Supplementary Information

An insight into the non-covalent interactions in the solid state structures of dinuclear cobalt(II) complexes with N,O-donor ligands: Application of the complexes in the fabrication of Schottky devices

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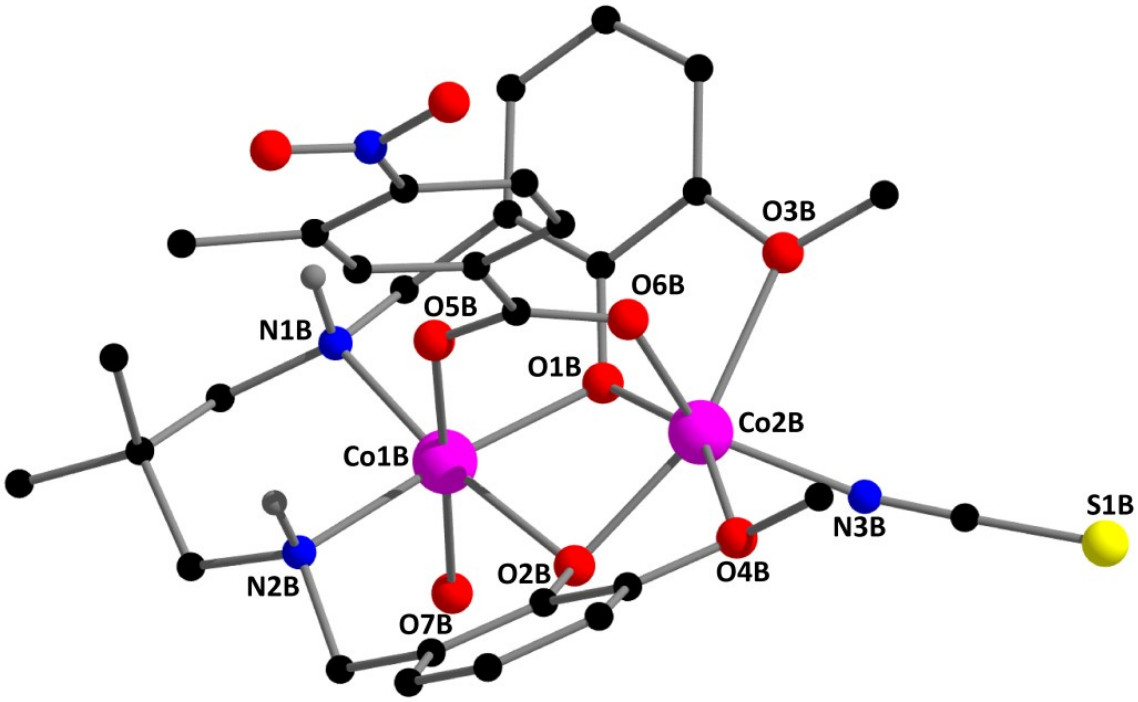

Fig. S1. Perspective view of the sub-unit B of complex **1**. Hydrogen atoms have been omitted for clarity.

