N)	108.7(16)
H(41N)-N(4)-H(43N)	108(2)
H(42N)-N(4)-H(43N)	110(2)
N(4)-C(41)-C(46)	110.50(15)
N(4)-C(41)-C(42)	109.26(15)
C(46)-C(41)-C(42)	111.71(16)
N(4)-C(41)-H(41)	108.4
C(46)-C(41)-H(41)	108.4
C(42)-C(41)-H(41)	108.4
C(41)-C(42)-C(43)	109.45(16)
C(41)-C(42)-H(42A)	109.8
C(43)-C(42)-H(42A)	109.8
C(41)-C(42)-H(42B)	109.8
C(43)-C(42)-H(42B)	109.8
H(42A)-C(42)-H(42B)	108.2

C(44)-C(43)-C(42)	111.19(17)
C(44)-C(43)-H(43A)	109.4
C(42)-C(43)-H(43A)	109.4
C(44)-C(43)-H(43B)	109.4
C(42)-C(43)-H(43B)	109.4
H(43A)-C(43)-H(43B)	108.0
C(43)-C(44)-C(45)	111.52(18)
C(43)-C(44)-H(44A)	109.3
C(45)-C(44)-H(44A)	109.3
C(43)-C(44)-H(44B)	109.3
C(45)-C(44)-H(44B)	109.3
H(44A)-C(44)-H(44B)	108.0
C(46)-C(45)-C(44)	111.34(18)
C(46)-C(45)-H(45A)	109.4
C(44)-C(45)-H(45A)	109.4
C(46)-C(45)-H(45B)	109.4
C(44)-C(45)-H(45B)	109.4
H(45A)-C(45)-H(45B)	108.0
C(41)-C(46)-C(45)	109.63(17)
C(41)-C(46)-H(46A)	109.7
C(45)-C(46)-H(46A)	109.7
C(41)-C(46)-H(46B)	109.7
C(45)-C(46)-H(46B)	109.7
H(46A)-C(46)-H(46B)	108.2
C(50B)-N(5)-H(51N)	121.7(18)
C(50A)-N(5)-H(51N)	100.3(18)
C(50B)-N(5)-H(52N)	113.1(19)
C(50A)-N(5)-H(52N)	109.4(18)
H(51N)-N(5)-H(52N)	106(2)
C(50B)-N(5)-H(53N)	94.5(18)
C(50A)-N(5)-H(53N)	119.1(18)
H(51N)-N(5)-H(53N)	110(2)
H(52N)-N(5)-H(53N)	111(2)
C(50B)-C(55)-C(54A)	115.3(3)
C(50A)-C(55)-C(54B)	111.1(3)
C(50B)-C(55)-H(55A)	108.4
C(54A)-C(55)-H(55A)	108.4
C(50B)-C(55)-H(55B)	108.4
C(54A)-C(55)-H(55B)	108.4
H(55A)-C(55)-H(55B)	107.5

C(50A)-C(55)-H(55C)	109.4
C(54B)-C(55)-H(55C)	109.4
C(50A)-C(55)-H(55D)	109.4
C(54B)-C(55)-H(55D)	109.4
H(55C)-C(55)-H(55D)	108.0
C(54A)-C(53A)-C(52B)	95.8(3)
C(54A)-C(53A)-H(53A)	112.6
C(52B)-C(53A)-H(53A)	112.6
C(54A)-C(53A)-H(53B)	112.6
C(52B)-C(53A)-H(53B)	112.6
H(53A)-C(53A)-H(53B)	110.1
C(55)-C(54A)-C(53A)	108.2(3)
C(55)-C(54A)-H(54A)	110.1
C(53A)-C(54A)-H(54A)	110.1
C(55)-C(54A)-H(54B)	110.1
C(53A)-C(54A)-H(54B)	110.1
H(54A)-C(54A)-H(54B)	108.4
C(51A)-C(52A)-C(53B)	113.5(3)
C(51A)-C(52A)-H(52A)	108.9
C(53B)-C(52A)-H(52A)	108.9
C(51A)-C(52A)-H(52B)	108.9
C(53B)-C(52A)-H(52B)	108.9
H(52A)-C(52A)-H(52B)	107.7
N(5)-C(50A)-C(51A)	108.5(3)
N(5)-C(50A)-C(55)	105.1(2)
C(51A)-C(50A)-C(55)	107.5(3)
N(5)-C(50A)-H(50A)	111.8
C(51A)-C(50A)-H(50A)	111.8
C(55)-C(50A)-H(50A)	111.8
C(52A)-C(51A)-C(50A)	109.9(3)
C(52A)-C(51A)-H(51A)	109.7
C(50A)-C(51A)-H(51A)	109.7
C(52A)-C(51A)-H(51B)	109.7
C(50A)-C(51A)-H(51B)	109.7
H(51A)-C(51A)-H(51B)	108.2
C(50B)-C(51B)-C(52B)	111.4(4)
C(50B)-C(51B)-H(51C)	109.3
C(52B)-C(51B)-H(51C)	109.3
C(50B)-C(51B)-H(51D)	109.3
C(52B)-C(51B)-H(51D)	109.3

