Supporting Information for

Cooperative Lone Pair-π and Coordination Interactions in Naphthalene Diimide Coordination Networks

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Table of Contents:

1. Single Crystal Structures

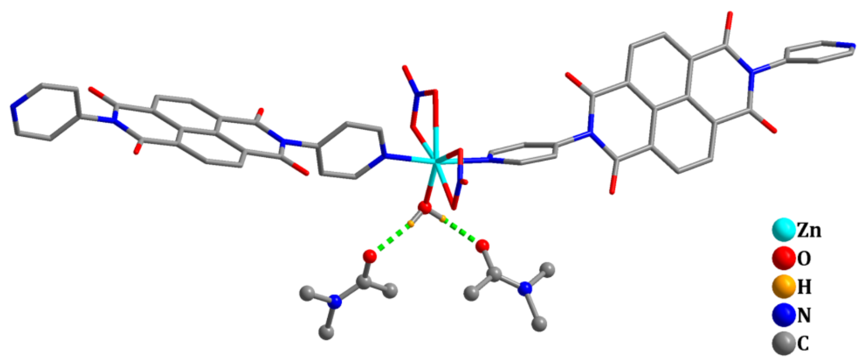

Figure S1. Hydrogen bonds (green dotted line) between the coordinated water and DMF molecules in complex **1**

