Supplementary Material (ESI) for New Journal of Chemistry

C_3 Symmetric Tris(phosphonate)-1,3,5-triazine Ligand: Homopolymetallic Complexes and its Radical Anion

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Supporting Information

X-Ray Structure Determinations

X-Ray structure of L

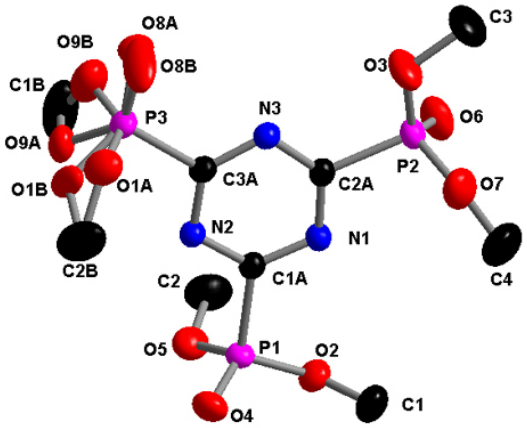

Figure S1. ORTEP view of **L** (thermal ellipsoids set at 50% probability, H atoms omitted).

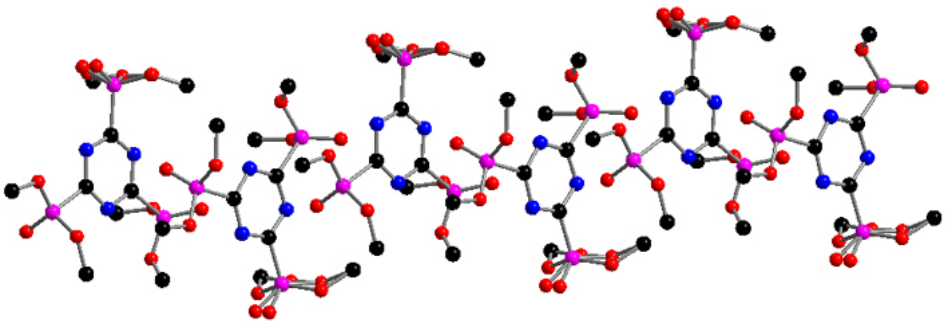

Figure S2. Supramolecular chain of **L** through short P=O---triazine contacts.

Bond Lengths (Å)

O9A O9B 1.293(16)	O9A O1B 1.480(19)	O9A P3 1.550(3)	O1A O1B 1.22(2)
O1A C2B 1.421(5)	O1A P3 1.576(3)	C1B O9B 1.307(15)	C1 O2 1.444(4)
C2 O5 1.447(4)	C3 O3 1.446(4)	C4 O7 1.420(6)	C1A N1 1.332(4)
C1A N2 1.335(4)	C1A P1 1.826(3)	N1 C2A 1.336(4)	C2A N3 1.331(4)
C2A P2 1.825(3)	N3 C3A 1.345(4)	C3A N2 1.329(4)	C3A P3 1.826(3)
O2 P1 1.559(2)	O3 P2 1.550(3)	O4 P1 1.455(2)	O5 P1 1.553(3)
O6 P2 1.438(3)	O7 P2 1.565(3)	O8A O8B 0.71(3)	O8A P3 1.438(6)
O8A O9B 1.835(19)	P3 O8B 1.45(3)	P3 O1B 1.518(13)	P3 O9B 1.603(17)

Bond Angles (°)

O9B O9A O1B 124.7(11)	O9B O9A P3 68.0(8)	O1B O9A P3 60.1(7)
O1B O1A C2B 69.0(7)	O1B O1A P3 64.3(6)	C2B O1A P3 123.9(3)
N1 C1A N2 125.3(3)	N1 C1A P1 119.0(2)	N2 C1A P1 115.7(2)
C1A N1 C2A 114.5(2)	N1 C2A N3 126.0(3)	N1 C2A P2 113.2(2)
N3 C2A P2 120.7(2)	C2A N3 C3A 113.7(2)	N2 C3A N3 125.8(3)

