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SUPPLEMENTARY MATERIAL TO

Solid–solid synthesis, characterization and thermal decomposition of a homodinuclear cobalt(II) complex

DI LI, GUO-QING ZHONG* and ZHI-XIAN WU

School of Material Science and Engineering, Southwest University of Science and Technology, Mianyang 621010, China

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TABLE S-I. Crystal data and structure refinement parameters for the title complex

Empirical formula	$Co_2C_{14}H_{20}O_{15}N_2$	Temperature, K	293(2)
Formula weight	574.18	Wavelength, Å	0.71073
Crystal system	Monoclinic	θ range, °	2.57–25.02
Space group	$P2(1)/c$	Limiting indices	$-9\leq h\leq 9$, $-32\leq k\leq 27$, $-11\leq l\leq 8$
a, Å	8.3680(5)	Reflections collected/unique	8367/3807 [R(int) = 0.0649]
b, Å	27.2976(14)	Completeness to theta = 25.02	99.9 %
c, Å	9.5826(4)	Absorption correction	Semi-empirical from equivalents
B, °	98.276(5)	Max. and min. transmission	0.6105 and 0.5652
V, Å^3	2166.12(19)	Refinement method	Full-matrix least-squares on F^2
Z	4	Data / restraints / parameters	3807 / 0 / 298
D_c, g cm^{-3}	1.761	Goodness-of-fit on F^2	1.031
μ (Cu K_α), mm^{-1}	1.610	Final R indices [$I>2\sigma(I)$]	R_1 = 0.0519, wR_2 = 0.0867
F(000)	1168	R indices (all data)	R_1 = 0.0915, wR_2 = 0.1086
Crystal size, mm	0.40×0.38×0.34	$\Delta\rho_{max}$ and $\Delta\rho_{min}$, e Å^{-3}	0.488 and –0.492

* Corresponding author. E-mail: zgq316@163.com

TABLE S-II. Selected bond lengths and angles for the title complex

Bond	Distance, Å	Bond	Angle, °	Bond	Angle, °
Co1–O12	2.051(3)	O12–Co1–O13	96.40(16)	N2–Co2–N1	172.19(16)
Co1–O13	2.051(4)	O12–Co1–O2	79.84(13)	N2–Co2–O5	76.77(16)
Co1–O2	2.075(3)	O13–Co1–O2	86.93(14)	N1–Co2–O5	105.03(15)
Co1–O10	2.076(3)	O12–Co1–O10	169.57(14)	N2–Co2–O7	75.72(15)
Co1–O9	2.080(3)	O13–Co1–O10	88.33(15)	N1–Co2–O7	103.67(15)
Co1–O11	2.172(3)	O2–Co1–O10	91.18(14)	O5–Co2–O7	150.48(14)
Co2–N1	2.012(4)	O12–Co1–O9	91.00(13)	N2–Co2–O3	112.15(15)
Co2–N2	2.012(4)	O13–Co1–O9	91.79(14)	N1–Co2–O3	75.64(14)
Co2–O5	2.110(4)	O2–Co1–O9	170.53(13)	O5–Co2–O3	85.96(14)
Co2–O7	2.175(4)	O10–Co1–O9	98.17(14)	O7–Co2–O3	94.63(14)
Co2–O3	2.178(3)	O12–Co1–O11	86.32(15)	N2–Co2–O1	96.13(14)
Co2–O1	2.215(3)	O13–Co1–O11	176.65(14)	N1–Co2–O1	76.15(14)
O1–C1	1.263(5)	O2–Co1–O11	95.49(13)	O5–Co2–O1	96.80(14)
O2–C1	1.252(5)	O10–Co1–O11	89.31(13)	O7–Co2–O1	96.56(13)
		O9–Co1–O11	86.19(13)	O3–Co2–O1	151.39(13)