H(51C)-C(51B)-H(51D)	108.0
C(51B)-C(50B)-N(5)	105.3(4)
C(51B)-C(50B)-C(55)	109.3(4)
N(5)-C(50B)-C(55)	108.3(3)
C(51B)-C(50B)-H(50B)	111.2
N(5)-C(50B)-H(50B)	111.2
C(55)-C(50B)-H(50B)	111.2
C(53B)-C(54B)-C(55)	107.7(4)
C(53B)-C(54B)-H(54C)	110.2
C(55)-C(54B)-H(54C)	110.2
C(53B)-C(54B)-H(54D)	110.2
C(55)-C(54B)-H(54D)	110.2
H(54C)-C(54B)-H(54D)	108.5
C(54B)-C(53B)-C(52A)	96.3(4)
C(54B)-C(53B)-H(53C)	112.5
C(52A)-C(53B)-H(53C)	112.5
C(54B)-C(53B)-H(53D)	112.5
C(52A)-C(53B)-H(53D)	112.5
H(53C)-C(53B)-H(53D)	110.0
C(51B)-C(52B)-C(53A)	113.0(3)
C(51B)-C(52B)-H(52C)	109.0
C(53A)-C(52B)-H(52C)	109.0
C(51B)-C(52B)-H(52D)	109.0
C(53A)-C(52B)-H(52D)	109.0
H(52C)-C(52B)-H(52D)	107.8

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+1,-z+2

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $(C_6 H_{14} N)_{10} (ReCl_6)_3 4(Cl) 2(H_2 O)$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Re(1)	12(1)	12(1)	11(1)	0(1)	-3(1)	-3(1)
Cl(1)	16(1)	14(1)	18(1)	-2(1)	-4(1)	-1(1)
Cl(2)	17(1)	17(1)	13(1)	0(1)	-1(1)	-4(1)
Cl(3)	16(1)	19(1)	17(1)	-1(1)	-7(1)	-4(1)
Re(2)	18(1)	12(1)	15(1)	-1(1)	2(1)	-1(1)
Cl(4)	18(1)	13(1)	20(1)	1(1)	-1(1)	-2(1)
Cl(5)	17(1)	15(1)	18(1)	-2(1)	-1(1)	-1(1)
Cl(6)	22(1)	17(1)	23(1)	-2(1)	5(1)	3(1)
Cl(7)	24(1)	31(1)	15(1)	0(1)	-4(1)	8(1)
Cl(8)	28(1)	34(1)	22(1)	-12(1)	-1(1)	-10(1)
Cl(11)	21(1)	24(1)	24(1)	2(1)	-9(1)	-3(1)
Cl(12)	18(1)	17(1)	20(1)	0(1)	-4(1)	-2(1)
O(1W)	25(1)	24(1)	20(1)	-1(1)	-6(1)	-5(1)
N(1)	28(1)	19(1)	18(1)	-4(1)	-3(1)	-3(1)
C(1)	22(1)	18(1)	18(1)	-2(1)	-4(1)	-5(1)
C(2)	37(1)	24(1)	21(1)	0(1)	-7(1)	-7(1)
C(3)	48(1)	24(1)	34(1)	3(1)	-15(1)	-14(1)
C(4)	59(2)	23(1)	36(1)	-7(1)	-20(1)	-9(1)
C(5)	70(2)	29(1)	22(1)	-4(1)	-14(1)	-17(1)
C(6)	38(1)	24(1)	19(1)	-4(1)	-3(1)	-11(1)
N(2)	22(1)	23(1)	17(1)	-1(1)	-6(1)	-2(1)
C(10)	17(1)	19(1)	12(1)	-1(1)	-3(1)	0(1)
C(11)	20(1)	18(1)	22(1)	-1(1)	-4(1)	-2(1)
C(12)	27(1)	24(1)	32(1)	-8(1)	-12(1)	0(1)
C(13)	37(1)	27(1)	26(1)	-11(1)	-10(1)	6(1)
C(14)	31(1)	28(1)	22(1)	-7(1)	0(1)	3(1)
C(15)	16(1)	26(1)	23(1)	-5(1)	0(1)	1(1)
N(3)	15(1)	18(1)	18(1)	-3(1)	-3(1)	-1(1)
C(30)	18(1)	13(1)	16(1)	-2(1)	-2(1)	-2(1)
C(31)	16(1)	30(1)	30(1)	-12(1)	-5(1)	3(1)
C(32)	21(1)	39(1)	44(1)	-20(1)	-4(1)	7(1)
C(33)	34(1)	30(1)	26(1)	-12(1)	6(1)	-2(1)
C(34)	33(1)	38(1)	25(1)	-15(1)	-9(1)	1(1)
C(35)	24(1)	34(1)	22(1)	-11(1)	-9(1)	5(1)
N(4)	18(1)	17(1)	21(1)	-1(1)	-6(1)	-4(1)