N2 C3A P3 116.7(2)	N3 C3A P3 117.5(2)	C3A N2 C1A 114.6(2)
C1 O2 P1 120.5(2)	C3 O3 P2 120.0(3)	C2 O5 P1 122.1(2)
C4 O7 P2 124.5(3)	O8B O8A P3 77(3)	O8B O8A O9B 130(3)
P3 O8A O9B 57.1(6)	O4 P1 O5 112.59(15)	O4 P1 O2 116.45(14)
O5 P1 O2 103.84(14)	O4 P1 C1A 112.05(14)	O5 P1 C1A 105.31(13)
O2 P1 C1A 105.64(13)	O6 P2 O3 118.34(16)	O6 P2 O7 115.74(17)
O3 P2 O7 102.20(17)	O6 P2 C2A 111.96(14)	O3 P2 C2A 102.22(14)
O7 P2 C2A 104.61(14)	O8A P3 O8B 28.4(11)	O8A P3 O1B 138.4(6)
O8B P3 O1B 122.6(13)	O8A P3 O9A 117.6(3)	O8B P3 O9A 136.6(12)
O1B P3 O9A 57.7(8)	O8A P3 O1A 112.1(3)	O8B P3 O1A 85.2(11)
O1B P3 O1A 46.3(8)	O9A P3 O1A 103.42(19)	O8A P3 O9B 74.0(6)
O8B P3 O9B 100.9(13)	O1B P3 O9B 103.9(10)	O9A P3 O9B 48.4(6)
O1A P3 O9B 143.0(6)	O8A P3 C3A 112.7(3)	O8B P3 C3A 114.0(12)
O1B P3 C3A 108.0(5)	O9A P3 C3A 104.76(16)	O1A P3 C3A 105.21(16)
O9B P3 C3A 105.3(6)	O9A O9B C1B 68.0(8)	O9A O9B P3 63.6(7)
C1B O9B P3 125.3(12)	O9A O9B O8A 108.4(11)	C1B O9B O8A 173.4(13)
P3 O9B O8A 48.9(5)	O1A O1B O9A 130.5(10)	O1A O1B P3 69.3(8)
O9A O1B P3 62.2(5)	O8A O8B P3 75(3)	

X-Ray structure of 1

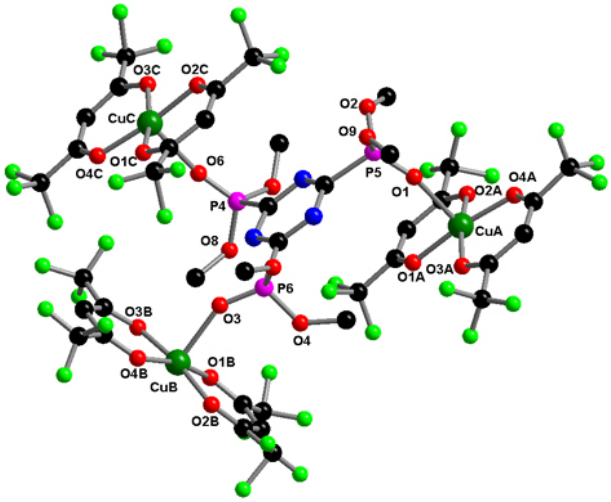

Figure S3. Crystalline structure of the complex **1** (H atoms omitted).

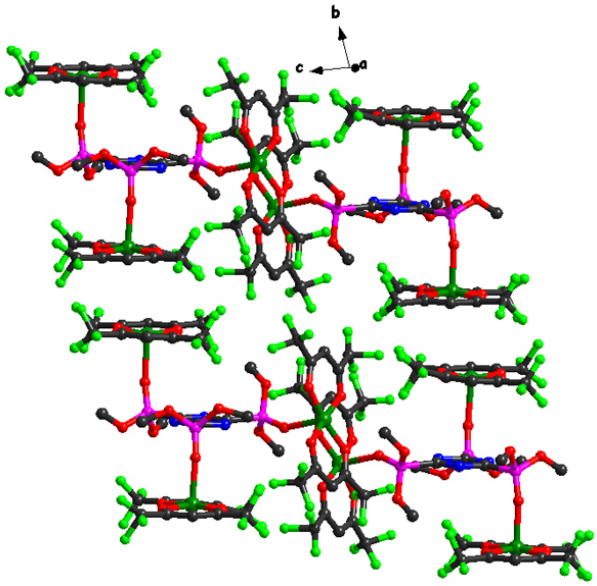

Figure S4. Packing diagram of **1**.

Bond Lengths (Å)

C10C F21C 1.193(13)	C10C F20C 1.21(3)	C10C C9C 1.465(11)
C10C F23C 1.47(3)	F8C C6C 1.312(10)	F10C C6C 1.275(11)
F9C C6C 1.305(11)	F14B C6B 1.268(11)	C8 O8 1.400(7)
F15B C6B 1.270(12)	F13B C6B 1.277(11)	F12B C20B 1.061(13)
F12B F21B 1.742(15)	F20A C10A 1.214(13)	F11C C1C 1.410(17)
C12B F20B 1.097(13)	C12B F5B 1.285(16)	C12B F6B 1.259(14)
C12B C4B 1.509(13)	C10 O9 1.369(12)	C20B F1B 1.110(12)
C20B F21B 1.42(2)	C20B C2B 1.581(18)	CuC O3C 1.923(5)
CuC O4C 1.928(5)	CuC O2C 1.932(5)	CuC O1C 1.948(5)
CuC O6 2.215(5)	CuA O4A 1.921(5)	CuA O1A 1.931(5)
CuA O2A 1.935(5)	CuA O3A 1.941(5)	CuA O1 2.220(6)
CuB O4B 1.912(5)	CuB O1B 1.919(5)	CuB O2B 1.937(5)
CuB O3B 1.944(5)	CuB O3 2.185(4)	P4 O6 1.424(5)
P4 O7 1.534(5)	P4 O8 1.556(5)	P4 C3 1.814(7)
P5 O1 1.436(5)	P5 O2 1.525(5)	P5 O9 1.567(6)

