



STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 75 (2019)

Supporting information for article:

**Influence of ligand positional isomerism on the molecular and
supramolecular structures of cobalt(II)-phenylimidazole complexes**

**Vasilios Duros, Constantina Papatriantafyllopoulou, Alexandros A. Kitos,
Anastasios J. Tasiopoulos and Vassilios Nastopoulos**

Table S1 $\pi \cdots \pi$ stacking distances (Å) and angles (°) in complexes **1–8**.

Structure	Rings involved*	Distance between ring centroids	Perpendicular distance between ring planes	Centroid offset	Dihedral angle between ring mean-planes
1	C1–B2	3.715(3)	3.699(3)	0.347(9)	8.4(2)
	D2–A2 ⁱ	3.720(2)	3.423(3)	1.448(6)	4.9(1)
2	A2–A2 ⁱⁱ	3.771(3)	3.530(3)	1.327(5)	5.8(2)
	A1–A1 ⁱⁱⁱ	3.515(2)	3.280(3)	1.265(5)	0.0
3	B2–A1 ^{iv}	3.871(2)	3.683(3)	1.191(6)	19.2(1)
4	–	–	–	–	–
5	B2–B2 ^v	3.899(5)	3.632(6)	1.419(9)	0.6(3)
6	A2–A2 ^{vi}	3.916(3)	3.654(4)	1.408(6)	4.4(2)
7	A2–A2 ^{vii}	3.709(2)	3.383(3)	1.519(4)	0.0
8	A2–A2 ^{viii}	3.710(2)	3.379(2)	1.531(3)	0.0

* C1: N1C to C5C; B2: C6B to C11B; D2: C6D to C11D; A2: C6A to C11A; A1: N1A to C5A.

Symmetry codes: (i) $3/2-x, y, -1/2+z$; (ii) $1-x, y, 1/2-z$; (iii) $1/2-x, 1/2-y, -z$; (iv) $x, 1/2-y, 1/2+z$; (v) $2-x, 1-y, z$; (vi) $-x, -y, z$; (vii) $-x, -y, 1-z$; (viii) $1/2-x, 1/2-y, 1-z$.