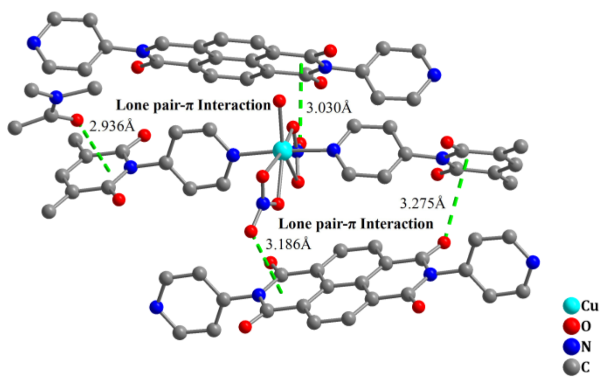

Figure S2. Lone pair-π interactions highlighted in complex **2**

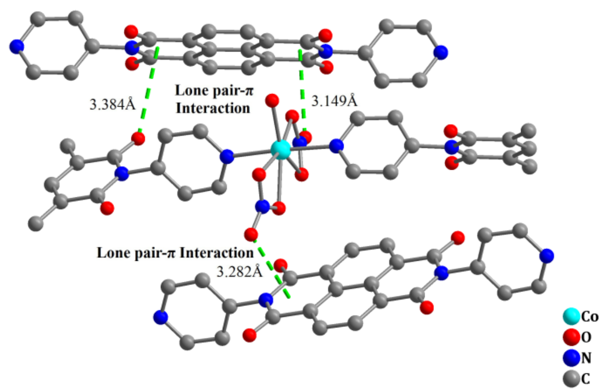

Figure S3. Lone pair-π interactions highlighted in complex **3**

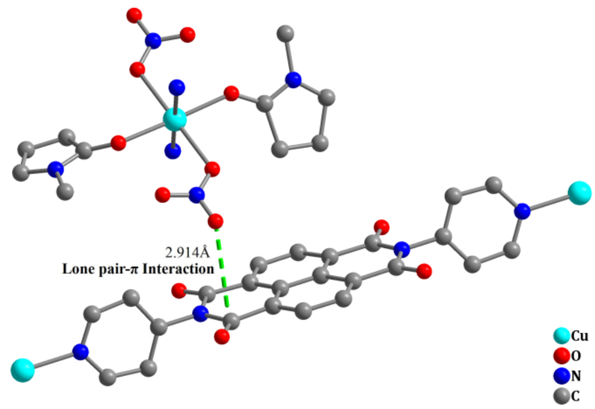

Figure S4. Lone pair-π interactions highlighted in complex **5**

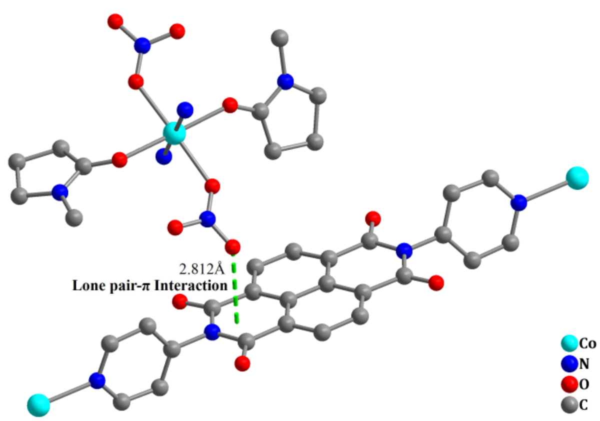

Figure S5. Lone pair-π interactions highlighted in complex **6**

