Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

Hydrothermal Synthesis of An *Ortho*-Metallated Co(III) Complex Anchored by Carboxylate Group with Selective Oxidation Catalytic Property

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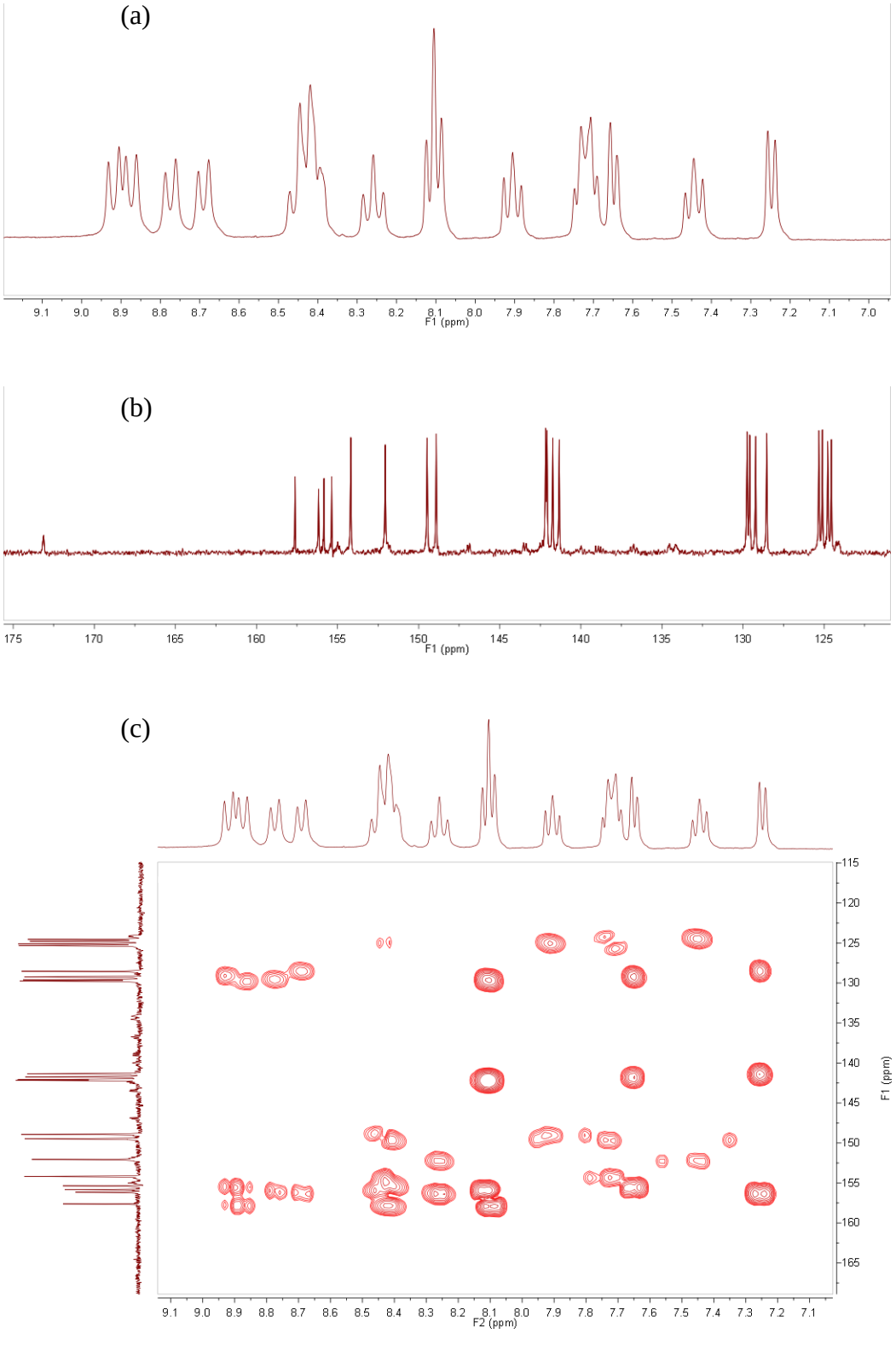

Figure S1. NMR spectra of complex **1**: (a) ^{1}H NMR; (b) ^{13}C NMR (c) HMBC.