C(41)	21(1)	17(1)	17(1)	-1(1)	-7(1)	-5(1)
C(42)	19(1)	21(1)	23(1)	-4(1)	-3(1)	-6(1)
C(43)	31(1)	27(1)	34(1)	-5(1)	-10(1)	-13(1)
C(44)	47(1)	22(1)	32(1)	-9(1)	-7(1)	-7(1)
C(45)	43(1)	31(1)	28(1)	-13(1)	0(1)	-2(1)
C(46)	25(1)	26(1)	28(1)	-9(1)	2(1)	-6(1)
N(5)	28(1)	23(1)	27(1)	3(1)	0(1)	-2(1)
C(55)	55(2)	24(1)	18(1)	6(1)	-6(1)	-9(1)
C(53A)	13(2)	22(2)	26(2)	2(2)	-2(2)	1(1)
C(54A)	7(2)	18(2)	26(2)	11(1)	0(1)	1(1)
C(52A)	12(2)	33(2)	20(2)	6(2)	-7(2)	3(2)
C(50A)	5(2)	20(2)	17(2)	8(1)	-6(1)	-1(1)
C(51A)	10(2)	27(2)	13(2)	9(1)	-3(1)	-2(1)
C(51B)	38(3)	26(2)	31(2)	3(2)	-10(2)	-1(2)
Cl(9A)	15(1)	14(1)	18(1)	2(1)	-5(1)	-2(1)
Cl(9B)	17(1)	12(1)	24(1)	2(1)	-1(1)	-2(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^3) for $(C_6H_{14}N)_{10}(ReCl_6)_3 \cdot 4(Cl) \cdot 2(H_2O)$.

	x	y	z	U(eq)
H(1W)	6256(14)	7542(13)	8727(13)	35
H(2W)	6940(20)	8384(7)	8593(12)	35
H(11N)	9010(20)	9479(19)	4121(17)	36(7)
H(12N)	9410(20)	10007(19)	3328(16)	31(6)
H(13N)	10190(30)	9258(19)	3652(16)	39(7)
H(1)	7974	8789	3326	24
H(2A)	8297	7678	4491	33
H(2B)	9662	7426	3956	33
H(3A)	8310	6116	3966	41
H(3B)	7397	6909	3618	41
H(4A)	8593	6149	2493	45
H(4B)	9847	6456	2681	45
H(5A)	8159	7860	2091	47
H(5B)	9510	7608	1537	47
H(6A)	10448	8359	2413	33
H(6B)	9548	9164	2060	33
H(21N)	-1690(20)	7101(18)	8339(15)	29(6)
H(22N)	-760(20)	6330(20)	8296(16)	39(7)
H(23N)	-420(20)	7325(19)	7958(16)	34(7)
H(10)	-1413	7344	6902	19
H(11A)	-2913	6111	7682	25
H(11B)	-1867	5257	7608	25
H(12A)	-2590	6393	6201	31
H(12B)	-2901	5223	6545	31
H(13A)	-788	4809	6110	35
H(13B)	-1173	5432	5316	35
H(14A)	-265	6903	5476	34
H(14B)	747	6028	5433	34
H(15A)	405	5791	6908	27
H(15B)	714	6959	6550	27
H(31N)	4010(20)	4682(19)	9408(15)	30(6)
H(32N)	3080(20)	3931(17)	9800(14)	24(6)
H(33N)	4160(20)	3992(18)	10087(16)	30(6)
H(30)	4309	2637	9341	19
H(31A)	6184	3395	9319	30