2. IR Studies

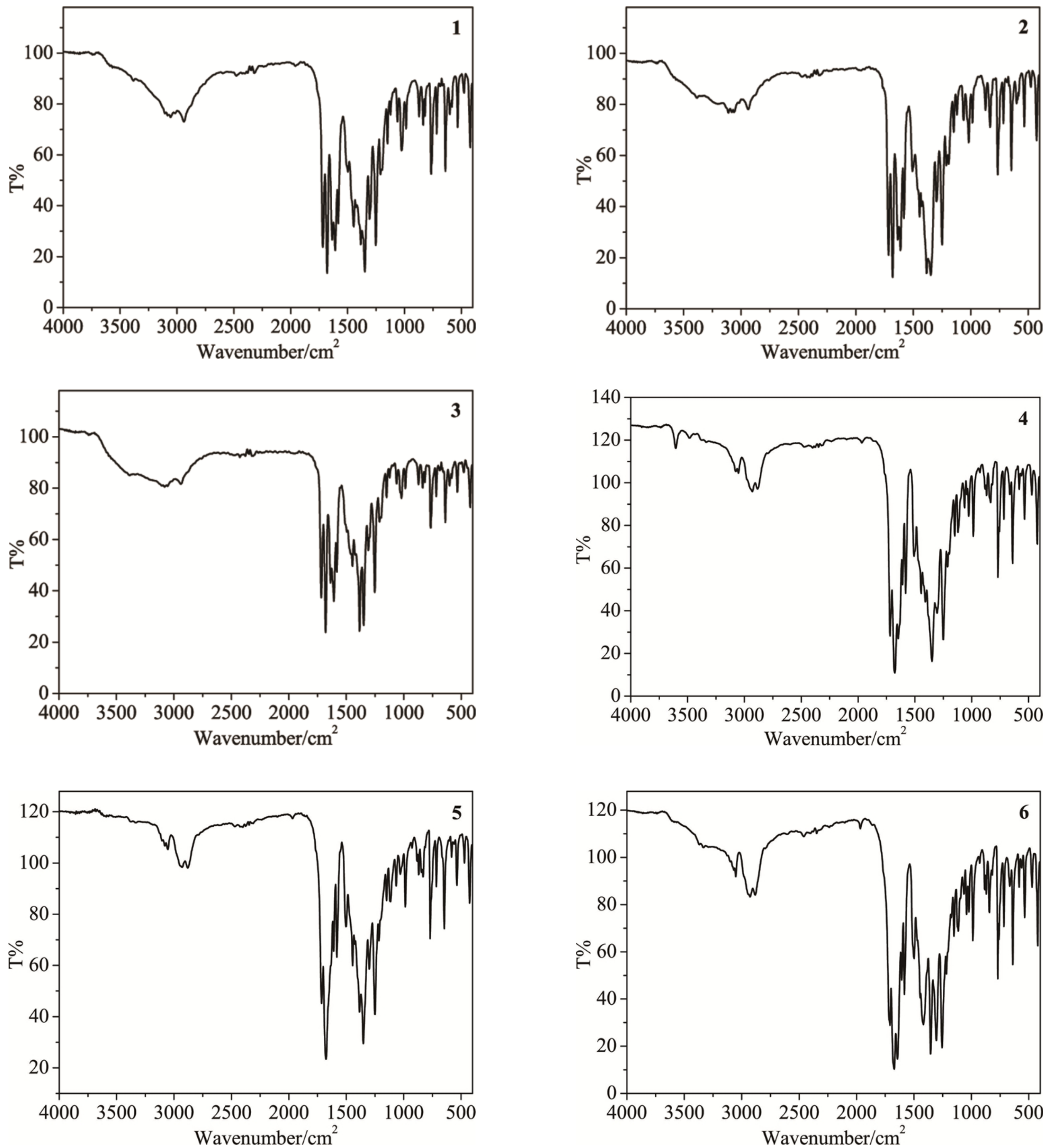

Figure S6. IR spectra of **1-6**

3. Powder X-ray Diffraction Studies

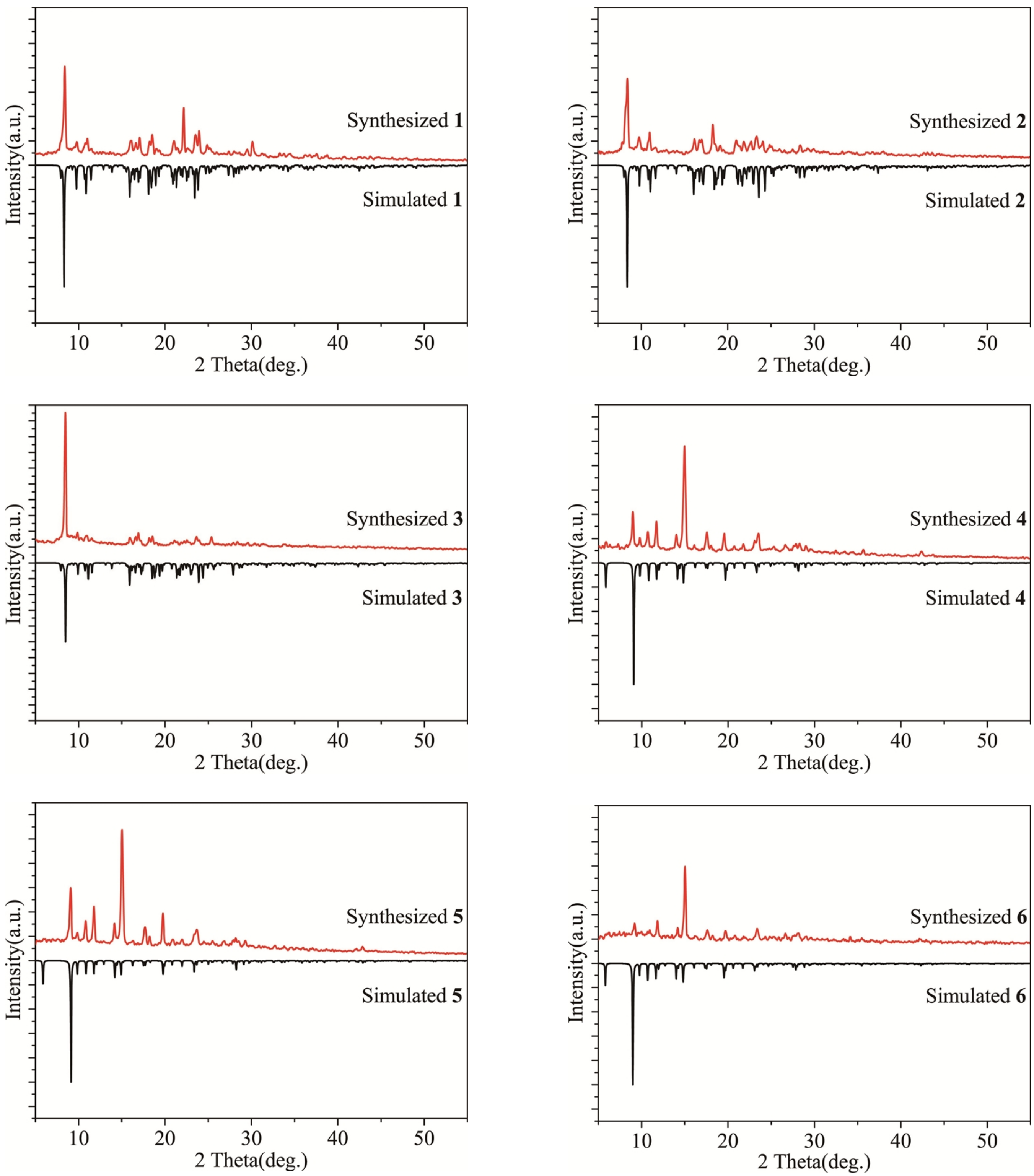

Figure S7. Comparison of the simulated and synthesized PXRD for **1-6**

4. TGA Studies

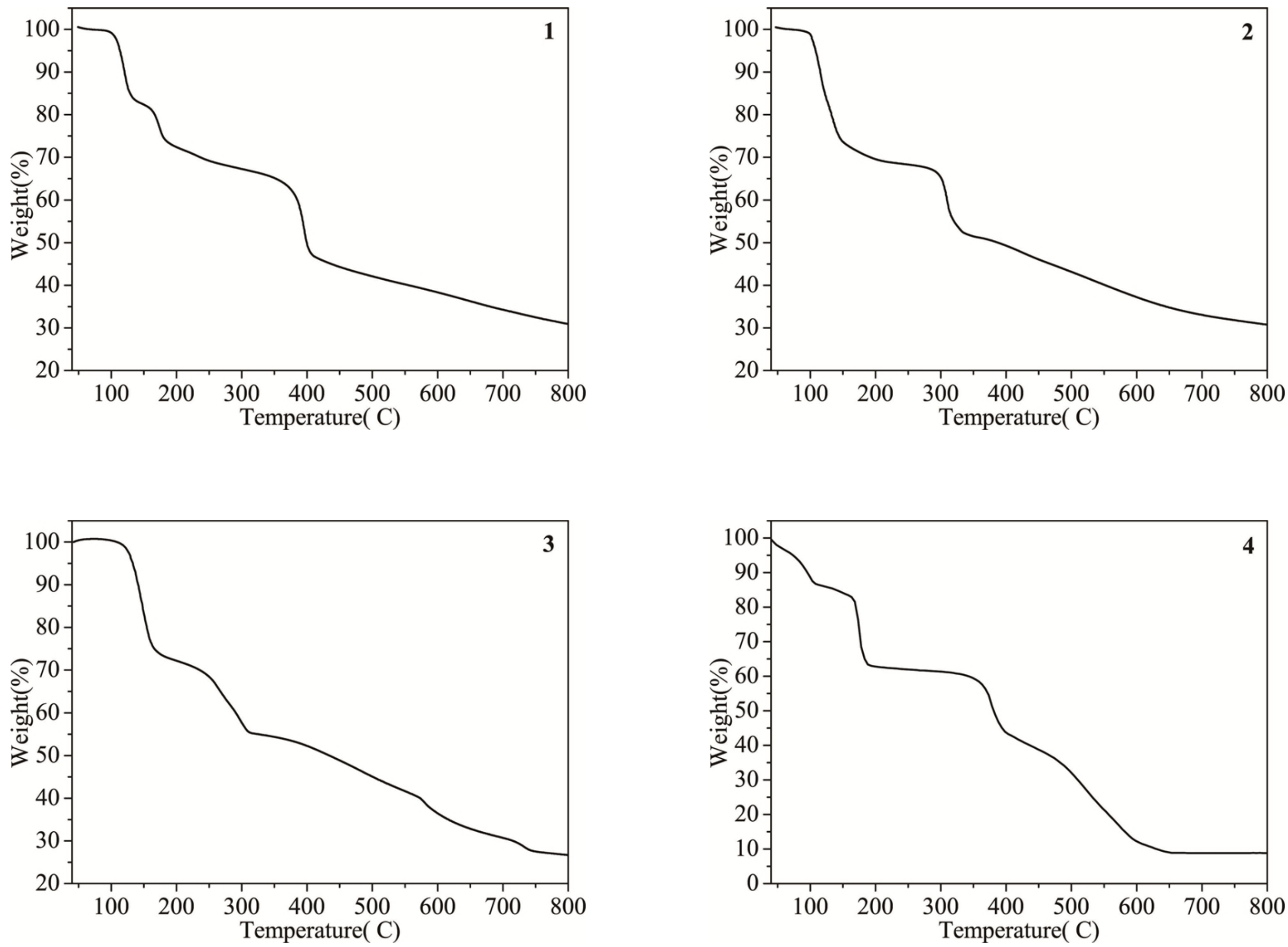

Figure S8. The TGA patterns for **1-4** under the N_2 with the rate of 5°C/min.