P5 C2 1.814(7)	P6 O3 1.437(4)	P6 O5 1.527(6)
P6 O4 1.544(6)	P6 C1 1.814(6)	O4C C7C 1.235(8)
C2B O2B 1.253(9)	C2B C3B 1.362(11)	N3 C3 1.334(7)
N3 C2 1.343(8)	O3A C1A 1.230(8)	N1 C1 1.329(7)
N1 C2 1.338(7)	O4B C7B 1.242(9)	C2C O1C 1.242(8)
C2C C3C 1.368(9)	C2C C1C 1.541(13)	O1A C7A 1.234(8)
O4A C4A 1.256(9)	N2 C1 1.342(7)	N2 C3 1.342(7)
O3B C9B 1.249(8)	F7A C6A 1.286(9)	C9A O2A 1.269(9)
C9A C8A 1.370(10)	C9A C10A 1.545(13)	F2C C5C 1.328(9)
C7A C8A 1.366(10)	C7A C6A 1.509(10)	O2C C4C 1.262(8)
C3B C4B 1.373(11)	F8A C6A 1.303(8)	O3C C9C 1.249(9)
C7C C8C 1.353(9)	C7C C6C 1.504(11)	F9A C6A 1.300(8)
F1C C5C 1.317(10)	F3C C5C 1.303(9)	O5 C5 1.407(8)
F7B C10B 1.289(12)	C4C C3C 1.361(9)	C4C C5C 1.504(10)
O1B C4B 1.259(9)	O7 C7 1.371(10)	C4A C3A 1.362(10)
C4A C5A 1.517(11)	F8B C10B 1.292(11)	C8C C9C 1.354(10)
F1A C5A 1.313(11)	O2 C6 1.412(9)	F2 C5A 1.345(10)
C3A C1A 1.386(10)	C2A F5A 1.238(11)	C2A F4A 1.252(11)
C2A F6A 1.300(12)	C2A C1A 1.500(11)	O4 C4 1.393(9)
F4C C1C 1.194(9)	C7B C8B 1.369(11)	C7B C6B 1.557(14)
C9B C8B 1.374(10)	C9B C10B 1.502(12)	F3A C5A 1.213(11)
C1C F5C 1.118(10)	F9B C10B 1.267(9)	F12A C10A 1.350(15)
F10A C10A 1.143(12)		

Bond Angles (°)

O3C CuC O4C 91.9(2)	O3C CuC O2C 87.2(2)	O4C CuC O2C 173.1(2)
O3C CuC O1C 167.2(2)	O4C CuC O1C 87.8(2)	O2C CuC O1C 91.5(2)
O3C CuC O6 99.2(2)	O4C CuC O6 94.8(2)	O2C CuC O6 92.2(2)
O1C CuC O6 93.5(2)	O4A CuA O1A 171.8(2)	O4A CuA O2A 87.3(2)
O1A CuA O2A 91.7(2)	O4A CuA O3A 92.3(2)	O1A CuA O3A 87.1(2)
O2A CuA O3A 168.7(3)	O4A CuA O1 94.6(2)	O1A CuA O1 93.6(2)
O2A CuA O1 95.9(2)	O3A CuA O1 95.4(2)	O4B CuB O1B 167.7(2)
O4B CuB O2B 86.1(2)	O1B CuB O2B 92.7(2)	O4B CuB O3B 92.2(2)
O1B CuB O3B 87.1(2)	O2B CuB O3B 171.4(2)	O4B CuB O3 96.4(2)
O1B CuB O3 95.88(19)	O2B CuB O3 94.23(19)	O3B CuB O3 94.33(18)
O6 P4 O7 117.3(3)	O6 P4 O8 117.7(3)	O7 P4 O8 98.6(3)
O6 P4 C3 111.1(3)	O7 P4 C3 104.9(3)	O8 P4 C3 105.6(3)
O1 P5 O2 118.2(3)	O1 P5 O9 115.7(3)	O2 P5 O9 100.9(4)
O1 P5 C2 110.2(3)	O2 P5 C2 106.1(3)	O9 P5 C2 104.4(3)
O3 P6 O5 117.1(3)	O3 P6 O4 110.6(3)	O5 P6 O4 108.5(4)
O3 P6 C1 113.0(3)	O5 P6 C1 102.7(3)	O4 P6 C1 103.8(3)
C7C O4C CuC 124.8(4)	O2B C2B C3B 128.3(8)	O2B C2B C20B 115.6(9)
C3B C2B C20B 115.1(9)	P6 O3 CuB 148.7(3)	C3 N3 C2 115.4(5)
C1A O3A CuA 125.5(5)	C1 N1 C2 115.8(6)	C7B O4B CuB 124.1(5)
O1C C2C C3C 126.5(7)	O1C C2C C1C 116.1(7)	C3C C2C C1C 116.8(8)
C7A O1A CuA 125.9(5)	C4A O4A CuA 124.5(5)	C2C O1C CuC 125.5(4)
C1 N2 C3 115.6(5)	C9B O3B CuB 124.8(5)	N1 C2 N3 124.4(6)
N1 C2 P5 115.9(6)	N3 C2 P5 119.5(5)	O2A C9A C8A 127.6(7)
O2A C9A C10A 115.4(9)	C8A C9A C10A 116.8(10)	C9A O2A CuA 124.6(5)
O1A C7A C8A 127.9(7)	O1A C7A C6A 113.4(7)	C8A C7A C6A 118.7(8)
C4C O2C CuC 124.9(4)	P5 O1 CuA 161.0(3)	C2B C3B C4B 122.3(7)
C9C O3C CuC 125.3(4)	O4C C7C C8C 128.0(7)	O4C C7C C6C 112.4(7)
C8C C7C C6C 119.6(9)	N1 C1 N2 124.3(5)	N1 C1 P6 118.4(5)
N2 C1 P6 117.1(5)	C8 O8 P4 122.5(5)	N3 C3 N2 124.3(6)
N3 C3 P4 118.9(5)	N2 C3 P4 116.8(5)	P4 O6 CuC 163.5(4)
C5 O5 P6 125.6(6)	O2C C4C C3C 126.9(7)	O2C C4C C5C 113.5(7)
C3C C4C C5C 119.5(8)	C4B O1B CuB 124.9(5)	C7 O7 P4 124.5(7)
C4C C3C C2C 123.7(7)	O4A C4A C3A 127.6(7)	O4A C4A C5A 112.2(8)
C3A C4A C5A 120.2(9)	C7C C8C C9C 123.0(8)	C2B O2B CuB 124.1(5)
C6 O2 P5 123.9(6)	C10 O9 P5 125.5(8)	C4A C3A C1A 122.9(8)
C4 O4 P6 127.1(6)	C7A C8A C9A 122.0(8)	O4B C7B C8B 130.0(8)
O4B C7B C6B 112.3(9)	C8B C7B C6B 117.6(9)	O3B C9B C8B 127.6(8)
O3B C9B C10B 112.4(9)	C8B C9B C10B 120.0(9)	C7B C8B C9B 120.6(8)