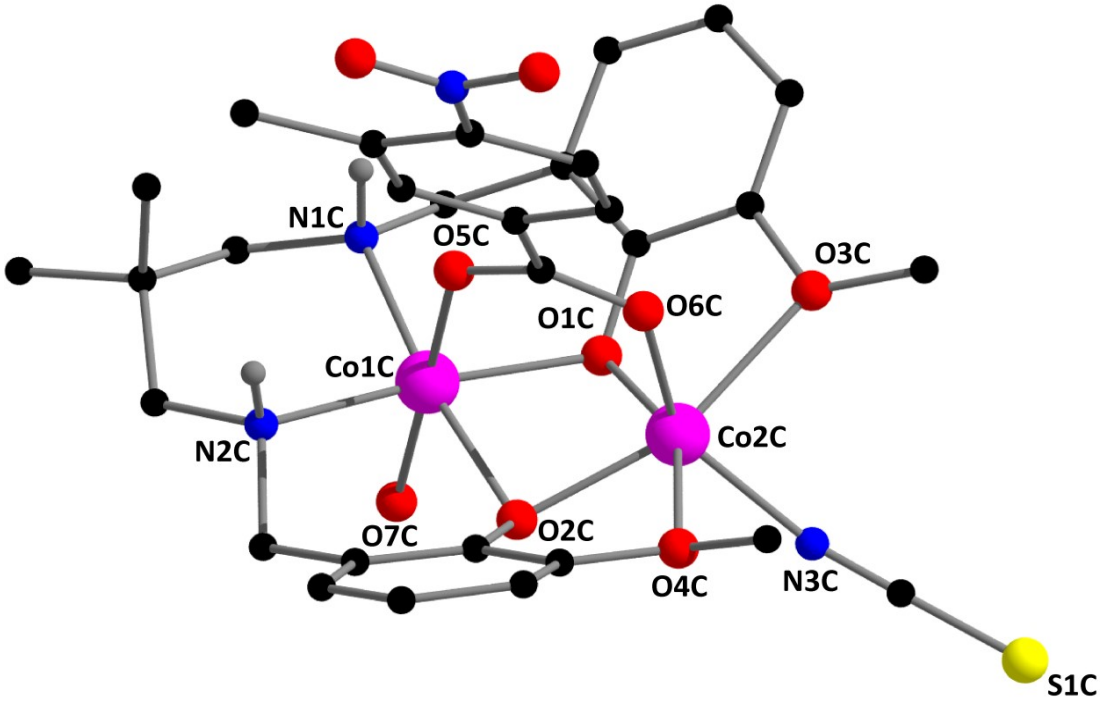

Fig. S2. Perspective view of the sub-unit C of complex **1**. Hydrogen atoms have been omitted for clarity.

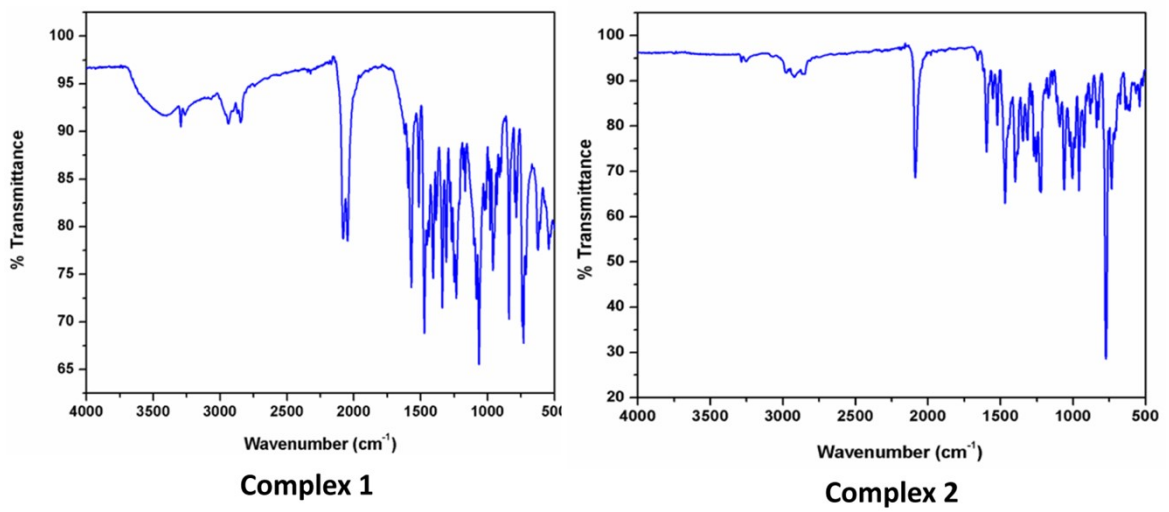

Fig. S3. IR spectra of complexes **1**(left) and **2** (right).