5. Crystallographic Data

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Zn(1)	8311(1)	6782(1)	2515(1)	44(1)	C(7)	2854(3)	1024(3)	901(3)	51(1)
O(1)	2507(2)	3672(2)	752(2)	62(1)	C(8)	4363(3)	3157(3)	1319(2)	46(1)
O(2)	3692(2)	783(2)	1174(2)	75(1)	C(9)	4983(3)	3866(3)	745(3)	58(1)
O(3)	6942(3)	7799(3)	2316(2)	77(1)	C(10)	6146(3)	4827(3)	1114(3)	59(1)
O(4)	6829(3)	8585(3)	1057(2)	82(1)	C(11)	6094(3)	4359(3)	2551(3)	56(1)
O(5)	7815(3)	7553(2)	1307(2)	63(1)	C(12)	4942(3)	3367(3)	2234(3)	55(1)
O(6)	7971(3)	6760(3)	3874(2)	70(1)	C(13)	10866(3)	9004(3)	2816(3)	61(1)
O(7)	9231(4)	6099(4)	3907(3)	112(1)	C(14)	9612(3)	9296(3)	3589(2)	49(1)
O(8)	8934(4)	6620(4)	5183(2)	112(1)	C(15)	10515(3)	10454(3)	3952(2)	49(1)
O(9)	9225(2)	6183(2)	1850(2)	61(1)	C(16)	11630(3)	10877(3)	3740(2)	44(1)
O(10)	13093(3)	11429(2)	5455(2)	67(1)	C(17)	11819(3)	10158(3)	3151(3)	62(1)
O(11)	12092(3)	12691(2)	2755(2)	70(1)	C(18)	13307(3)	12258(3)	5022(2)	49(1)
O(12)	1685(3)	7100(3)	2054(3)	88(1)	C(19)	14300(3)	13507(3)	5392(2)	45(1)
O(13)	8282(3)	3805(3)	1488(2)	84(1)	C(20)	15018(4)	13758(3)	6285(3)	58(1)
O(14)	5295(5)	2335(5)	4130(3)	137(2)	C(21)	14513(3)	14409(3)	4824(2)	41(1)
N(1)	3089(2)	2222(2)	959(2)	43(1)	C(22)	13780(3)	14180(3)	3910(2)	46(1)
N(2)	6681(2)	5116(2)	2016(2)	44(1)	C(23)	14018(4)	15076(3)	3370(2)	59(1)
N(3)	9775(2)	8561(2)	3040(2)	45(1)	C(24)	12763(3)	12950(3)	3528(2)	49(1)
N(4)	12607(2)	12086(2)	4109(2)	45(1)	C(25)	4100(5)	8397(5)	2190(5)	119(2)
N(5)	7182(3)	7999(3)	1557(2)	55(1)	C(26)	3862(5)	6815(7)	986(5)	123(2)
N(6)	8729(3)	6482(3)	4342(2)	65(1)	C(27)	2128(4)	6703(4)	1545(4)	78(1)
N(7)	3290(4)	7249(4)	1556(3)	88(1)	C(28)	1348(5)	5572(5)	878(4)	111(2)
N(8)	8099(5)	2079(4)	1870(4)	132(2)	C(29)	6872(6)	1457(5)	1150(6)	136(3)
N(9)	6887(8)	2208(10)	4708(7)	204(5)	C(30)	8569(10)	1320(7)	2382(8)	237(7)
C(1)	1251(3)	-1092(3)	403(3)	59(1)	C(31)	8687(5)	3229(5)	1991(4)	94(2)
C(2)	1543(3)	101(3)	494(2)	44(1)	C(32)	9922(6)	3856(6)	2706(5)	138(3)
C(3)	622(3)	448(3)	200(2)	40(1)	C(33)	6030(14)	2038(16)	4398(10)	250(9)
C(4)	899(3)	1665(3)	282(2)	42(1)	C(34)	5620(20)	720(20)	3840(20)	860(50)
C(5)	-18(3)	1982(3)	-13(3)	55(1)	C(35)	7837(10)	1773(10)	5045(10)	300(9)
C(6)	2202(3)	2611(3)	672(2)	46(1)	C(36)	7450(10)	3573(9)	5295(9)	221(6)

Table S2. Selected bond lengths (Å) and bond angles (°) for **1**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Zn(1)-O(9)	2.021(3)	Zn(1)-N(2)	2.120(3)
Zn(1)-N(3)	2.135(3)	Zn(1)-O(6)	2.166(3)
Zn(1)-O(5)	2.186(3)	Zn(1)-O(7)	2.528(5)
Zn(1)-O(3)	2.537(4)		
Atoms	Angles (º)	Atoms	Angles (º)
O(9)-Zn(1)-N(2)	88.99(11)	O(9)-Zn(1)-N(3)	98.65(11)
N(2)-Zn(1)-N(3)	171.73(11)	O(9)-Zn(1)-O(6)	136.34(12)
N(2)-Zn(1)-O(6)	91.08(11)	N(3)-Zn(1)-O(6)	85.57(11)
O(9)-Zn(1)-O(5)	90.62(12)	N(2)-Zn(1)-O(5)	91.31(11)
N(3)-Zn(1)-O(5)	85.49(11)	O(6)-Zn(1)-O(5)	133.01(12)
O(9)-Zn(1)-O(7)	84.74(13)	N(2)-Zn(1)-O(7)	96.20(13)
N(3)-Zn(1)-O(7)	87.68(13)	O(6)-Zn(1)-O(7)	51.86(12)
O(5)-Zn(1)-O(7)	171.08(13)	O(9)-Zn(1)-O(3)	143.50(12)
N(2)-Zn(1)-O(3)	88.31(11)	N(3)-Zn(1)-O(3)	83.68(11)
O(6)-Zn(1)-O(3)	80.11(11)	O(5)-Zn(1)-O(3)	53.08(10)
O(7)-Zn(1)-O(3)	131.72(12)		