O3A C1A C3A 126.6(7)	O3A C1A C2A 114.4(8)	C3A C1A C2A 118.9(9)
O3C C9C C8C 126.9(7)	O3C C9C C10C 116.5(9)	C8C C9C C10C 116.2(10)
O1B C4B C3B 127.4(8)	O1B C4B C12B 115.1(11)	C3B C4B C12B 117.4(11)

X-Ray structure of 2

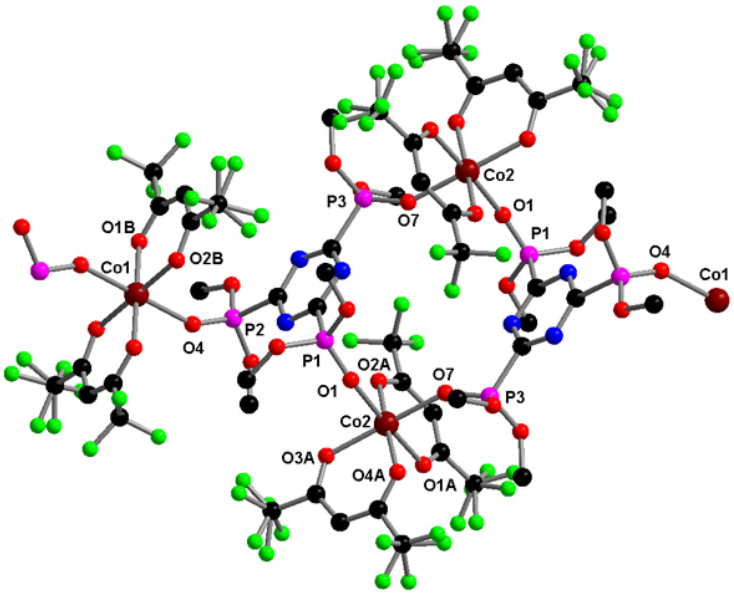

Figure S5. Crystalline structure of the complex **2** (H atoms omitted).

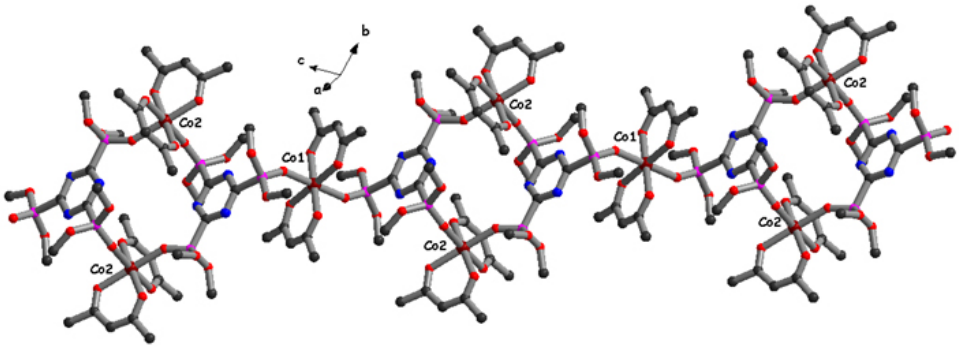

Figure S6. Coordination polymeric chain in **2** (H and F atoms omitted).