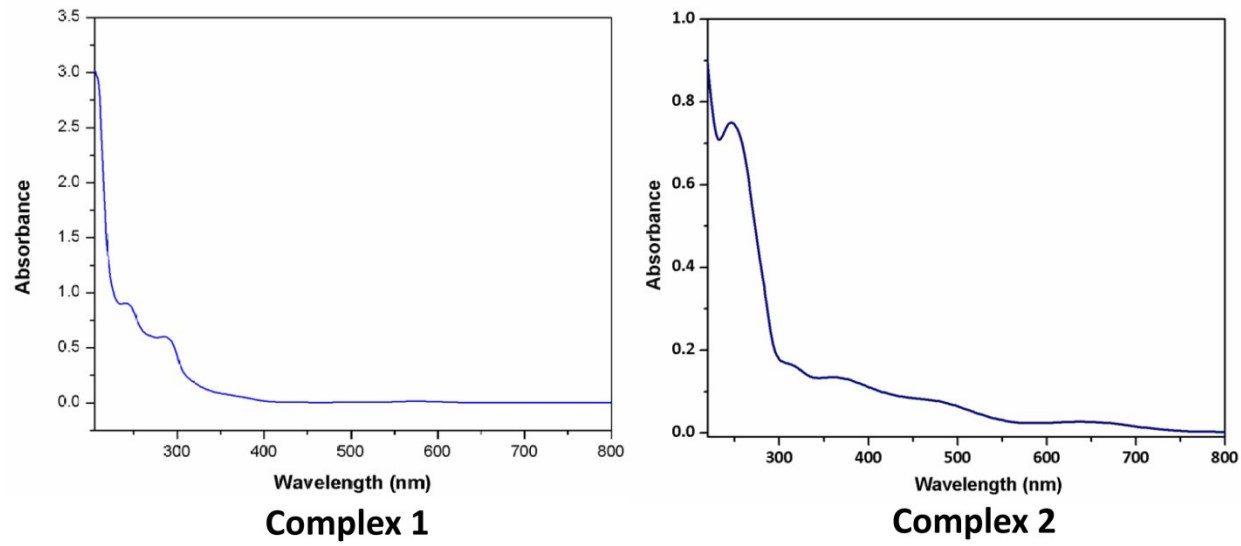

Fig. S4. UV-vis spectra of complexes **1** and **2**.

Hirshfeld Surface analysis

Hirshfeld surfaces[1-3] and the fingerprint[4-5](2D) plots were calculated using Crystal Explorer.[6-7]

Hirshfield surface analysis

The Hirshfeld surfaces of both complexes, mapped over d_{norm} (range -0.1 Å to 1.5 Å), have been shown in Figure 4. Red spots on these surfaces are indicative of the principal interactions (Figure **S5**) which include C···H/H···C, N···H/H···N and O···H/H···O (for **1**), C···H/H···C,O···H/H···O and S···H/H···S (for **2**) interactions. These interactions appear as distinct spikes in the 2D fingerprint plots (Figure **S6**).

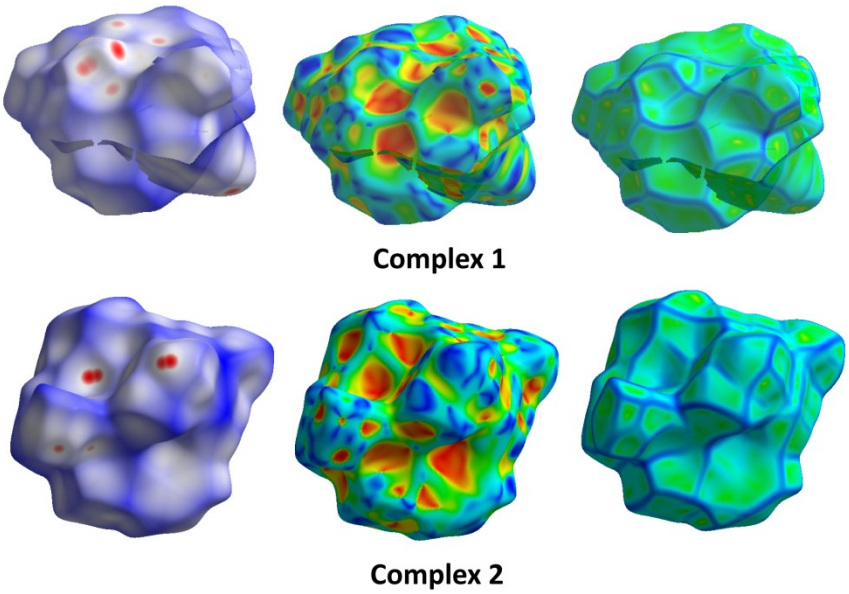

Figure S5. Hirshfeld surfaces mapped with d_{norm} (left), shape index (middle) and curvedness (right) for complex **1** (top) and complex **2** (bottom)