H(31B)	6076	4225	8537	30
H(32A)	7434	2949	8016	41
H(32B)	6403	2101	8484	41
H(33A)	6428	2426	7056	38
H(33B)	6263	3609	7088	38
H(34A)	4419	2091	7927	36
H(34B)	4337	2937	7151	36
H(35A)	4124	4211	8001	30
H(35B)	3085	3365	8459	30
H(41N)	1970(20)	7801(18)	8688(16)	32(7)
H(42N)	1600(20)	7202(18)	9485(16)	32(6)
H(43N)	2840(20)	7197(18)	8966(15)	32(7)
H(41)	2967	8093	9971	22
H(42A)	3261	9350	8364	26
H(42B)	4311	8622	8613	26
H(43A)	4418	9568	9670	36
H(43B)	4639	10311	8790	36
H(44A)	2598	10883	9165	40
H(44B)	3226	11013	9898	40
H(45A)	2210	9562	10749	42
H(45B)	1189	10293	10466	42
H(46A)	873	8585	10311	33
H(46B)	1103	9319	9423	33
H(51N)	3160(20)	8623(19)	6655(16)	32(7)
H(52N)	3920(20)	9030(20)	5925(18)	40(7)
H(53N)	4490(30)	8530(20)	6591(19)	60(9)
H(55A)	2851	6954	7097	41
H(55B)	4209	6534	7074	41
H(55C)	2798	6615	7154	41
H(55D)	4232	6867	7015	41
H(53A)	4221	4887	5492	26
H(53B)	5139	5667	5688	26
H(54A)	2463	5790	6344	23
H(54B)	3261	5150	6911	23
H(52A)	5194	6110	4772	26
H(52B)	4074	6602	4426	26
H(50A)	2713	7628	5887	17
H(51A)	4598	8008	4758	22
H(51B)	5397	7429	5352	22
H(51C)	3913	8118	4871	39

H(51D)	2677	7656	5545	39
H(50B)	5090	7484	5798	33
H(54C)	4895	5644	6140	43
H(54D)	3709	5095	6818	43
H(53C)	2521	5924	5822	45
H(53D)	3368	4973	5532	45
H(52C)	4435	6661	4417	32
H(52D)	3021	6343	4863	32