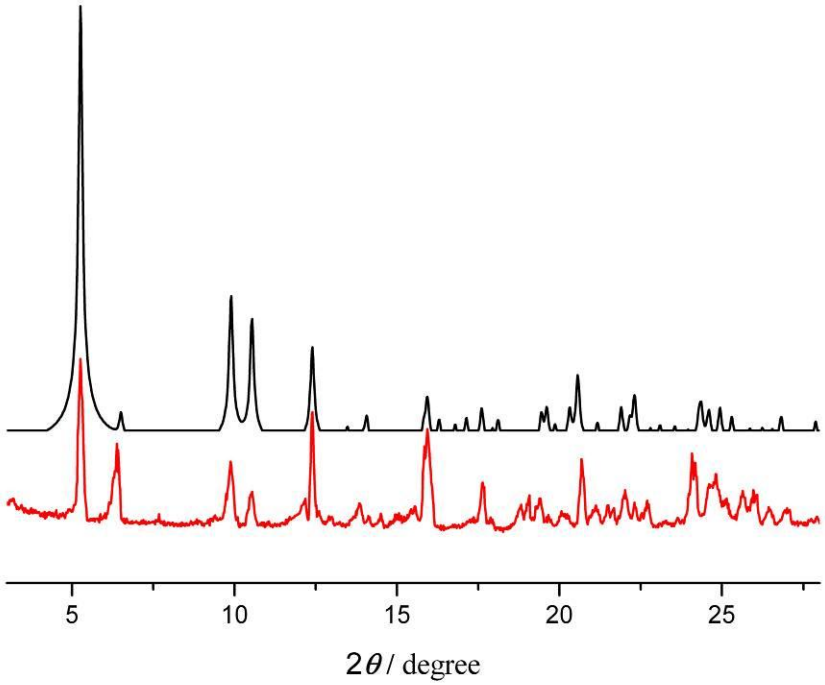

Figure S2. Powder X-ray diffraction spectra comparison of complex **1**. Red color line responses the experimental data, black color line responses the simulated data.

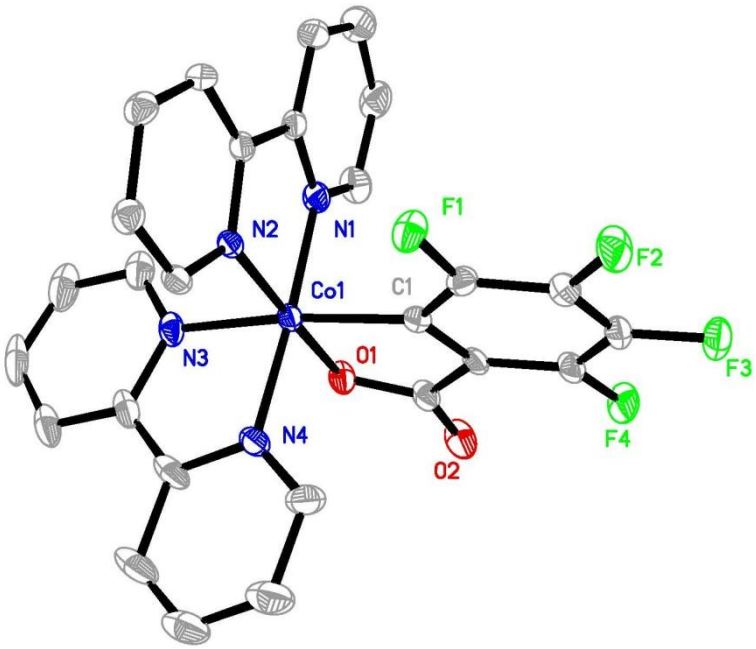

Figure S3. Coordination geometry of the Co(III) ion in **1**. H atoms have been omitted for clarity.

