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SUPPORTING INFORMATION

Crystal structures, magnetic properties and DFT study of cobalt(II) azido complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

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Table S1

Selected bond lengths (Å) and angles (°) for **1** and **2**.

1			
Co1–N1	2.003(2)	O1–Co1–N1	163.65(10)
Co1–N2	1.854(2)	O1–Co1–N2	81.62(10)
Co1–N5	1.951(3)	O1–Co1–N5	90.17(12)
Co1–N8	1.958(3)	O1–Co1–N8	92.17(10)
Co1–N11	1.967(3)	O1–Co1–N11	91.04(13)
Co1–O1	1.917(2)	N1–Co1–N2	82.09(10)
N2–N3	1.381(3)	N2–Co1–N8	173.03(10)
N2–C10	1.274(4)	N5–Co1–N11	178.76(12)
2			
Co1–N1	2.1860(19)	O1–Co1–N1	147.51(8)
Co1–N2	2.058(2)	O1–Co1–N2	73.85(8)
Co1–N9	2.132(3)	O1–Co1–N9	90.34(10)
Co1–N15	2.098(2)	O1–Co1–N15	91.18(8)
Co1–N18	2.167(3)	O1–Co1–N18	100.11(9)
Co1–O1	2.1271(19)	N1–Co1–N2	75.39(8)
Co2–N5	2.248(2)	N1–Co1–N9	87.81(9)
Co2–N6	2.062(2)	O2–Co2–N5	147.18(8)
Co2–N12	2.107(3)	O2–Co2–N6	73.52(8)
Co2–N15	2.160(2)	O2–Co2–N12	89.20(10)
Co2–N18	2.091(2)	O2–Co2–N15	96.17(9)
Co2–O2	2.1700(19)	O2–Co2–N18	101.14(8)
N2–N3	1.383(3)	N5–Co2–N6	75.00(9)
N6–N7	1.384(3)	N5–Co2–N12	87.84(11)
C11–N3	1.323(4)	Co1–N15–Co2	103.37(10)
C26–N7	1.318(4)	Co1–N18–Co2	103.36(11)

Table S2

Intermolecular π···π interaction parameters for complex **1**.

Cg(*I*)[a]	Cg(*J*)[a]	Cg(*I*) –Cg(*J*)[b] (Å)	α[c] (°)	β[d] (°)	γ[e] (°)	Sym. code on (*J*)
Cg(1)	Cg(1)	4.1197(16)	0.0	35.0	35.0	3-*x*,-*y*,1-*z*
Cg(1)	Cg(2)	3.7260(17)	1.58(13)	23.8	24.5	3-*x*,-*y*,1-*z*
Cg(2)	Cg(2)	4.7312(19)	0.0	44.8	44.8	3-*x*,-*y*,1-*z*

[a] Labels of aromatic rings: (1) = N(1),C(1)–C(4),C(9); (2) = C(4)–C(9).
[b] Cg(*I*) – Cg(*J*) = Distance between ring centroids (Ang.).
[c] α = Dihedral angle between planes (*I*) and (*J*) (Deg).
[d] β = Angle between Cg(*I*)–Cg(*J*) vector and normal to plane (I) (Deg).
[e] γ = Angle between Cg(I) –Cg(*J*) vector and normal to plane (J) (Deg).

Table S3

Intermolecular C–H···π(quinoline) interaction parameters for complex **1**.

C–H	Cg(*J*)	H···Cg (Å)	H···(quinoline *J*)[a] (Å)	C–H···Cg (°)	γ[b] (°)	Sym. code on (*J*)
C15–H15B	Cg(2)	2.66	2.62	145	10.32	1+*x*, *y*, *z*

[a] Perpendicular distance of H to ring plane (*J*) (Ang.).
[b] γ = Angle between H···Cg line and perpendicular H···(ring plane) line (Deg).