Bond Lengths (Å)

Co1 O2B 2.040(2)	Co1 O1B 2.063(2)	Co1 O4 2.110(3)
Co2 O2A 2.035(2)	Co2 O4A 2.065(2)	Co2 O1A 2.076(3)
Co2 O3A 2.081(2)	Co2 O7 2.085(2)	Co2 O1 2.093(3)
P1 O1 1.453(3)	P1 O2 1.541(3)	P1 O3 1.546(3)
P1 C1 1.828(3)	P2 O4 1.454(3)	P2 O5 1.542(3)
P2 O6 1.549(3)	P2 C2 1.821(3)	P3 O7 1.448(2)
P3 O8 1.542(3)	P3 O9 1.542(3)	P3 C6 1.822(3)
N1 C2 1.331(4)	N1 C1 1.338(4)	N2 C1 1.331(4)
N3 C6 1.337(4)	O1A C6A 1.230(5)	O1B C1B 1.252(4)
O2 C9 1.456(5)	O2A C8A 1.244(4)	O2B C3B 1.252(5)
O3 C3 1.437(5)	O3A C3A 1.245(4)	O4A C1A 1.252(4)
O5 C4 1.454(4)	O6 C11 1.461(6)	O8 C7 1.401(5)
O9 C10 1.409(6)	F1 C9A 1.308(5)	F1B C2B 1.307(5)
F2 C9A 1.308(5)	F2B C2B 1.303(5)	F3 C9A 1.335(5)
F3B C2B 1.311(5)	F4A F4D 1.003(15)	F4A C10A 1.353(13)
F4A F6D 1.40(5)	F4D C10A 1.290(11)	F4D F5A 1.569(18)
F4B F4C 0.76(4)	F4B C4B 1.260(11)	F4B F6C 1.48(3)
F4C C4B 1.36(2)	F4C F5B 1.74(3)	F5A F5D 0.70(3)
F5A C10A 1.251(13)	F5D C10A 1.35(2)	F5D F6A 1.66(4)

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F5B F5C 0.64(4)          F5B C4B 1.333(13)        F5C C4B 1.23(2)
F5C F6B 1.57(3)          F6A F6D 0.72(7)          F6A C10A 1.252(11)
F6D C10A 1.25(2)         F6B F6C 0.87(3)          F6B C4B 1.294(12)
F6C C4B 1.28(2)          F7A F7B 0.66(3)          F7A C5A 1.214(11)
F8 C5A 1.370(9)          F8 F9B 1.667(11)         F9A F9B 1.101(17)
F9A C5A 1.345(11)        F9A F7B 1.70(2)          F7B C5A 1.256(16)
F9B C5A 1.262(8)         F10A F10B 0.78(4)        F10A C4A 1.296(14)
F10A F12B 1.40(5)        F10B C4A 1.26(2)         F10B F11A 1.53(3)
F11A F11B 0.88(3)        F11A C4A 1.32(2)         F11B C4A 1.255(19)
F11B F12A 1.61(3)        F12A F12B 0.97(5)        F12A C4A 1.324(13)
F12B C4A 1.32(3)         C1A C2A 1.374(5)         C1A C5A 1.515(6)
C1B C5B 1.378(5)         C1B C2B 1.516(6)         C2 N3 1.338(4)
C2A C3A 1.385(5)         C3A C4A 1.522(6)         C3B C5B 1.377(5)
C3B C4B 1.523(6)         C6 N2 1.336(4)           C6A C7A 1.404(6)
C6A C10A 1.526(6)        C7A C8A 1.384(5)         C8A C9A 1.520(5)
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Bond Angles (°)