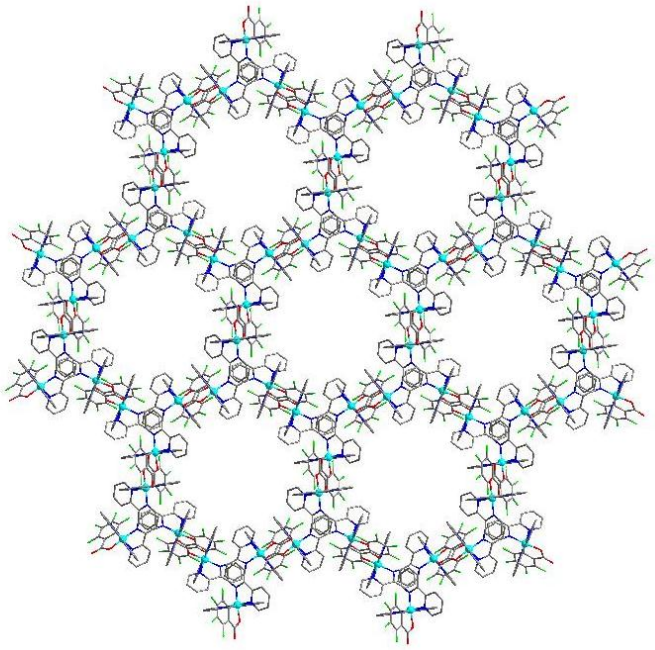

Figure S4. Molecule packing of **1** in the crystal structure highlighting the 3D arrangement of Co(III) unit (viewed along c axis). H atoms, NO_3^- counter ions and the water solvent molecules have been omitted for clarity.

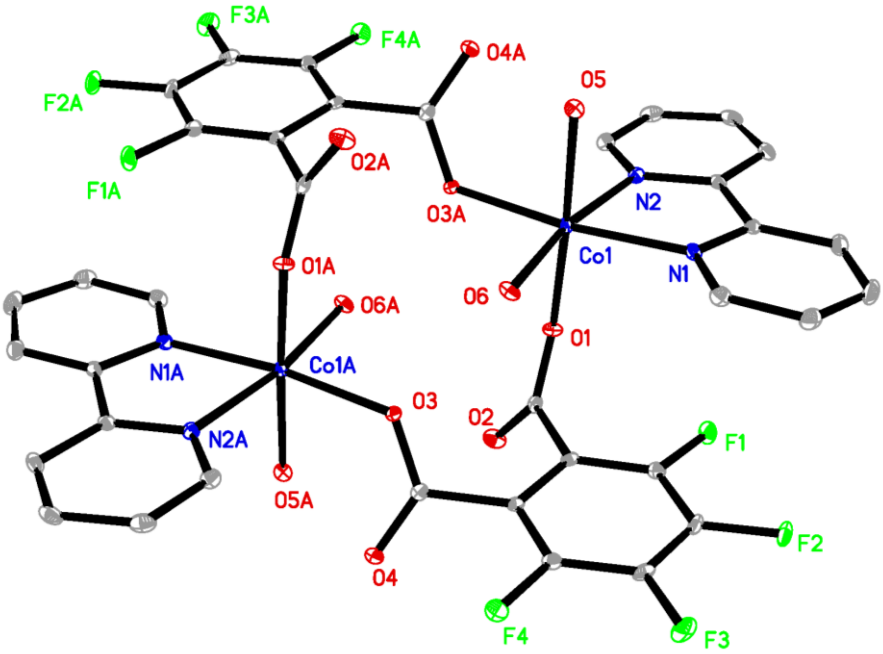

Figure S5. Coordination geometry of the Co(II) ion in **2**. H atoms have been omitted for clarity.

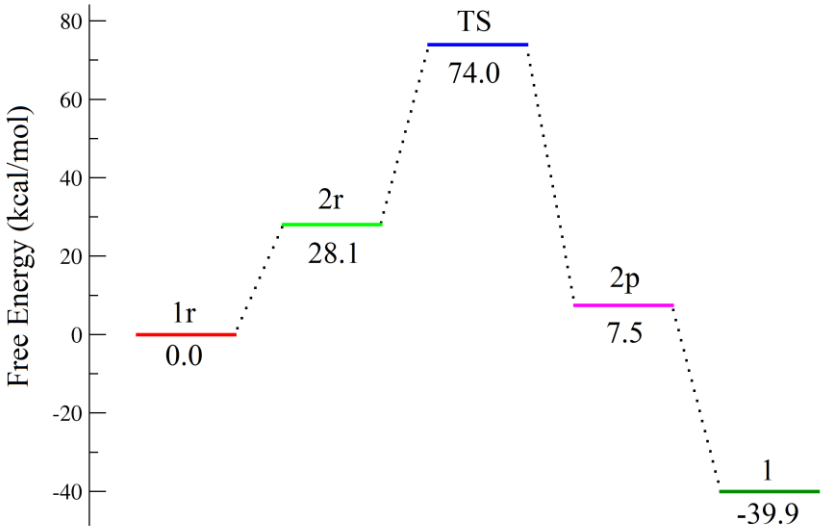

Figure S6. DFT calculation results for the energy profile from **1r** to **1** at 243K.