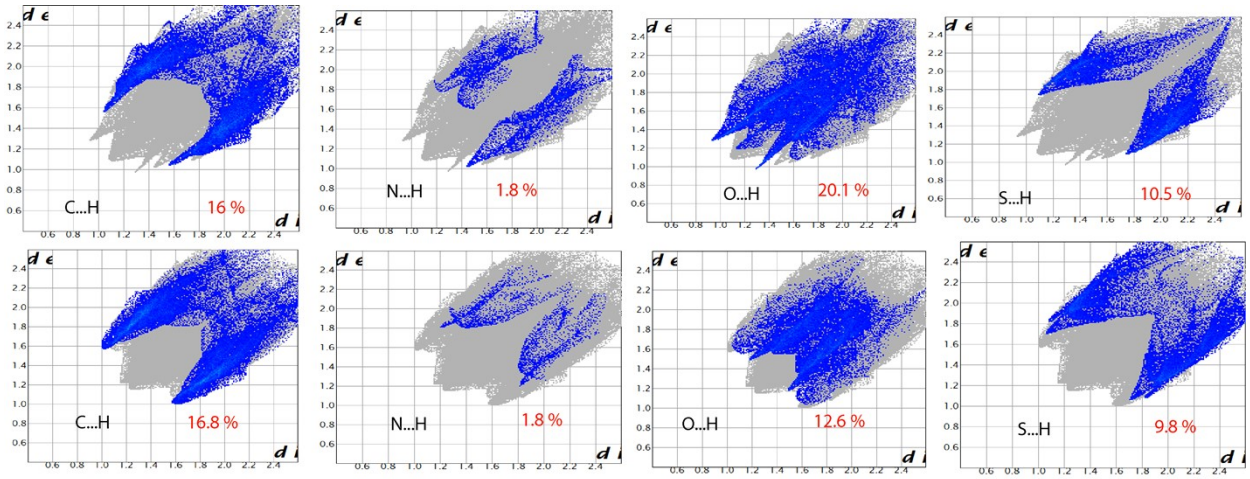

Figure S6. Fingerprint plots: different contacts contributed to the total Hirshfeld surface area of complexes **1(top)** and **2(bottom)**

Table S1. Selected bond lengths (Å) of complexes **1** and **2**

	Complex – 1			**Complex - 2**
	Subunit A	Subunit B	Subunit C	
Co(1)–O(1)	2.087(4)	2.086(4)	2.088(4)	2.111(2)
Co(1)–O(2)	2.103(4)	2.108(4)	2.101(4)	2.046(2)
Co(1)–O(5)	2.124(4)	2.123(3)	2.122(4)	2.118(2)
Co(1)–O(7)	2.141(4)	2.146(4)	2.135(4)	2.125(2)
Co(1)–N(1)	2.106(5)	2.119(4)	2.105(5)	2.100(2)

Co(1)–N(2)	2.113(5)	2.106(4)	2.109(5)	2.125(2)
Co(2)–O(1)	2.015(4)	2.018(4)	2.013(4)	2.023(2)
Co(2)–O(2)	2.048(4)	2.042(4)	2.040(4)	2.004(2)
Co(2)–O(3)	2.314(6)	2.319(6)	2.321(6)	2.518(2)
Co(2)–O(4)	2.350(5)	2.348(5)	2.347(5)	2.387(4)
Co(2)–O(6)	2.032(4)	2.025(4)	2.027(4)	2.030(2)
Co(2)–N(3)	1.997(6)	1.995(6)	1.998(6)	1.980(3)