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O2B Co1 O2B 180.00(8)      O2B Co1 O1B 89.14(10)      O2B Co1 O1B 90.86(10)
O2B Co1 O1B 90.86(10)      O2B Co1 O1B 89.14(10)      O1B Co1 O1B 180.00(13)
O2B Co1 O4 89.31(11)       O2B Co1 O4 90.69(11)       O1B Co1 O4 88.82(11)
O1B Co1 O4 91.18(11)       O2B Co1 O4 90.69(11)       O2B Co1 O4 89.31(11)
O1B Co1 O4 91.18(11)       O1B Co1 O4 88.82(11)       O4 Co1 O4 180.000(1)
O2A Co2 O4A 173.10(11)     O2A Co2 O1A 88.27(11)      O4A Co2 O1A 84.91(12)
O2A Co2 O3A 92.51(10)      O4A Co2 O3A 86.95(10)      O1A Co2 O3A 94.05(11)
O2A Co2 O7 91.58(9)        O4A Co2 O7 89.29(9)        O1A Co2 O7 88.64(11)
O3A Co2 O7 175.17(12)      O2A Co2 O1 89.82(10)       O4A Co2 O1 97.03(11)
O1A Co2 O1 177.14(11)      O3A Co2 O1 88.16(11)       O7 Co2 O1 89.29(11)
O1 P1 O2 116.22(16)        O1 P1 O3 110.80(15)        O2 P1 O3 104.78(16)
O1 P1 C1 112.84(16)        O2 P1 C1 104.01(15)        O3 P1 C1 107.48(15)
O4 P2 O5 117.43(15)        O4 P2 O6 113.54(16)        O5 P2 O6 104.88(17)
O4 P2 C2 110.64(17)        O5 P2 C2 103.39(14)        O6 P2 C2 105.89(15)
O7 P3 O8 116.58(17)        O7 P3 O9 115.68(16)        O8 P3 O9 105.39(18)
O7 P3 C6 110.81(14)        O8 P3 C6 100.11(16)        O9 P3 C6 106.77(15)
C2 N1 C1 115.4(3)          C1 N2 C6 114.4(3)          C6 N3 C2 114.2(3)
P1 O1 Co2 152.18(17)       C6A O1A Co2 123.8(2)       C1B O1B Co1 125.5(2)
C9 O2 P1 122.8(3)          C8A O2A Co2 124.6(2)       C3B O2B Co1 124.8(3)
C3 O3 P1 124.7(2)          C3A O3A Co2 125.6(2)       P2 O4 Co1 147.77(18)
C1A O4A Co2 124.7(2)       C4 O5 P2 120.4(3)          C11 O6 P2 122.0(3)
P3 O7 Co2 148.76(15)       C7 O8 P3 126.8(4)          C10 O9 P3 124.2(3)
N2 C1 N1 125.0(3)          N2 C1 P1 120.0(2)          N1 C1 P1 115.0(2)
O4A C1A C2A 128.1(3)       O4A C1A C5A 114.1(3)       C2A C1A C5A 117.7(4)
O1B C1B C5B 127.4(4)       O1B C1B C2B 113.8(3)       C5B C1B C2B 118.8(4)
N1 C2 N3 125.0(3)          N1 C2 P2 112.9(2)          N3 C2 P2 122.1(3)
C1A C2A C3A 123.5(3)       C1A C2A H2A 118.2          O3A C3A C2A 127.6(3)
O3A C3A C4A 114.5(4)       C2A C3A C4A 117.9(4)       O2B C3B C5B 129.0(3)
O2B C3B C4B 112.3(4)       C5B C3B C4B 118.7(4)       C3B C5B C1B 124.1(4)
N2 C6 N3 126.0(3)          N2 C6 P3 116.6(2)          N3 C6 P3 117.4(2)
O1A C6A C7A 129.0(4)       O1A C6A C10A 115.6(4)      C7A C6A C10A 115.4(5)
C8A C7A C6A 121.5(4)       O2A C8A C7A 129.5(4)       O2A C8A C9A 113.2(3)
C7A C8A C9A 117.2(4) . . ?
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X-Ray structure of 3

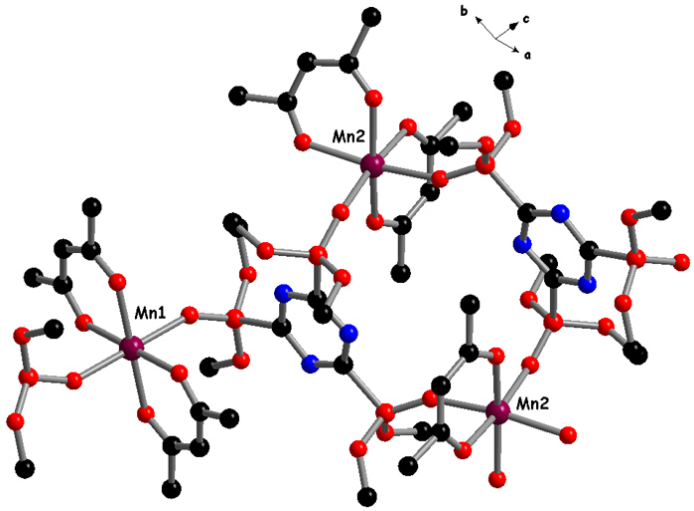

Figure S7. Crystalline structure of the complex **3** (H and F atoms omitted).