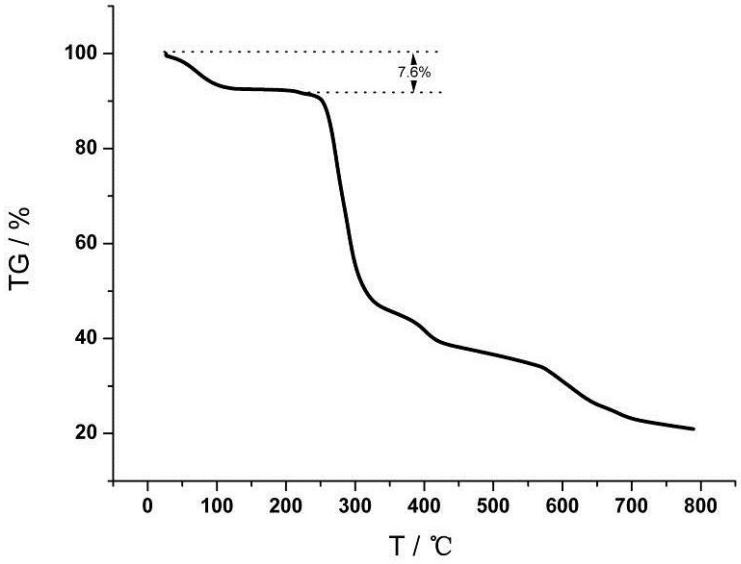

Figure S7. TGA curve of **1**.

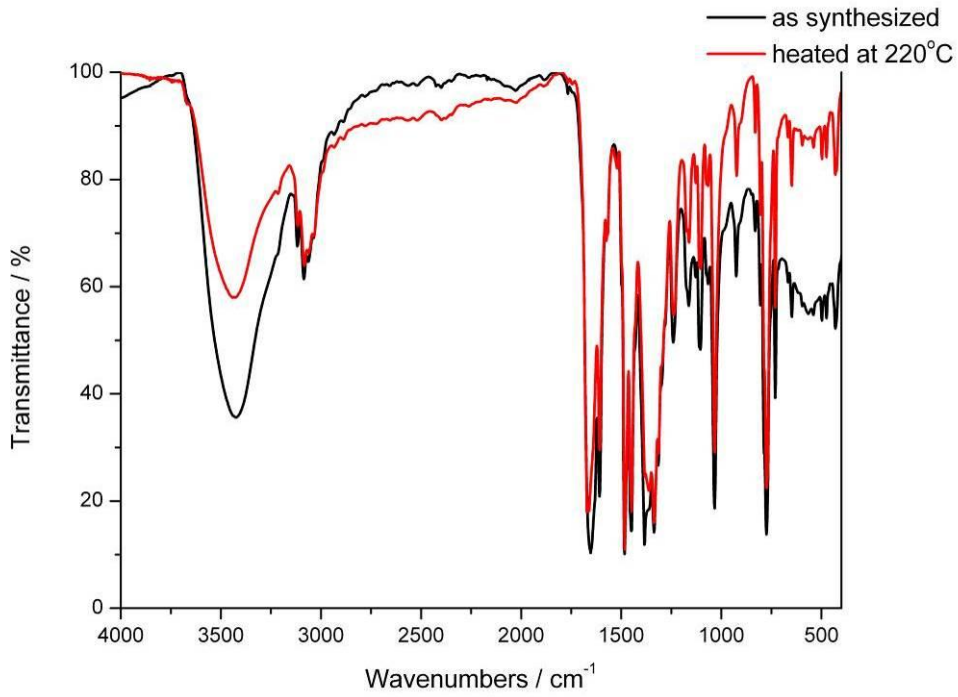

Figure S8. IR spectra of **1** before and after heating.

Table S1. Cartesian coordinates and the vibrational frequency of the TS.