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	6682(1)	3212(1)	2463(1)	27(1)	C(7)	12101(3)	8971(3)	4059(2)	29(1)
O(1)	12434(2)	6287(2)	4264(2)	31(1)	C(8)	9977(3)	6608(3)	2707(2)	31(1)
O(2)	11260(2)	9212(2)	3756(2)	40(1)	C(9)	10573(3)	6820(3)	3651(2)	26(1)
O(3)	5776(2)	3795(2)	3238(2)	38(1)	C(10)	9941(3)	6093(3)	4252(2)	32(1)
O(4)	7239(2)	2446(2)	3663(2)	34(1)	C(11)	8767(3)	5109(3)	3874(2)	31(1)
O(5)	8157(2)	2105(3)	2683(2)	42(1)	C(12)	8812(3)	5588(3)	2379(2)	33(1)
O(6)	8183(3)	1362(3)	4009(2)	43(1)	C(13)	4166(4)	1078(3)	2191(3)	42(1)
O(7)	6994(3)	3239(3)	1085(3)	55(1)	C(14)	3200(3)	-91(3)	1860(3)	41(1)
O(8)	5728(4)	3946(4)	977(4)	95(2)	C(15)	3391(3)	-828(3)	1285(2)	28(1)
O(9)	6041(4)	3324(4)	-279(2)	79(1)	C(16)	4535(3)	-397(3)	1070(2)	29(1)
O(10)	1925(2)	-1388(2)	-483(2)	38(1)	C(17)	5449(3)	778(3)	1423(2)	30(1)
O(11)	2953(2)	-2647(2)	2301(2)	40(1)	C(18)	1703(3)	-2232(3)	-30(2)	30(1)
O(12)	3280(3)	2932(3)	2897(3)	52(1)	C(19)	700(3)	-3492(3)	-407(2)	29(1)
O(13)	6785(3)	6202(2)	3576(2)	45(1)	C(20)	494(3)	-4403(3)	177(2)	25(1)
O(14)	9692(4)	7627(5)	808(3)	82(1)	C(21)	-24(3)	-3752(3)	-1324(2)	34(1)
N(1)	11859(2)	7761(2)	4017(2)	26(1)	C(22)	1002(3)	-5067(3)	1684(2)	35(1)
N(2)	8230(2)	4818(2)	2945(2)	26(1)	C(23)	1242(3)	-4165(3)	1116(2)	28(1)
N(4)	7868(3)	1953(2)	3450(2)	30(1)	C(24)	2269(3)	-2920(3)	1509(2)	29(1)
N(5)	5270(2)	1517(2)	1967(2)	28(1)	C(25)	3671(5)	4470(5)	4100(4)	67(1)
N(6)	2406(2)	-2044(2)	907(2)	27(1)	C(26)	2858(4)	3321(4)	3432(3)	46(1)
N(7)	1662(3)	2734(4)	3447(3)	51(1)	C(27)	826(4)	1603(4)	2813(4)	64(1)
N(8)	6956(4)	7965(3)	3182(4)	71(1)	C(28)	1123(5)	3146(5)	4070(4)	63(1)
N(9)	8270(7)	8244(7)	494(7)	146(3)	C(29)	5082(6)	6115(5)	2341(4)	87(2)
N(10)	6216(3)	3505(3)	583(2)	40(1)	C(30)	6346(4)	6764(4)	3068(3)	50(1)
C(1)	15003(3)	7999(3)	5040(3)	31(1)	C(31)	8179(5)	8616(4)	3895(5)	72(2)
C(2)	14080(3)	8321(3)	4722(2)	26(1)	C(32)	6433(8)	8710(6)	2676(7)	137(4)
C(3)	12753(3)	7364(3)	4329(2)	26(1)	C(33)	7572(7)	6376(6)	-302(6)	91(2)
C(4)	14364(3)	9552(3)	4797(2)	24(1)	C(34)	8567(8)	7470(7)	350(5)	89(2)
C(5)	13435(3)	9901(3)	4485(2)	27(1)	C(35)	9377(14)	9407(13)	1089(15)	345(13)
C(6)	13741(3)	11108(3)	4563(3)	33(1)	C(36)	7107(10)	8253(9)	33(12)	261(11)

Table S4. Selected bond lengths (Å) and bond angles (°) for **2**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Cu(1)-N(2)	2.005(3)	Cu(1)-N(5)	2.016(3)
Cu(1)-O(3)	2.092(3)	Cu(1)-O(7)	2.139(4)
Cu(1)-O(4)	2.152(3)	Cu(1)-O(8)	2.629(6)
Cu(1)-O(5)	2.727(3)		
Atoms	**Angles (º)**	**Atoms**	**Angles (º)**
N(2)-Cu(1)-N(5)	173.02(11)	N(2)-Cu(1)-O(3)	87.67(11)
N(5)-Cu(1)-O(3)	98.48(11)	N(2)-Cu(1)-O(7)	91.84(12)
N(5)-Cu(1)-O(7)	85.64(12)	O(3)-Cu(1)-O(7)	139.43(11)
N(2)-Cu(1)-O(4)	91.00(11)	N(5)-Cu(1)-O(4)	85.83(11)
O(3)-Cu(1)-O(4)	89.12(11)	O(7)-Cu(1)-O(4)	131.44(11)
N(2)-Cu(1)-O(8)	95.22(13)	N(5)-Cu(1)-O(8)	88.28(13)
O(3)-Cu(1)-O(8)	88.52(12)	O(7)-Cu(1)-O(8)	51.11(12)
O(4)-Cu(1)-O(8)	173.25(11)	N(2)-Cu(1)-O(5)	89.65(10)
N(5)-Cu(1)-O(5)	83.52(10)	O(3)-Cu(1)-O(5)	140.02(10)
O(7)-Cu(1)-O(5)	80.51(10)	O(4)-Cu(1)-O(5)	51.04(9)
O(8)-Cu(1)-O(5)	131.43(10)		