Bond Lengths (Å)

Mn1 O2B 2.150(5)	Mn1 O2B 2.150(5)	Mn1 O1B 2.149(5)
Mn1 O1B 2.149(5)	Mn1 O4 2.169(5)	Mn1 O4 2.169(5)
Mn2 O2A 2.128(4)	Mn2 O1A 2.189(5)	Mn2 O4A 2.170(4)
Mn2 O1 2.145(5)	Mn2 O3A 2.166(5)	Mn2 O7 2.132(4)
P1 O1 1.449(5)	P1 O3 1.558(5)	P1 O2 1.552(5)
P1 C1 1.824(6)	P2 O4 1.456(5)	P2 O6 1.551(5)
P2 O5 1.542(5)	P2 C2 1.813(7)	P3 O7 1.445(5)
P3 O9 1.538(6)	P3 O8 1.548(6)	P3 C6 1.827(6)
N1 C2 1.343(8)	N1 C1 1.329(8)	N2 C1 1.330(8)
N2 C6 1.340(8)	N3 C2 1.338(8)	N3 C6 1.334(8)
O1A C6A 1.246(9)	O1B C1B 1.246(9)	O2 C9 1.448(10)
O2A C8A 1.255(8)	O2B C3B 1.244(9)	O3 C3 1.430(9)
O3A C3A 1.230(8)	O4A C1A 1.250(8)	O5 C4 1.455(9)
O6 C11 1.429(11)	O8 C7 1.389(10)	O9 C10 1.386(11)
C1A C2A 1.375(10)	C1A C5A 1.559(12)	C1B C5B 1.390(10)
C1B C2B 1.535(10)	C2 N3 1.338(8)	C2A C3A 1.388(10)
C3A C4A 1.542(12)	C3B C5B 1.386(10)	C3B C4B 1.514(11)
C6 N2 1.340(8)	C6A C7A 1.390(10)	C6A C10A 1.545(11)
C7A C8A 1.370(10)	C8A C9A 1.507(10)	

Bond Angles (°)

O2B Mn1 O2B 180.00(13)	O2B Mn1 O1B 84.5(2)	O2B Mn1 O1B 95.5(2)
O2B Mn1 O1B 95.5(2)	O2B Mn1 O1B 84.5(2)	O1B Mn1 O1B 180.0(2)
O2B Mn1 O4 89.9(2)	O2B Mn1 O4 90.1(2)	O1B Mn1 O4 90.9(2)
O1B Mn1 O4 89.1(2)	O2B Mn1 O4 90.1(2)	O2B Mn1 O4 89.9(2)
O1B Mn1 O4 89.1(2)	O1B Mn1 O4 90.9(2)	O4 Mn1 O4 180.000(1)
O2A Mn2 O1A 82.73(19)	O2A Mn2 O4A 166.82(19)	O1A Mn2 O4A 84.68(19)
O2A Mn2 O1 88.70(17)	O1A Mn2 O1 171.18(18)	O4A Mn2 O1 104.00(18)
O2A Mn2 O3A 95.66(19)	O1A Mn2 O3A 95.5(2)	O4A Mn2 O3A 81.66(18)
O1 Mn2 O3A 87.3(2)	O2A Mn2 O7 95.81(18)	O1A Mn2 O7 88.1(2)
O4A Mn2 O7 87.67(18)	O1 Mn2 O7 90.7(2)	O3A Mn2 O7 168.31(19)
O1 P1 O3 111.6(3)	O1 P1 O2 116.1(3)	O3 P1 O2 105.0(3)
O1 P1 C1 112.0(3)	O3 P1 C1 107.7(3)	O2 P1 C1 103.7(3)
O4 P2 O6 113.5(3)	O4 P2 O5 116.7(3)	O6 P2 O5 105.1(3)
O4 P2 C2 111.0(3)	O6 P2 C2 106.1(3)	O5 P2 C2 103.4(3)
O7 P3 O9 115.5(3)	O7 P3 O8 116.4(4)	O9 P3 O8 105.8(4)

O7 P3 C6 111.7(3)	O9 P3 C6 106.6(3)	O8 P3 C6 99.2(3)
C2 N1 C1 115.0(5)	C1 N2 C6 113.8(5)	C2 N3 C6 113.8(5)
P1 O1 Mn2 155.0(3)	C6A O1A Mn2 125.4(4)	C1B O1B Mn1 127.1(5)
C9 O2 P1 121.5(5)	C8A O2A Mn2 126.7(4)	C3B O2B Mn1 127.5(5)
C3 O3 P1 126.0(5)	C3A O3A Mn2 127.9(5)	P2 O4 Mn1 150.1(4)
C1A O4A Mn2 125.9(4)	C4 O5 P2 121.2(5)	C11 O6 P2 123.7(6)
P3 O7 Mn2 153.1(3)	C7 O8 P3 126.8(7)	C10 O9 P3 125.8(6)
N2 C1 N1 125.7(6)	N2 C1 P1 119.3(5)	N1 C1 P1 115.0(5)
O4A C1A C2A 128.7(7)	O4A C1A C5A 111.7(8)	C2A C1A C5A 119.6(8)
O1B C1B C5B 129.0(7)	O1B C1B C2B 112.3(7)	C5B C1B C2B 118.7(7)
N1 C2 N3 125.0(6)	N1 C2 P2 113.7(5)	N3 C2 P2 121.3(5)
C1A C2A C3A 122.2(7)	O3A C3A C2A 128.3(7)	O3A C3A C4A 115.1(8)
C2A C3A C4A 116.5(8)	O2B C3B C5B 128.7(7)	O2B C3B C4B 113.2(8)
C5B C3B C4B 118.2(8)	C1B C5B C3B 123.1(7)	N2 C6 N3 126.5(6)
N2 C6 P3 116.0(5)	N3 C6 P3 117.4(5)	O1A C6A C7A 128.7(6)
O1A C6A C10A 115.0(8)	C7A C6A C10A 116.3(8)	C8A C7A C6A 121.8(7)
O2A C8A C7A 129.7(7)	O2A C8A C9A 112.9(6)	C7A C8A C9A 117.3(7)

