Supporting information

Exclusive selectivity of multidentate ligands independent on the oxidation state of cobalt: influence of steric hindrance on dioxygen binding and phenoxazinone synthase activity

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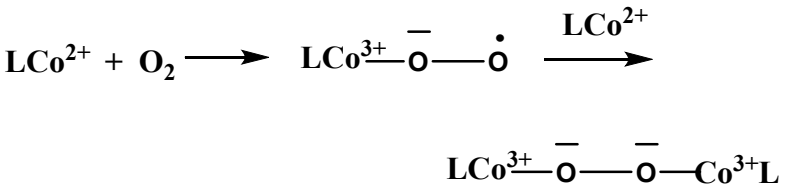
Contents

Table S1. Selected bond angles (º) for complexes **1**–**5**

N1–Co1–N2	81.2(2)	81.53(19)	74.5(2)	79.5(3)	77.26(5)
N1–Co1–N3	179.4(2)	178.8(2)	153.1(2)	166.1(3)	169.74(5)
N1–Co1–N4	93.8(2)	96.20(18)	126.4(2)	105.7(2)	104.81(5)
N1–Co1–N5	86.2(2)	86.04(18)	95.1(2)	89.2(2)	87.59(5)
N2–Co1–N3	99.0(2)	99.3(2)	78.9(3)	91.7(4)	94.36(5)
N2–Co1–N4	172.8(2)	175.35(19)	157.3(3)	174.8(3)	177.73(5)
N2–Co1–N5	93.1(2)	94.93(18)	113.3(3)	101.7(2)	104.56(5)
N3–Co1–N4	86.0(2)	82.92(19)	79.3(3)	83.4(3)	83.49(5)
N3–Co1–N5	94.3(2)	92.96(19)	99.3(2)	103.2(3)	100.38(5)
N4–Co1–N5	81.3(2)	80.83(17)	76.6(2)	78.0(2)	76.61(5)
O1/N6–Co1–N1	92.56(19)	94.29(17)	79.3(2)	82.3(2)	83.84(5)
O1/N6–Co1–N2	92.9(2)	88.59(19)	88.4(2)	87.0(2)	87.85(5)
O1/N6–Co1–N3	86.9(2)	86.67(18)	95.9(2)	86.6(2)	90.01(5)
O1/N6–Co1–N4	92.5(2)	95.65(18)	87.6(2)	94.3(2)	91.40(5)
O1/N6–Co1–N5	173.6(2)	176.48(18)	155.5(2)	166.6(2)	163.00(5)
Co1–O1–O1a	112.4(4)	113.0(4)	-	-	-