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **3**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Co(1)	8274(1)	1813(1)	2545(1)	21(1)	C(6)	2179(3)	-2389(3)	685(2)	25(1)
O(1)	2478(2)	-1325(2)	761(2)	30(1)	C(7)	2880(3)	-3985(3)	911(2)	26(1)
O(2)	3737(2)	-4232(2)	1185(2)	39(1)	C(8)	4365(3)	-1850(3)	1341(2)	25(1)
O(3)	6802(2)	3623(2)	1090(2)	39(1)	C(9)	4937(3)	-1638(3)	2280(2)	30(1)
O(4)	7821(2)	2567(2)	1267(2)	30(1)	C(10)	4986(3)	-1140(3)	739(2)	32(1)
O(5)	6957(2)	2745(2)	2349(2)	32(1)	C(11)	6147(3)	-174(3)	1115(2)	29(1)
O(6)	9188(2)	1221(2)	1811(2)	30(1)	C(12)	6088(3)	-637(3)	2602(2)	30(1)
O(7)	7919(2)	1837(2)	3928(2)	30(1)	C(13)	10852(3)	4015(3)	2821(3)	33(1)
O(8)	9189(3)	1132(3)	3810(2)	44(1)	C(14)	9587(3)	4345(3)	3612(2)	24(1)
O(9)	8937(3)	1506(3)	5202(2)	52(1)	C(15)	10492(3)	5505(3)	3968(2)	24(1)
O(10)	12009(2)	7721(2)	2748(2)	38(1)	C(16)	11818(3)	5155(3)	3159(3)	34(1)
O(11)	13166(2)	6407(2)	5469(2)	32(1)	C(17)	11627(3)	5902(3)	3745(2)	23(1)
O(12)	1681(2)	2106(2)	2096(2)	41(1)	C(18)	13354(3)	7257(3)	5032(2)	24(1)
O(13)	8252(2)	8842(2)	1422(2)	36(1)	C(19)	12714(3)	7979(3)	3529(2)	29(1)
N(1)	3094(2)	-2785(2)	971(2)	24(1)	C(20)	13937(3)	10108(3)	3355(3)	36(1)
N(2)	6677(2)	121(2)	2042(2)	23(1)	C(21)	13739(3)	9200(3)	3909(2)	26(1)
N(3)	7181(3)	3001(2)	1562(2)	28(1)	C(22)	14513(3)	9415(3)	4822(2)	22(1)
N(4)	8697(3)	1486(3)	4343(2)	32(1)	C(23)	14346(3)	8494(3)	5398(2)	25(1)
N(5)	9754(2)	3598(2)	3051(2)	24(1)	C(24)	15091(3)	8739(3)	6301(2)	34(1)
N(6)	12605(2)	7102(2)	4117(2)	24(1)	C(25)	3891(4)	1832(5)	981(3)	58(1)
N(7)	3334(3)	2274(3)	1591(2)	39(1)	C(26)	4142(4)	3393(4)	2212(3)	49(1)
N(8)	8056(4)	7073(3)	1811(3)	76(2)	C(27)	2125(3)	1708(3)	1577(3)	34(1)
C(1)	1295(3)	-6099(3)	401(3)	33(1)	C(28)	1324(4)	589(4)	902(3)	50(1)
C(2)	1571(3)	-4902(3)	499(2)	27(1)	C(29)	6830(5)	6446(4)	1110(5)	78(2)
C(3)	623(3)	-4552(3)	197(2)	23(1)	C(30)	8578(7)	6321(5)	2300(7)	164(5)
C(4)	882(3)	-3334(3)	292(2)	23(1)	C(31)	8666(4)	8265(3)	1933(3)	42(1)
C(5)	-58(3)	-3008(3)	-5(3)	31(1)	C(32)	9901(5)	8888(4)	2666(4)	65(2)

Table S6. Selected bond lengths (Å) and bond angles (°) for **3**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Co(1)-O(6)	2.042(2)	Co(1)-N(2)	2.130(3)
Co(1)-N(5)	2.150(3)	Co(1)-O(7)	2.164(2)
Co(1)-O(4)	2.191(2)	Co(1)-O(8)	2.331(3)
Co(1)-O(5)	2.348(3)		
Atoms	**Angles (º)**	**Atoms**	**Angles (º)**
O(6)-Co(1)-N(2)	87.24(10)	O(6)-Co(1)-N(5)	97.83(10)
N(2)-Co(1)-N(5)	174.07(10)	O(6)-Co(1)-O(7)	140.29(10)
N(2)-Co(1)-O(7)	92.25(10)	N(5)-Co(1)-O(7)	85.83(10)
O(6)-Co(1)-O(4)	85.33(10)	N(2)-Co(1)-O(4)	92.34(10)
N(5)-Co(1)-O(4)	85.04(10)	O(7)-Co(1)-O(4)	134.32(9)
O(6)-Co(1)-O(8)	83.96(10)	N(2)-Co(1)-O(8)	94.81(11)
N(5)-Co(1)-O(8)	88.81(11)	O(7)-Co(1)-O(8)	56.49(9)
O(4)-Co(1)-O(8)	166.81(9)	O(6)-Co(1)-O(5)	141.26(10)
N(2)-Co(1)-O(5)	89.36(9)	N(5)-Co(1)-O(5)	84.76(10)
O(7)-Co(1)-O(5)	78.38(9)	O(4)-Co(1)-O(5)	56.26(9)
O(8)-Co(1)-O(5)	134.77(9)		