Table T1 Selected bond lengths (Å) and angles (º) for compounds **L** and **1-3**

L		**1**		**2**		**3**	
C1 O2	1.449(4)	CuC O3C	1.922(5)	Co1 O2B	2.039(3)	Mn1 O2B	2.135(5)
C2 O5	1.447(4)	CuC O4C	1.928(5)	Co1 O1B	2.066(3)	Mn1 O1B	2.148(5)
C3 O3	1.448(4)	CuC O2C	1.933(5)	Co1 O6	2.111(3)	Mn1 O6	2.167(5)
C4 O7	1.421(6)	CuC O1C	1.948(5)	Co2 O2A	2.041(3)	Mn2 O2A	2.127(4)
C1A N1	1.333(3)	CuC O6	2.214(5)	Co2 O4A	2.067(2)	Mn2 O4A	2.166(5)
C1A N2	1.335(3)	CuA O4A	1.922(5)	Co2 O5A	2.078(3)	Mn2 O5A	2.170(4)
C1A P1	1.825(3)	CuA O1A	1.933(5)	Co2 O3A	2.082(2)	Mn2 O4	2.145(5)
N1 C2A	1.335(4)	CuA O2A	1.936(5)	Co2 O8A	2.081(2)	Mn2 O3A	2.171(5)
C2A N3	1.330(4)	CuA O3A	1.941(5)	Co2 O4	2.095(3)	Mn2 O8A	2.130(4)
C2A P2	1.825(3)	CuA O1	2.221(6)	P1 O5	1.454(3)	P1 O4	1.450(4)
N3 C3A	1.345(4)	CuB O4B	1.913(5)	P2 O6	1.454(3)	P2 O6	1.454(4)
C3A N2	1.330(4)	CuB O1B	1.919(5)	O2B Co1 O1B	89.15(12)	O2B Mn1 O1B	84.48(18)
C3A P3	1.827(3)	CuB O2B	1.939(5)	O2B Co1 O6	90.69(12)	O2B Mn1 O6	90.4(2)
O2 P1	1.558(2)	CuB O3B	1.944(5)	O1B Co1 O6	88.82(11)	O1B Mn1 O6	89.1(2)
O3 P2	1.549(3)	CuB O3	2.185(4)	O2A Co2 O4A	173.08(13)	O2A Mn2 O4A	166.69(19)
O4 P1	1.457(2)	P4 O6	1.425(5)	O2A Co2 O5A	88.16(12)	O2A Mn2 O5A	82.75(17)
O5 P1	1.554(3)	P6 O3	1.437(4)	O4A Co2 O3A	87.01(11)	O5A Mn2 O4	171.09(18)
O6 P2	1.439(3)	P5 O1	1.435(5)	O5A Co2 O3A	93.95(11)	O4A Mn2 O4	104.24(18)
O7 P2	1.565(3)	O3C CuC O2C	87.2(2)	O2A Co2 O8A	91.58(11)	O2A Mn2 O3A	95.56(19)
C1 O2	1.444(4)	O4C CuC O2C	173.1(2)	O3A Co2 O8A	175.29(13)	O8A Mn2 O3A	168.42(18)
N1 C1A N2	125.3(3)	O3C CuC O1C	167.2(2)				
N1 C1A P1	119.0(2)	O4C CuC O1C	87.2(2)				
N2 C1A P1	115.7(2)	O4A CuA O1A	171.8(2)				
C1A N1 C2A	114.5(2)	O4A CuA O2A	87.3(2)				
N1 C2A N3	126.0(3)	O1A CuA O2A	91.7(2)				
N1 C2A P2	113.2(2)	O4A CuA O3A	92.3(2)				
N3 C2A P2	120.7(2)	O4B CuB O1B	167.8(2)				
C2A N3 C3A	113.7(2)	O4B CuB O2B	86.1(2)				
N2 C3A N3	125.8(3)	O1B CuB O2B	92.7(2)				
N2 C3A P3	116.6(2)	O4B CuB O3B	92.2(2)				
N3 C3A P3	117.6(2)						

Theoretical calculations.

Table T2. Spin distribution for the four minima of $\mathbf{L}^{-\bullet}$.

	TZ	3*PO(OMe)$_2$
Min **1**	90.6%	9.4%
Min **2**	89.62%	10.37%
Min **3**	90.23%	9.77%
Min **4**	90.4%	9.6%
average	90.21%	9.78%