Scheme 2. Mechanism of peroxo-bridging where L is multidentate ligand

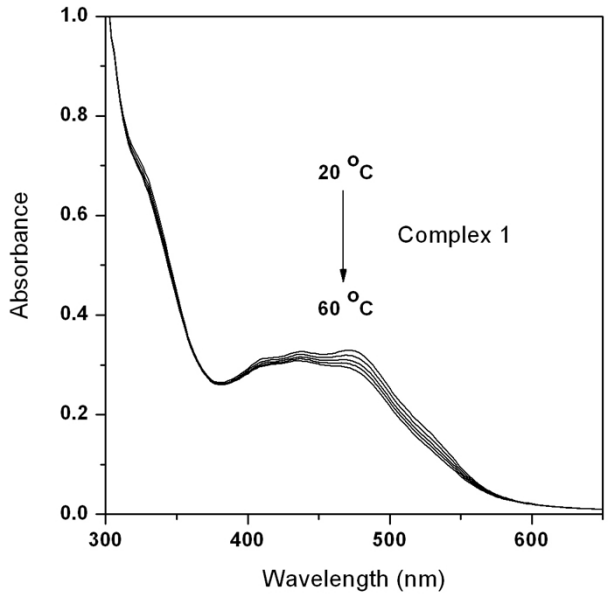


Fig. S1. UV-vis spectra of complex **1** at variable temperature

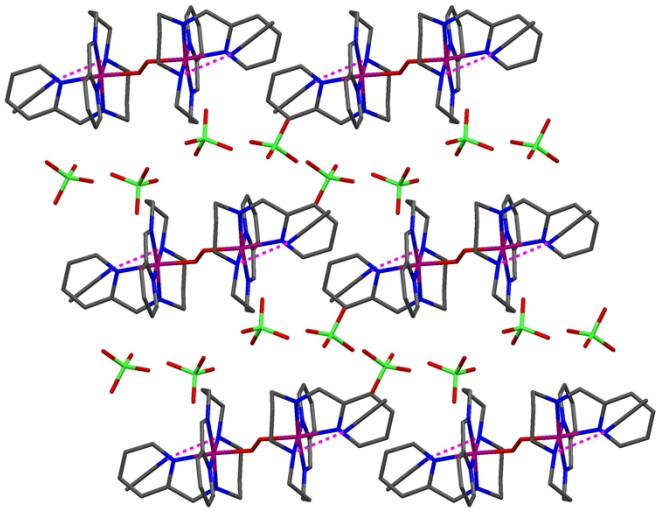


Fig. S2. Packing diagram of complex **1** in ac plane showing hydrogen bonding interaction

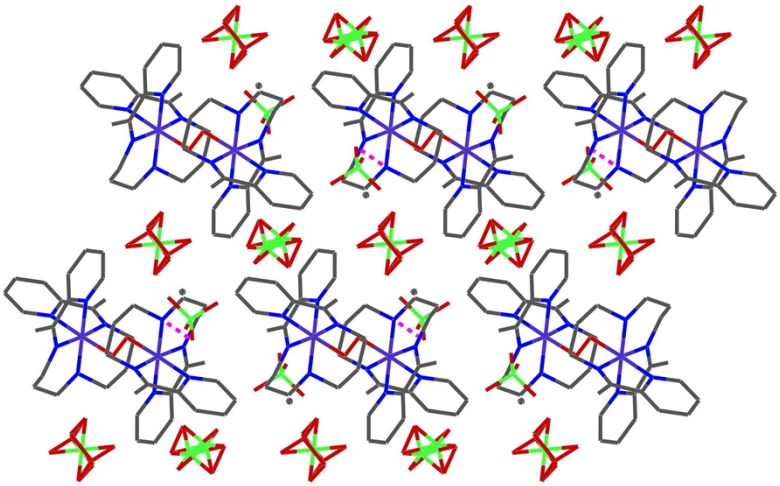


Fig. S3. Packing diagram of **2** viewed along the b axis showing alternate layers of cations and anions and also hydrogen bonding interaction.

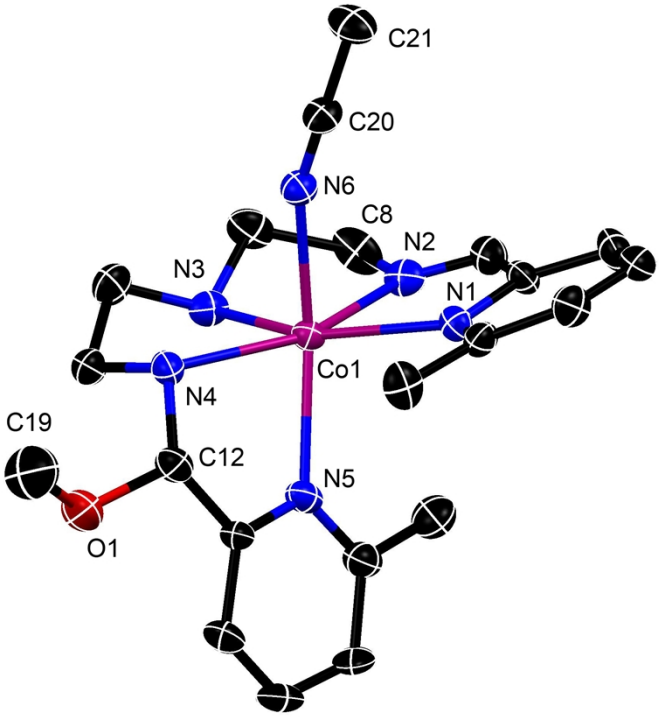


Fig. S4. Molecular structure of **3** showing atom numbering scheme. Ellipsoids are drawn in 30% probability level and hydrogen atoms are omitted from clarity.