TABLE S-III. Hydrogen bond lengths and bond angles for the title complex

D–H	*d*(D–H), Å	*d*(H···A), Å	*d*(D···A), Å	∠DHA, °	A symmetry operation
O9–H9C	0.850	1.919	2.764	172.28	O3 (*x*–1, *y*, *z*–1)
O9–H9D	0.850	1.808	2.652	171.56	O15 (*x*, *y*, *z*–1)
O10–H10C	0.850	1.985	2.831	173.26	O1
O10–H10C	0.850	2.470	2.965	117.97	O2
O10–H10D	0.850	1.848	2.695	173.45	O8 (*x*–1, *y*, *z*–1)
O11–H11C	0.850	1.831	2.675	171.39	O4 (–x+1, –y+1, z+1)
O11–H11D	0.850	1.939	2.782	171.32	O7 (*x*–1, *y*, *z*)
O12–H12C	0.850	1.801	2.635	166.60	O4 (x–1, *y*, *z*–1)
O12–H12D	0.850	2.127	2.936	167.46	O14
O13–H13C	0.850	1.886	2.726	169.72	O6 (*x*, *y*, *z*–1)
O13–H13D	0.850	1.982	2.823	170.12	O14 (–*x*+1, –*y*+1, –*z*)
O14–H14C	0.850	2.232	3.060	164.82	O5 (–*x*+1, –*y*+1, –*z*+1)
O14–H14D	0.850	2.103	2.933	165.10	O11 (–*x*, –*y*+1, –*z*)
O15–H10C	0.850	1.918	2.764	173.53	O6
O15–H10D	0.850	1.929	2.775	173.95	O8 (*x*–1, –*y*+3/2, *z*+1/2)

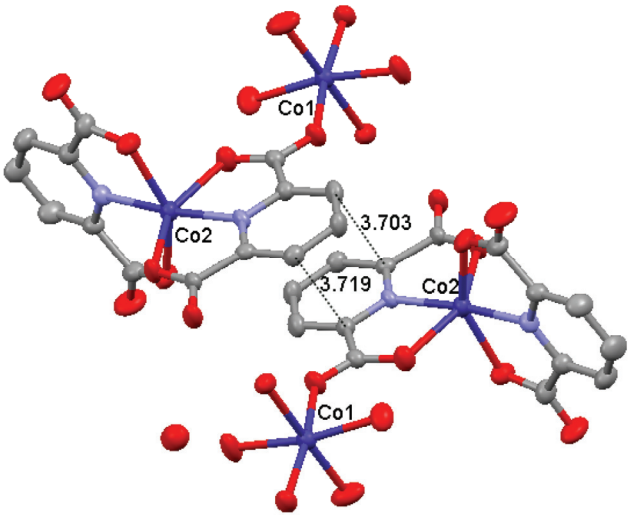

Fig. S-1. Weak spatial π–π stacking interactions of the title complex.

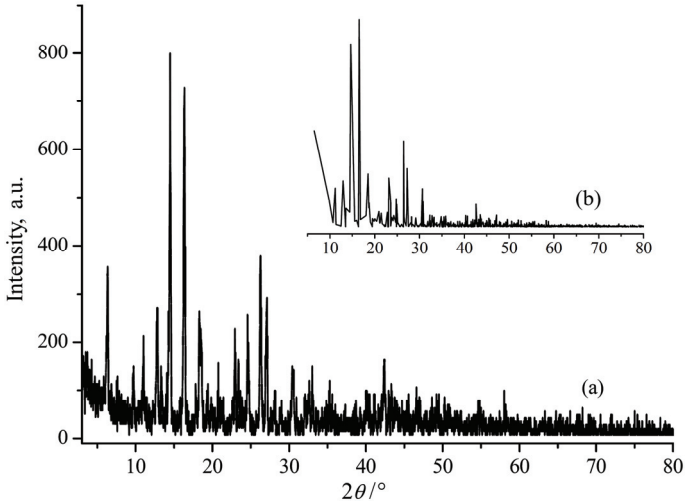

Fig. S-2. XRD patterns for the title complex (a) generated from the experimental data and (b) simulated from the single crystal X-ray data.