	X	Y	Z		X	Y	Z
Co	-0.72543	-0.09743	-0.02779	H	-5.54289	-1.33468	0.267366
O	-0.57234	1.034434	-1.60459	C	-4.75783	-2.3774	-1.43774
H	-1.38584	1.49267	-1.86318	H	-5.67766	-2.91511	-1.64054
H	-0.29834	0.403119	-2.34243	C	-3.64309	-2.5234	-2.25495
C	3.535478	-1.98273	0.482397	H	-3.65145	-3.16412	-3.12881
C	3.514359	-0.99188	-0.48657	C	-2.47869	-1.82564	-1.94072
C	2.329388	-2.57583	0.910359	H	-1.62381	-1.91896	-2.58585
C	2.292417	-0.61981	-1.04857	N	-2.16874	0.848656	0.968054
C	1.129029	-2.21343	0.347713	N	-2.37671	-1.01139	-0.87611
C	1.062875	-1.25332	-0.73092	C	-0.60948	4.42842	-1.23469
F	4.651271	-0.40961	-0.87655	H	-1.61078	4.841074	-1.13515
F	4.681797	-2.33999	1.042827	C	0.230575	4.843886	-2.27151
F	2.416206	-3.42985	1.940594	H	-0.1128	5.577808	-2.99287
F	2.356253	0.311426	-2.0018	C	1.512784	4.298456	-2.34241
C	-0.16341	-2.58966	1.025386	H	2.200721	4.595724	-3.12773
O	-0.42535	-3.71135	1.436753	C	1.90239	3.362639	-1.3833
O	-0.93097	-1.53883	1.207859	H	2.892624	2.921761	-1.40779
C	0.523608	-1.83638	-2.27014	C	0.980047	2.99282	-0.39806
O	0.245898	-0.92611	-3.07186	C	1.379053	2.090737	0.730489
O	0.532974	-3.05422	-2.32624	C	2.44705	2.533805	1.522125

C	-2.00468	1.897986	1.791762	H	2.980062	3.425875	1.214622
H	-1.0601	2.413194	1.751128	C	2.780673	1.882607	2.705632
C	-3.01695	2.337752	2.640493	H	3.602681	2.236943	3.318593
H	-2.8346	3.192789	3.280781	C	2.004205	0.795933	3.095764
C	-4.23346	1.660854	2.645982	H	2.176468	0.268612	4.026841
H	-5.03801	1.963898	3.307323	C	0.984892	0.370072	2.254264
C	-4.41154	0.592454	1.77093	H	0.369135	-0.47362	2.529457
H	-5.35762	0.068773	1.7423	N	-0.25086	3.523385	-0.31435
C	-3.36487	0.211793	0.928389	N	0.686651	0.962662	1.073366
C	-3.48481	-0.81942	-0.10838	C	-4.67754	-1.49924	-0.36064
C	-4.67754	-1.49924	-0.36064				

The vibrational frequency of TS is -123.35.

Table S2. The Coordination Environment of the Cobalt Atom in Complexes **1** and **2**. Selected Interatomic Distances (Å) and Angles (deg).

		1			
Co(1)-O(1)	1.898(2)	O(1)-Co(1)-N(2)	176.66(8)	N(2)-Co(1)-N(4)	94.91(8)
Co(1)-N(1)	1.919(2)	N(1)-Co(1)-N(2)	83.06(8)	C(1)-Co(1)-N(4)	94.92(9)
Co(1)-N(2)	1.924(2)	O(1)-Co(1)-C(1)	84.74(9)	O(1)-Co(1)-N(3)	87.44(8)
Co(1)-C(1)	1.935(2)	N(1)-Co(1)-C(1)	87.23(9)	N(1)-Co(1)-N(3)	95.31(9)
Co(1)-N(4)	1.941(2)	N(2)-Co(1)-C(1)	96.52(9)	N(2)-Co(1)-N(3)	91.40(8)
Co(1)-N(3)	1.989(2)	O(1)-Co(1)-N(4)	88.05(8)	C(1)-Co(1)-N(3)	171.93(9)
O(1)-Co(1)-N(1)	93.93(8)	N(1)-Co(1)-N(4)	177.20(9)	N(4)-Co(1)-N(3)	82.80(10)
		2			
Co(1)-O(1)	2.0759(14)	O(6)-Co(1)-O(1)	90.20(5)	O(1)-Co(1)-N(2)	87.90(5)
Co(1)-N(1)	2.1139(16)	O(3)-Co(1)-O(1)	88.44(5)	N(1)-Co(1)-N(2)	77.31(6)
Co(1)-N(2)	2.1173(15)	O(6)-Co(1)-N(1)	93.48(6)	O(6)-Co(1)-O(5)	89.11(5)
Co(1)-O(3)	2.0735(14)	O(3)-Co(1)-N(1)	173.04(5)	O(3)-Co(1)-O(5)	89.20(5)
Co(1)-O(6)	2.0664(14)	O(1)-Co(1)-N(1)	96.00(6)	O(1)-Co(1)-O(5)	177.52(5)
Co(1)-O(5)	2.1466(15)	O(6)-Co(1)-N(2)	170.34(6)	N(1)-Co(1)-O(5)	86.41(6)
O(6)-Co(1)-O(3)	91.85(6)	O(3)-Co(1)-N(2)	97.56(6)	N(2)-Co(1)-O(5)	93.18(6)