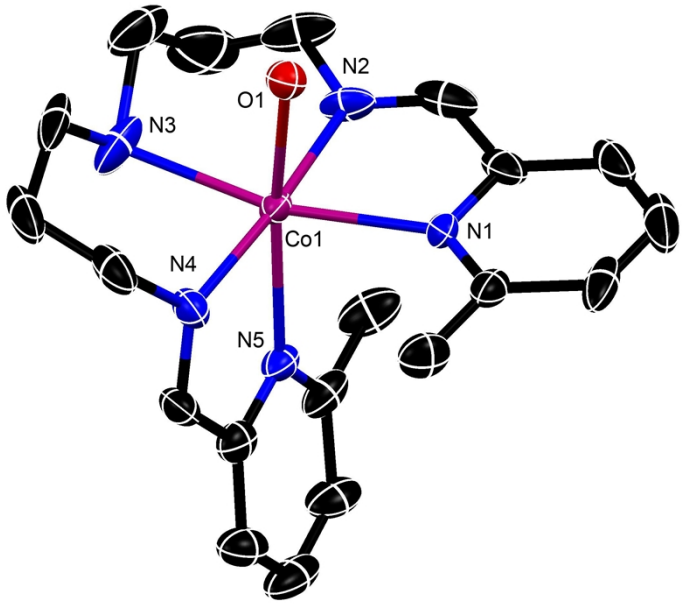


Fig. S5. Crystal structure of **4** showing atom labeling scheme. Ellipsoids are drawn in 30% probability level and hydrogen atoms are omitted from clarity.

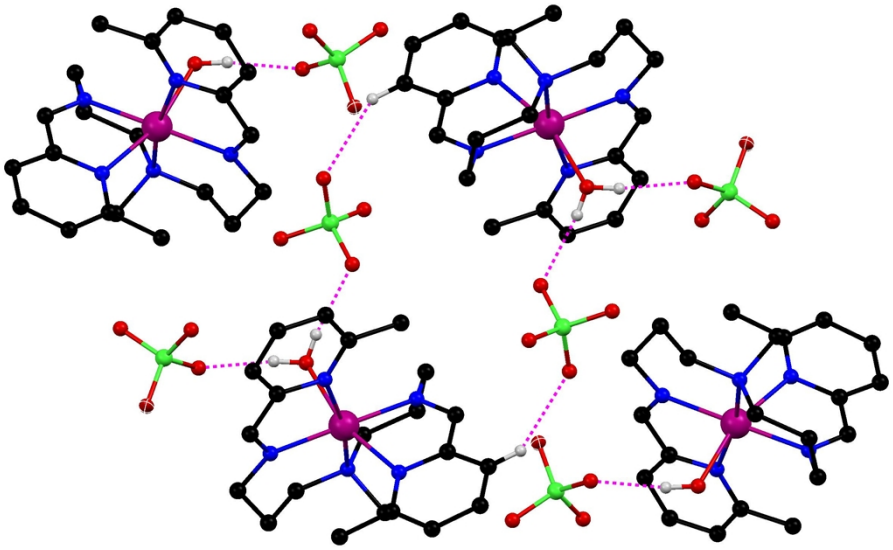


Fig. S6. Crystal packing of **5** viewed along the *b* axis showing hydrogen bonding scheme.