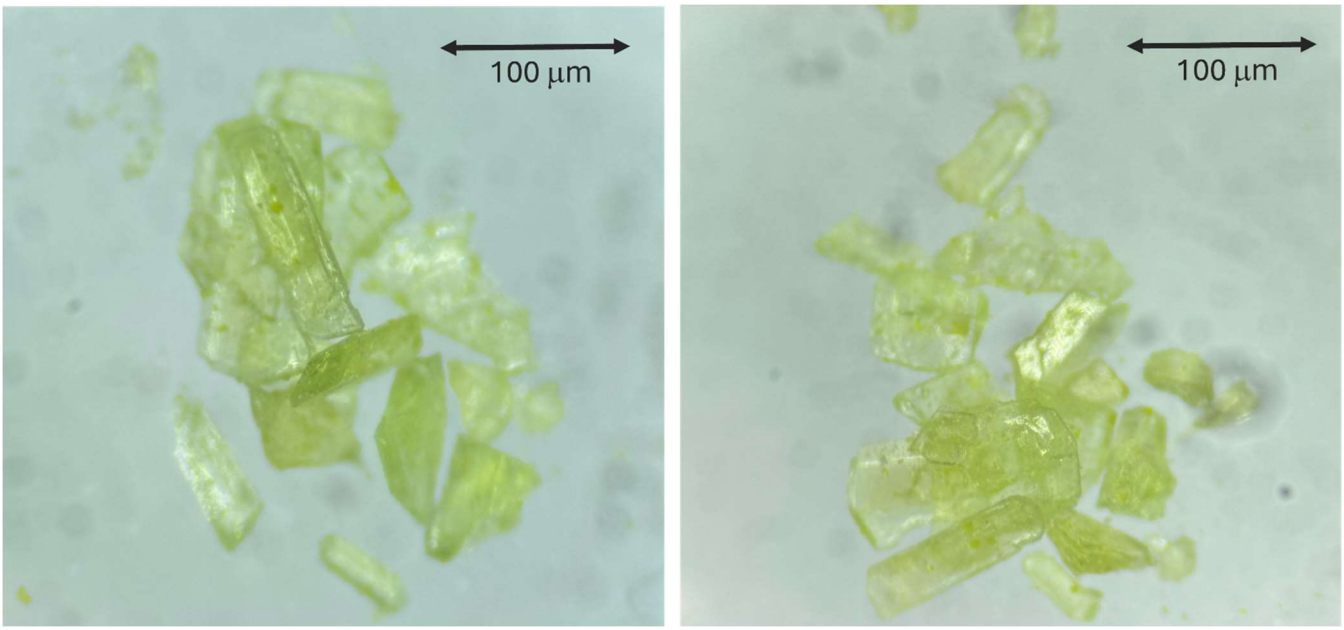


Figure S1. Photographies of the investigated crystals.

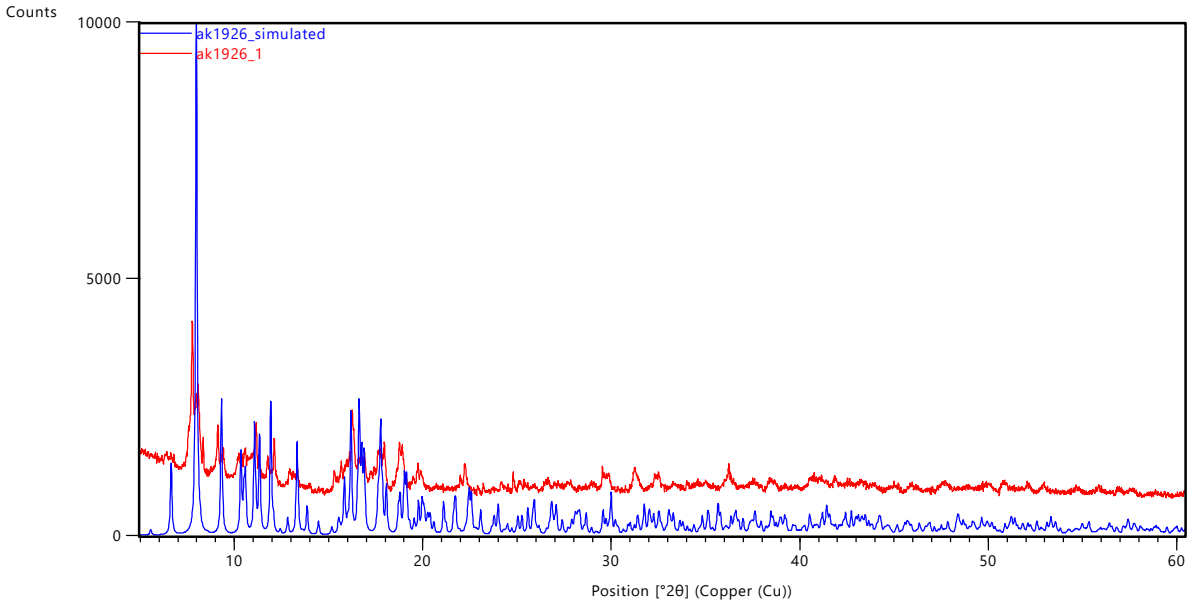


Figure S2. Powder XRD patterns of the investigated compound.