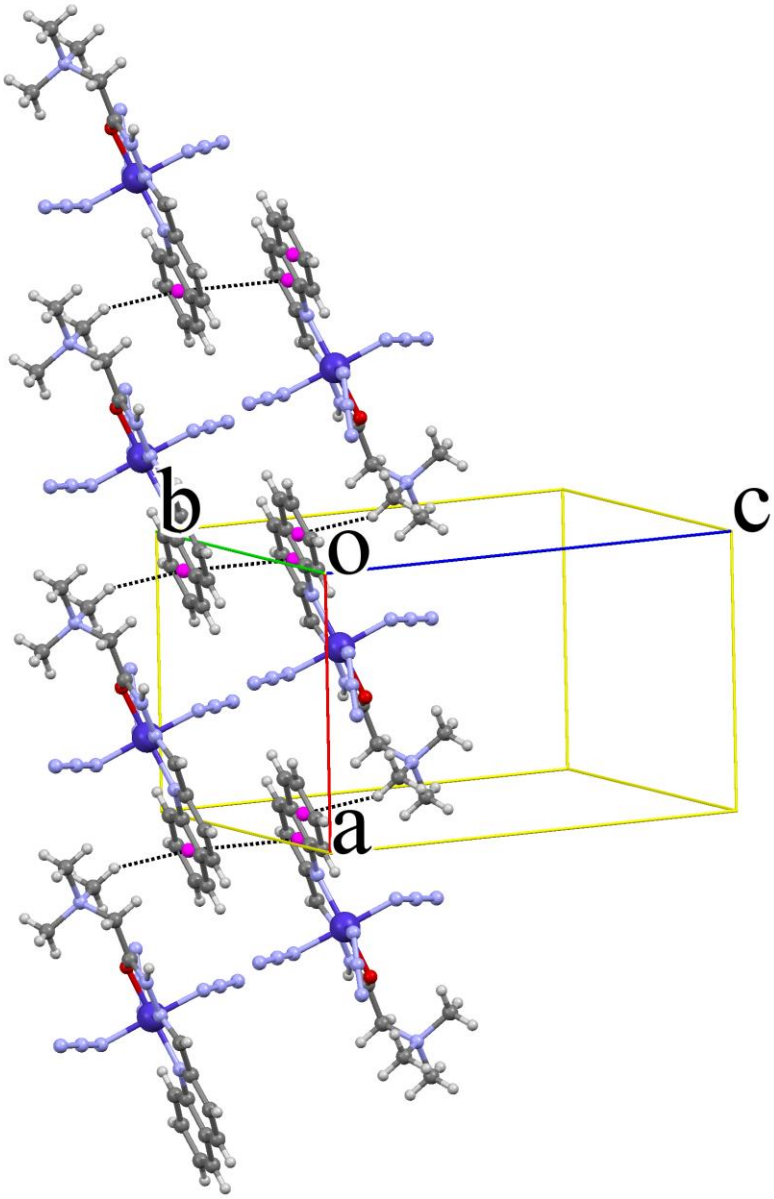

Fig. S1. Perspective view of the crystal structure of **1** showing complex molecules linked through π···π and C–H···π(ring) interactions.

Table S4

The experimental and the theoretical calculated average values of selected bond lengths (Å) and bond angles (°) obtained for the complexes **1** and **2**.

Compound	**1**			**2**	
Distance, Å			Distance, Å		
Co1–N8	1.958[a]	1.967[b]	Co2-N6	2.062[a]	1.880[b]
Co1–O1	1.917[a]	1.972[b]	Co2-O2	2.170[a]	1.998[b]
Co1–Co2	–	–		3.341[a]	3.127[b]
Angle, °			Angle, °		
Trans			*Trans*		
N5–Co1–N11	178.76[a]	178.55[b]	N15-Co2-N5	164.59[a]	167.65[b]
Cis			*Cis*		
N1–Co1–N2	82.11[a]	82.22[b]	N5-Co2-N6	75.00[a]	78.00[b]
N1–Co1–N5	89.97[a]	87.94[b]	N5-Co2-N12	87.84[a]	89.25[b]
N1–Co1–N11	88.94[a]	91.83[b]	N15-Co2-N18	76.80[a]	77.73[b]
N2–Co1–O1	81.61[a]	81.94[b]	O2-Co2-N6	73.52[a]	81.30[b]
N2–Co1–N5	95.25[a]	90.99[b]	O2-Co2-N12	89.20[a]	89.20[b]
N2–Co1–N11	85.17[a]	87.56[b]	Co1–N18–Co2	103.40[a]	102.16[b]

[a] Crystal structure data obtained by XRD in the present work;
[b] Optimized geometries parameters obtained by DFT/B3LYP/6-31G

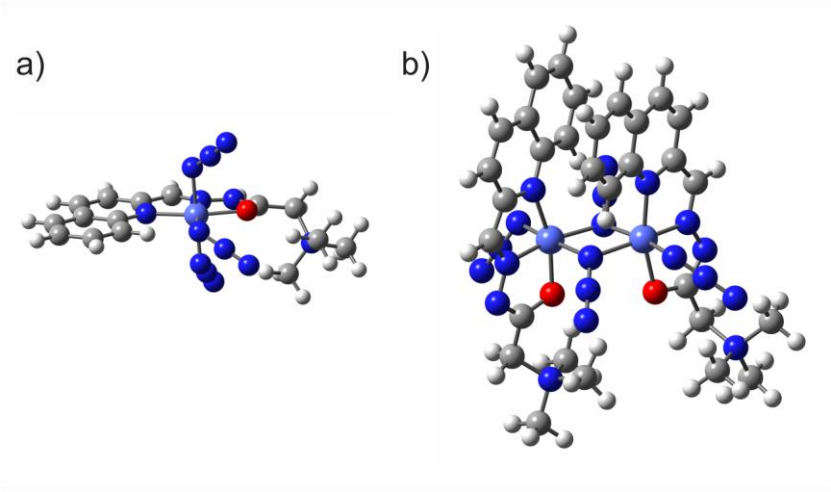

Fig. S2. Optimized the ground state geometries of a) complex **1** and b) complex **2**.

Table S5

Selected highest values of the condensed Fukui functions (f^+ and f^-) for the complexes **1** and **2**, considering DFT / NBO charges according to equations (2 and 3).

Compound / atom		Co1	N_{13}	N_{11}	N_{10}	N_7
1	f^+	**0.090**	0.120	0.040	**0.099**	**0.100**
	f^-	**0.079**	**0.437**	**0.519**	0.008	0.013
		Co1	N_{11}	N_9	N_{20}	N_{17}
2	f^+	**0.175** **0.278**	0.026	0.026	**0.110**	**0.128**
	f^-	0.079 0.094	**0.477**	**0.477**	0.007	0.010