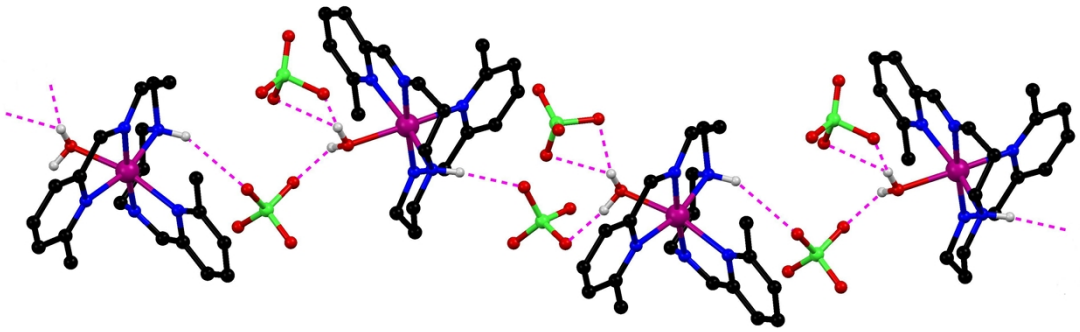


Fig. S7. One dimensional (1D) supramolecular hydrogen-bonded wavy chain of **4** propagating along the *a* axis.

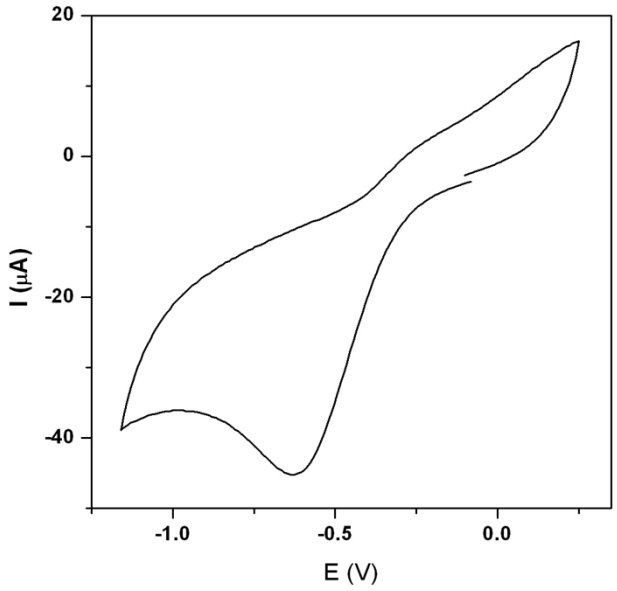


Fig. S8. Cyclic voltammogram of **2** in methanol containing tetraethylammonium perchlorate as the supporting electrolyte at a scan rate of 100 mV s^{-1}.

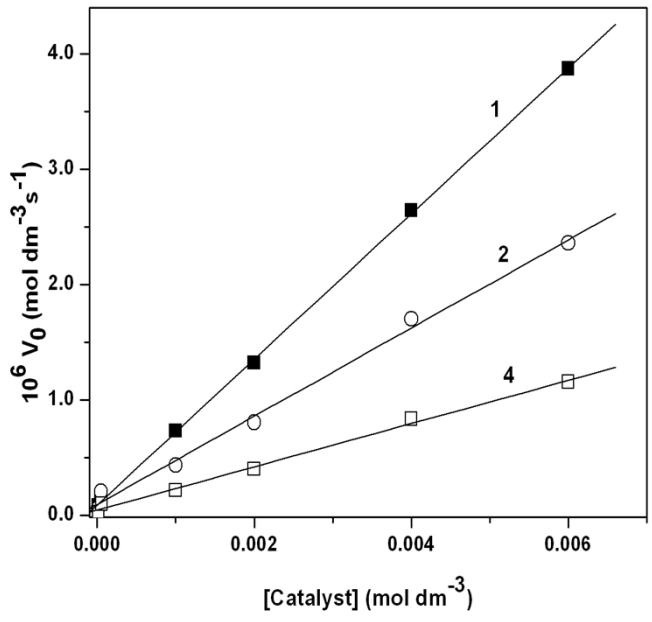


Fig. S9. Plot of initial rates on the complex concentrations for the oxidation of *o*-aminophenol catalyzed by **1**, **2** and **4** in dioxygen-saturated methanol at 25 ºC