TABLE S-IV. Experimental data and calculated results for powder X-ray diffraction pattern of the title complex (monoclinic: a = 8.397 Å, b = 27.409 Å, c = 9.609 Å and β = 98.22°)

No.	2θ, °	h	k	l	d_{exp}, Å	d_{cal}, Å	I/I_0	No.	2θ, °	h	k	l	d_{exp}, Å	d_{cal}, Å	I/I_0
1	6.44	0	2	0	13.710	13.705	37.7	9	18.43	1	4	–1	4.811	4.810	34.0
2	9.84	0	1	1	8.980	8.985	13.2	10	18.65	0	0	–2	4.755	4.755	19.1
3	11.12	1	1	0	7.950	7.953	18.6	11	19.44	0	6	0	4.563	4.568	9.5
4	12.92	0	4	0	6.845	6.852	38.3	12	20.88	1	5	–1	4.250	4.256	9.6
5	13.48	1	1	–1	6.565	6.559	8.5	13	21.39	2	0	0	4.151	4.155	6.3

TABLE S-IV. Continued

No.	2θ, °	h	k	l	d_{exp}, Å	d_{cal}, Å	I/I_0	No.	2θ, °	h	k	l	d_{exp}, Å	d_{cal}, Å	I/I_0
6	14.60	1	2	–1	6.061	6.059	100	14	23.04	1	1	2	3.857	3.856	22.0
7	16.45	1	2	1	5.386	5.386	97.4	15	23.51	2	3	0	3.782	3.783	14.6
8	17.97	1	3	1	4.933	4.931	7.2	16	24.17	2	3	–1	3.680	3.683	6.3
17	24.74	0	5	2	3.596	3.592	17.4	26	40.14	1	4	–4	2.245	2.246	9.8
18	26.38	2	0	–2	3.376	3.377	56.0	27	41.83	3	8	0	2.158	2.154	6.2
19	27.17	2	2	–2	3.279	3.279	37.6	28	42.45	2	8	–3	2.128	2.128	13.1
20	30.52	1	7	–2	2.927	2.927	16.0	29	47.06	3	2	–4	1.929	1.928	6.3
21	32.23	1	9	–1	2.775	2.776	6.1	30	50.39	4	6	1	1.809	1.810	7.1
22	32.67	0	5	3	2.739	2.744	8.3	31	57.94	4	4	3	1.590	1.589	6.0
23	33.12	1	3	3	2.703	2.703	8.6	32	65.18	5	4	–4	1.430	1.432	6.4
24	38.36	2	7	2	2.345	2.345	7.4	33	76.94	2	1	7	1.238	1.239	7.5
25	38.87	3	5	–2	2.315	2.318	6.7								

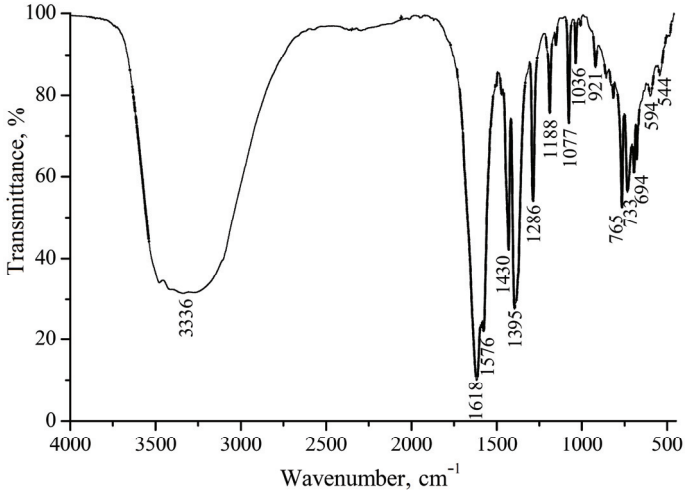

Fig. S-3. FT-IR spectrum of the title complex.