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **4**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Zn(1)	1347(1)	2500	1250	60(1)	C(4)	1946(10)	5190(7)	1064(6)	210(9)
O(1)	1310(2)	3574(2)	1294(2)	85(1)	C(5)	1068(9)	4773(8)	1841(6)	198(8)
O(2)	1372(3)	2671(3)	365(2)	90(1)	C(6)	2766(3)	2161(3)	856(3)	59(1)
O(3)	1188(8)	1708(5)	-4(4)	222(6)	C(7)	3482(3)	2157(3)	848(3)	60(2)
O(4)	1399(4)	2497(5)	-517(3)	145(3)	C(8)	3832(3)	2500	1250	51(2)
O(5)	4547(2)	3218(3)	503(2)	76(1)	C(9)	4884(2)	2896(3)	843(2)	53(1)
O(6)	8149(2)	3217(2)	513(2)	69(1)	C(10)	5631(2)	2902(3)	858(3)	54(1)
N(1)	1505(6)	4677(4)	1324(5)	152(4)	C(11)	6000(3)	3285(3)	474(3)	61(2)
N(2)	1309(3)	2298(4)	-39(3)	83(2)	C(12)	6003(4)	2500	1250	56(2)
N(3)	2417(3)	2500	1250	58(2)	C(13)	6712(2)	2500	1250	37(1)
N(4)	4553(3)	2500	1250	54(2)	C(14)	6708(2)	3280(3)	478(2)	53(1)
N(5)	8129(2)	2500	1250	49(1)	C(15)	7054(2)	2899(3)	851(2)	46(1)
N(6)	10274(2)	2500	1250	52(2)	C(16)	7813(2)	2897(3)	855(3)	53(1)
C(1)	1615(4)	4081(4)	1123(3)	80(2)	C(17)	8891(3)	2500	1250	43(2)
C(2)	2125(5)	4132(5)	670(4)	110(3)	C(18)	9222(2)	2037(3)	922(3)	62(2)
C(3)	2254(10)	4864(6)	578(6)	195(8)	C(19)	9933(3)	2082(3)	938(3)	65(2)

Table S8. Selected bond lengths (Å) and bond angles (°) for **4**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Zn(1)-N(3)	2.097(6)	Zn(1)-N(6)#1	2.101(5)
Zn(1)-O(1)	2.108(5)	Zn(1)-O(1)#2	2.108(5)
Zn(1)-O(2)	2.156(5)	Zn(1)-O(2)#2	2.156(5)
Atoms	**Angles (º)**	**Atoms**	**Angles (º)**
N(3)-Zn(1)-N(6)#1	180.0	N(3)-Zn(1)-O(1)	91.93(12)
N(6)#1-Zn(1)-O(1)	88.07(12)	N(3)-Zn(1)-O(1)#2	91.93(12)
N(6)#1-Zn(1)-O(1)#2	88.07(12)	O(1)-Zn(1)-O(1)#2	176.1(2)
N(3)-Zn(1)-O(2)	88.71(16)	N(6)#1-Zn(1)-O(2)	91.29(16)
O(1)-Zn(1)-O(2)	84.0(2)	O(1)#2-Zn(1)-O(2)	96.1(2)
N(3)-Zn(1)-O(2)#2	88.71(16)	N(6)#1-Zn(1)-O(2)#2	91.29(16)
O(1)-Zn(1)-O(2)#2	96.1(2)	O(1)#2-Zn(1)-O(2)#2	84.0(2)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z; #2 x,-y+1/2,-z+1/4.

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **5**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Cu(1)	1384(1)	2500	1250	87(1)	C(4)	1900(19)	-165(12)	1413(15)	281(14)
O(1)	1348(3)	1438(4)	1149(4)	142(3)	C(5)	1167(18)	212(12)	600(11)	281(14)
O(2)	1386(4)	2737(6)	338(4)	130(3)	C(6)	2767(3)	2149(4)	884(4)	83(2)
O(3)	1237(14)	1740(12)	125(16)	410(20)	C(7)	3483(3)	2135(4)	863(4)	81(2)
O(4)	1353(9)	2412(11)	-463(9)	249(8)	C(8)	3833(3)	2500	1250	62(2)
O(5)	4558(2)	3225(3)	503(2)	88(2)	C(9)	4887(3)	2901(4)	842(3)	70(2)
O(6)	8192(2)	3202(3)	498(3)	100(2)	C(10)	5660(3)	2897(4)	839(3)	75(2)
N(1)	1559(9)	317(8)	1147(8)	214(8)	C(11)	6032(3)	3278(4)	456(4)	86(2)
N(2)	1340(7)	2297(9)	8(10)	168(7)	C(12)	6032(3)	2500	1250	69(2)
N(3)	2415(3)	2500	1250	77(2)	C(13)	6759(3)	2500	1250	57(2)
N(4)	4578(3)	2500	1250	62(2)	C(14)	6747(3)	3265(4)	467(3)	81(2)
N(5)	8191(3)	2500	1250	86(3)	C(15)	7096(3)	2901(3)	847(3)	64(2)
N(6)	10347(3)	2500	1250	83(3)	C(16)	7858(3)	2887(4)	821(3)	78(2)
C(1)	1640(6)	915(8)	1327(7)	146(4)	C(17)	8942(4)	2500	1250	81(3)
C(2)	2166(8)	867(9)	1839(8)	173(6)	C(18)	9283(3)	2045(5)	893(5)	99(3)
C(3)	2269(13)	170(12)	1892(14)	254(12)	C(19)	9999(3)	2093(5)	927(4)	100(3)