Table S2. Selected bond angles (°) of complexes **1-2.**

	Complex **1**			Complex **2**
	Subunit A	Subunit B	Subunit C	
O(1)–Co(1)–O(2)	80.33(16)	80.14(16)	79.94(16)	80.28(8)
O(1)–Co(1)–O(5)	92.74(15)	92.76(16)	92.90(16)	88.74(8)
O(1)–Co(1)–O(7)	89.77(19)	90.02(18)	89.2(2)	93.66(8)

O(1)–Co(1)–N(1)	91.81(17)	91.84(18)	92.10(18)	91.62(8)
O(1)–Co(1)–N(2)	172.78(17)	172.89(19)	172.72(17)	172.03(9)
O(2)–Co(1)–O(5)	90.47(15)	90.62(15)	90.38(15)	92.09(8)
O(2)–Co(1)–O(7)	87.67(18)	87.6(2)	87.53(19)	90.97(8)
O(2)–Co(1)–N(1)	172.12(18)	171.96(17)	172.00(18)	171.88(8)
O(2)–Co(1)–N(2)	92.61(17)	92.87(17)	92.88(17)	91.93(9)
O(5)–Co(1)–O(7)	176.6(2)	176.4(2)	176.8(2)	176.40(8)
O(5)–Co(1)-N(1)	89.23(16)	89.19(16)	89.22(16)	87.15(9)
O(5)–Co(1)–N(2)	85.75(17)	85.98(15)	85.85(17)	89.87(9)
O(7)–Co(1)–N(1)	93.0(2)	93.1(2)	93.2(2)	90.12(9)
O(7)–Co(1)–N(2)	91.5(2)	91.0(2)	91.8(2)	88.12(9)
N(1)–Co(1)–N(2)	95.22(17)	95.13(18)	95.06(18)	96.15(9)
O(1)–Co(2)–O(2)	83.39(16)	83.37(17)	83.20(16)	83.47(8)
O(1)–Co(2)–O(6)	99.34(17)	99.21(18)	99.42(18)	98.04(9)
O(1)–Co(2)–N(3)	114.8(2)	114.8(2)	114.8(3)	106.73(12)
O(2)–Co(2)–O(6)	97.42(17)	97.55(16)	97.25(17)	99.18(9)

O(2)–Co(2)–N(3)	112.3(3)	112.1(3)	112.1(3)	114.24(12)
O(6)–Co(2)–N(3)	136.3(3)	136.4(2)	136.6(3)	139.97(12)
O(3)-Co(2)-O(1)	73.52(17)	73.56(18)	73.86(18)	71.05(8)
O(3)-Co(2)-O(2)	156.29(17)	156.25(18)	156.29(17)	153.22(8)
O(3)-Co(2)-O(6)	81.4(2)	81.0(2)	81.0(2)	77.01(9)
O(3)-Co(2)-N(3)	83.0(3)	83.3(3)	83.6(3)	81.87(11)
O(3)-Co(2)-O(4)	129.72(17)	129.77(18)	129.50(19)	133.26(9)
O(4)-Co(2)-O(1)	154.98(17)	154.92(17)	154.89(18)	155.34(9)
O(4)-Co(2)-O(2)	72.37(17)	72.29(17)	72.39(17)	71.87(9)
O(4)-Co(2)-O(6)	78.26(18)	78.63(18)	78.45(18)	86.10(11)
O(4)-Co(2)-N(3)	81.0(2)	80.8(2)	80.8(2)	84.16(13)

Table S3. Bond valence sum calculation and the related parameters of subunit **A** in complex **1.**

i−*j* *reported*	r_0	*i*−*j* *this complex*	r_{ij}	S_{ij}	Z_j
O−Co^{2+}	1.68	O(1)-Co(1)	2.087	0.332	2.103
O−Co^{2+}	1.68	O(2)-Co(1)	2.103	0.318	
O−Co^{2+}	1.68	O(5)-Co(1)	2.124	0.301	
O−Co^{2+}	1.68	O(7)-Co(1)	2.141	0.287	
N−Co^{2+}	1.80	N(1)−Co(1)	2.106	0.436	
N−Co^{2+}	1.80	N(2)−Co(1)	2.113	0.429	
O−Co^{2+}	1.68	O(1)-Co(2)	2.015	0.404	2.093
O−Co^{2+}	1.68	O(2)-Co(2)	2.048	0.369	
O−Co^{2+}	1.68	O(3)-Co(2)	2.314	0.180	
O−Co^{2+}	1.68	O(4)-Co(2)	2.350	0.163	