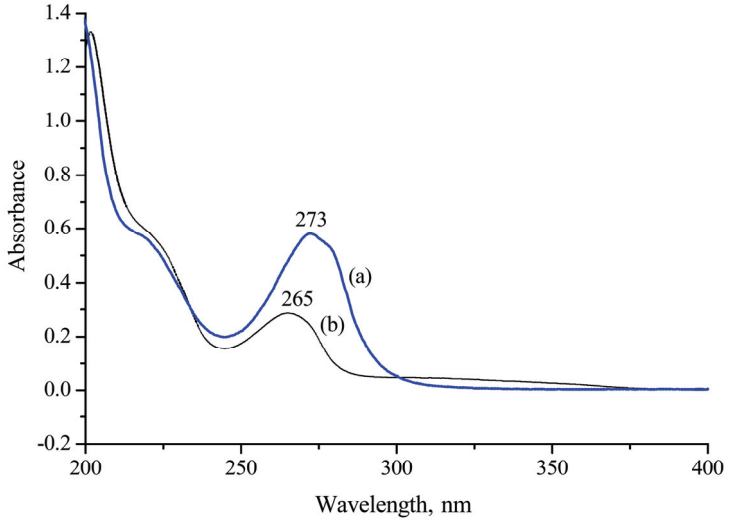

Fig. S-4. UV spectra of (a) the ligand and (b) the title complex.

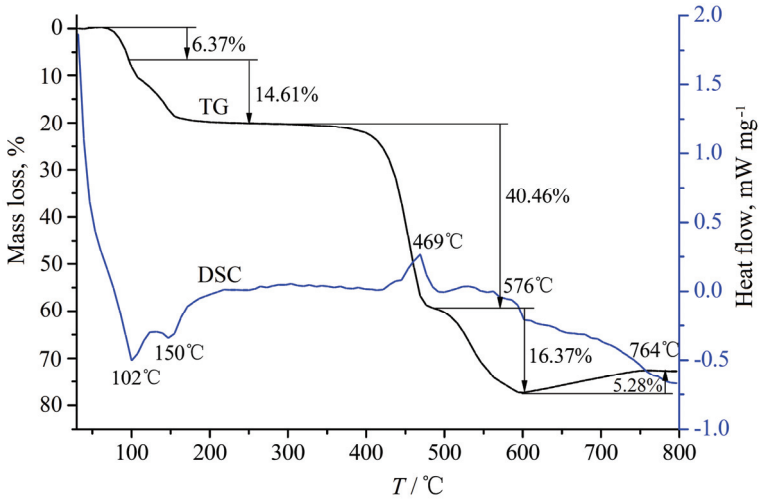

Fig. S-5. TG–DSC curves of the title complex obtained under a air atmosphere.

TABLE S-V. Thermal decomposition data of the title complex

Reaction	T_{DSC}, °C	Mass loss, %	
		m_{exp}	m_{theor}
$[Co_2(C_7H_3O_4N)_2(H_2O)_5]\cdot 2H_2O$ ↓ $-2H_2O$	102 (endo.)	6.37	6.28
$[Co_2(C_7H_3O_4N)_2(H_2O)_5]$ ↓ $-5H_2O$	150 (endo.)	14.61	15.69
$[Co_2(C_7H_3O_4N)_2]$ ↓$-2C_5H_3N$, $-2CO_2$	469 (exo.)	40.46	42.17
CoC_2O_4 + Co ↓ $-2CO_2$	576 (exo.)	16.37	15.33
2Co ↓ $+O_2$	764 (exo.)	5.28[a]	5.57[a]
2CoO		27.47[b]	26.10[c]

[a]The increased mass percentage; [b]the experimental mass percentage of the residue in the sample, [c]the calculated mass percentage of the residue in the sample