Table S10. Selected bond lengths (Å) and bond angles (°) for **5**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Cu(1)-N(3)	1.998(6)	Cu(1)-N(6)#1	2.009(6)
Cu(1)-O(1)	2.074(7)	Cu(1)-O(1)#2	2.074(7)
Cu(1)-O(2)	2.214(9)	Cu(1)-O(2)#2	2.214(9)
Atoms	Angles (º)	Atoms	Angles (º)
N(3)-Cu(1)-N(6)#1	180.0	N(3)-Cu(1)-O(1)	91.92(16)
N(6)#1-Cu(1)-O(1)	88.08(17)	N(3)-Cu(1)-O(1)#2	91.92(17)
N(6)#1-Cu(1)-O(1)#2	88.08(16)	O(1)-Cu(1)-O(1)#2	176.2(3)
N(3)-Cu(1)-O(2)	89.9(2)	N(6)#1-Cu(1)-O(2)	90.1(2)
O(1)-Cu(1)-O(2)	95.3(4)	O(1)#2-Cu(1)-O(2)	84.7(4)
N(3)-Cu(1)-O(2)#2	89.9(2)	N(6)#1-Cu(1)-O(2)#2	90.1(2)
O(1)-Cu(1)-O(2)#2	84.7(4)	O(1)#2-Cu(1)-O(2)#2	95.3(4)
O(2)-Cu(1)-O(2)#2	179.7(5)		

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z; #2 x,-y+1/2,-z+1/4.

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **6**

Atom	x	y	z	U(eq)	Atom	x	y	z	U(eq)
Co(1)	1350(1)	2500	1250	44(1)	C(4)	1944(9)	5168(5)	1085(4)	229(8)
N(1)	1528(4)	4655(3)	1351(3)	116(2)	C(5)	1105(7)	4776(5)	1846(4)	179(6)
N(2)	1310(2)	2312(2)	-37(2)	67(1)	C(6)	2780(2)	2182(2)	853(2)	52(1)
N(3)	2437(2)	2500	1250	50(1)	C(7)	3492(2)	2161(2)	838(2)	51(1)
N(4)	4564(2)	2500	1250	47(1)	C(8)	3842(2)	2500	1250	44(1)
N(5)	8127(2)	2500	1250	38(1)	C(9)	4884(2)	2899(2)	844(2)	49(1)
N(6)	10264(2)	2500	1250	42(1)	C(10)	5645(2)	2898(2)	854(2)	43(1)
O(1)	1315(2)	3557(2)	1302(1)	66(1)	C(11)	5998(2)	2500	1250	42(1)
O(2)	1388(2)	2670(2)	373(1)	73(1)	C(12)	6000(2)	3296(2)	482(2)	49(1)
O(3)	1173(6)	1711(3)	-3(2)	184(4)	C(13)	6707(2)	3295(2)	476(2)	47(1)
O(4)	1398(3)	2505(3)	-512(2)	123(2)	C(14)	6714(2)	2500	1250	34(1)
O(5)	4556(1)	3222(2)	510(1)	65(1)	C(15)	7060(2)	2905(2)	864(1)	37(1)
O(6)	8147(1)	3230(2)	523(1)	58(1)	C(16)	7811(2)	2903(2)	854(2)	42(1)
C(1)	1615(3)	4062(3)	1124(2)	72(1)	C(17)	8876(2)	2500	1250	39(1)
C(2)	2124(4)	4106(3)	661(3)	95(2)	C(18)	9215(2)	2033(2)	928(2)	54(1)
C(3)	2227(7)	4848(4)	574(5)	172(5)	C(19)	9918(2)	2062(2)	942(2)	55(1)

Table S12. Selected bond lengths (Å) and bond angles (°) for **6**

Atoms	Dist. (Å)	Atoms	Dist. (Å)
Co(1)-O(1)#1	2.081(3)	Co(1)-O(1)	2.081(3)
Co(1)-O(2)#1	2.124(3)	Co(1)-O(2)	2.124(3)
Co(1)-N(6)#2	2.132(3)	Co(1)-N(3)	2.135(4)
Atoms	Angles (º)	Atoms	Angles (º)
O(1)#1-Co(1)-O(1)	176.30(17)	O(1)#1-Co(1)-O(2)#1	84.40(13)
O(1)-Co(1)-O(2)#1	95.73(13)	O(1)#1-Co(1)-O(2)	95.73(13)
O(1)-Co(1)-O(2)	84.40(13)	O(2)#1-Co(1)-O(2)	175.9(2)
O(1)#1-Co(1)-N(6)#2	88.15(8)	O(1)-Co(1)-N(6)#2	88.15(8)
O(2)#1-Co(1)-N(6)#2	92.03(11)	O(2)-Co(1)-N(6)#2	92.03(11)
O(1)#1-Co(1)-N(3)	91.85(8)	O(1)-Co(1)-N(3)	91.85(8)
O(2)#1-Co(1)-N(3)	87.97(11)	O(2)-Co(1)-N(3)	87.97(11)
N(6)#2-Co(1)-N(3)	180.0		

Symmetry transformations used to generate equivalent atoms: #1 x,-y+1/2,-z+1/4; #2 x-1,y,z.