O−Co^{2+}	1.68	O(6)-Co(2)	2.031	0.387	
N−Co^{2+}	1.80	N(3)−Co(2)	1.997	0.587	

Table S4. Bond valence sum calculation and the related parameters of subunit **B** in complex **1.**

i−*j* *reported*	r_0	*i*−*j* *this complex*	r_{ij}	S_{ij}	Z_j
O−Co^{2+}	1.68	O(1)-Co(1)	2.086	0.333	2.091
O−Co^{2+}	1.68	O(2)-Co(1)	2.108	0.314	
O−Co^{2+}	1.68	O(5)-Co(1)	2.123	0.302	
O−Co^{2+}	1.68	O(7)-Co(1)	2.146	0.283	
N−Co^{2+}	1.80	N(1)−Co(1)	2.119	0.422	
N−Co^{2+}	1.80	N(2)−Co(1)	2.106	0.437	
O−Co^{2+}	1.68	O(1)-Co(2)	2.018	0.401	2.100
O−Co^{2+}	1.68	O(2)-Co(2)	2.042	0.375	
O−Co^{2+}	1.68	O(3)-Co(2)	2.319	0.177	

O−Co^{2+}	1.68	O(4)-Co(2)	2.348	0.164	
O−Co^{2+}	1.68	O(6)-Co(2)	2.025	0.393	
N−Co^{2+}	1.80	N(3)−Co(2)	1.995	0.590	

Table S5. Bond valence sum calculation and the related parameters of subunit **C** in complex **1.**

i−*j* *reported*	r_0	*i*−*j* *this complex*	r_{ij}	S_{ij}	Z_j
O−Co^{2+}	1.68	O(1)-Co(1)	2.088	0.331	2.144
O−Co^{2+}	1.68	O(2)-Co(1)	2.101	0.320	
O−Co^{2+}	1.68	O(5)-Co(1)	2.122	0.302	
O−Co^{2+}	1.68	O(7)-Co(1)	2.135	0.291	
N−Co^{2+}	1.80	N(1)−Co(1)	2.105	0.437	
N−Co^{2+}	1.80	N(2)−Co(1)	2.109	0.433	
O−Co^{2+}	1.68	O(1)-Co(2)	2.103	0.331	2.002

O−Co^{2+}	1.68	O(2)-Co(2)	2.040	0.377	
O−Co^{2+}	1.68	O(3)-Co(2)	2.321	0.176	
O−Co^{2+}	1.68	O(4)-Co(2)	2.347	0.164	
O−Co^{2+}	1.68	O(6)-Co(2)	2.027	0.369	
N−Co^{2+}	1.80	N(3)−Co(2)	1.998	0.585	

Table S6. Bond valence sum calculation and the related parameters of complex **2.**

i−*j* *reported*	r_0	*i*−*j* *this complex*	r_{ij}	S_{ij}	Z_j
O−Co^{2+}	1.68	O(1)-Co(1)	2.111	0.311	2.146
O−Co^{2+}	1.68	O(2)-Co(1)	2.046	0.370	
O−Co^{2+}	1.68	O(5)-Co(1)	2.118	0.306	
O−Co^{2+}	1.68	O(7)-Co(1)	2.125	0.300	
N−Co^{2+}	1.80	N(1)−Co(1)	2.100	0.444	
N−Co^{2+}	1.80	N(2)−Co(1)	2.125	0.415	
O−Co^{2+}	1.68	O(1)-Co(2)	2.023	0.395	2.065
O−Co^{2+}	1.68	O(2)-Co(2)	2.004	0.416	

$O-Co^{2+}$	1.68	O(3)-Co(2)	2.518	0.103	
$O-Co^{2+}$	1.68	O(4)-Co(2)	2.387	0.147	
$O-Co^{2+}$	1.68	O(6)-Co(2)	2.030	0.388	
$N-Co^{2+}$	1.80	N(3)−Co(2)	1.979	0.616	

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