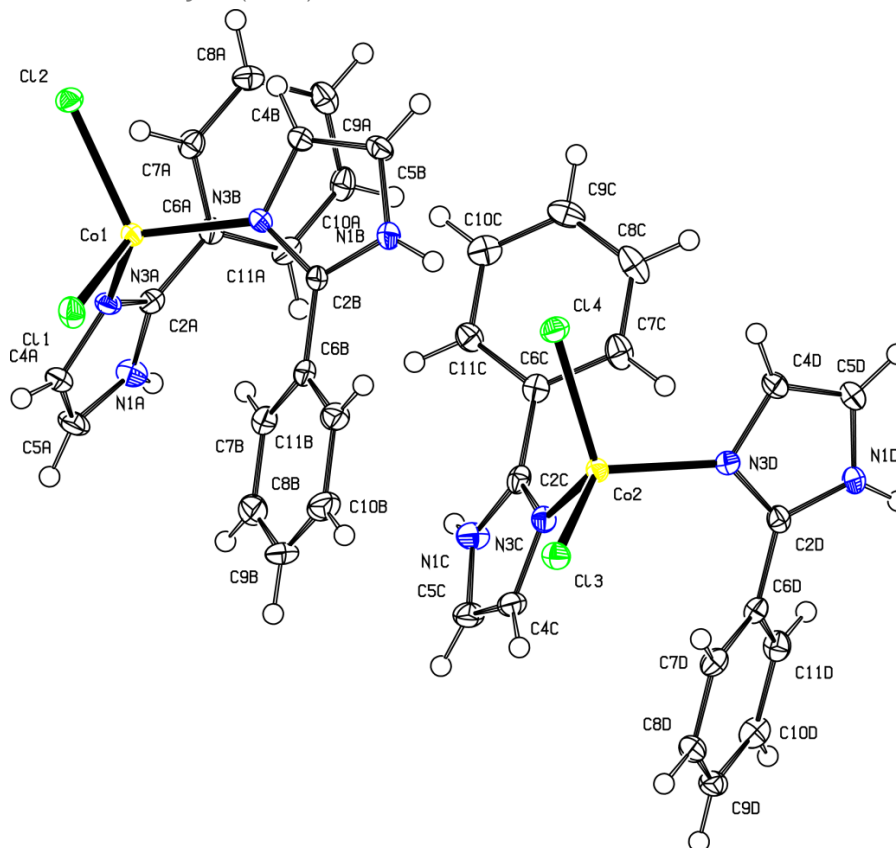


Figure S1 View of the asymmetric unit of compound **1** with atom labelling and displacement ellipsoids drawn at the 50% probability level.

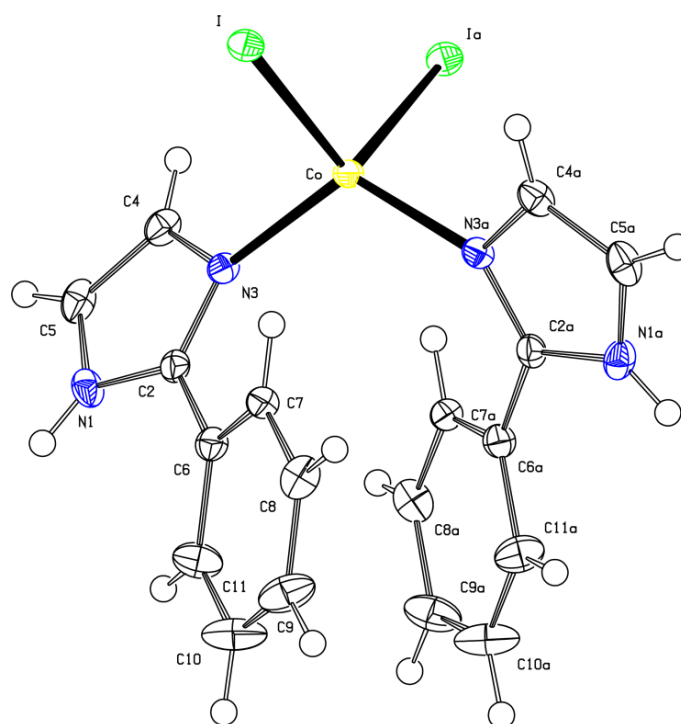


Figure S2 A view of the structure of compound **2** with atom labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (a) $1 - x, y, 1/2 - z$.

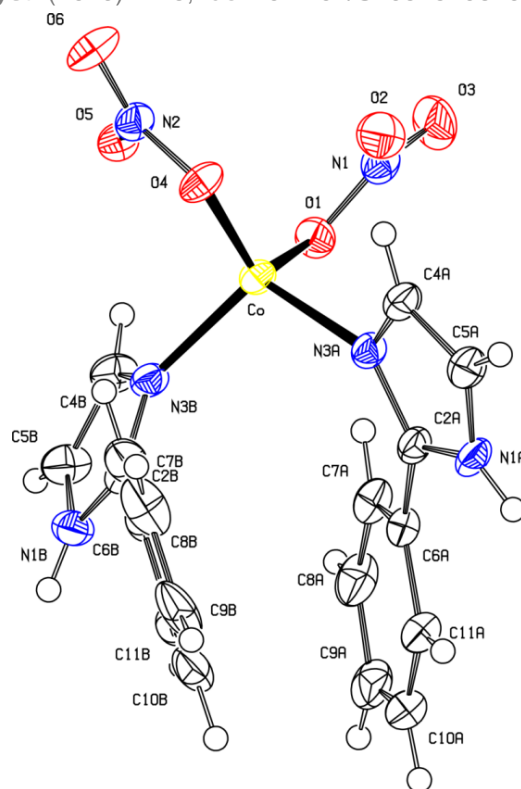


Figure S3 A view of the structure of compound **3** with atom labelling and displacement ellipsoids drawn at the 50% probability level.

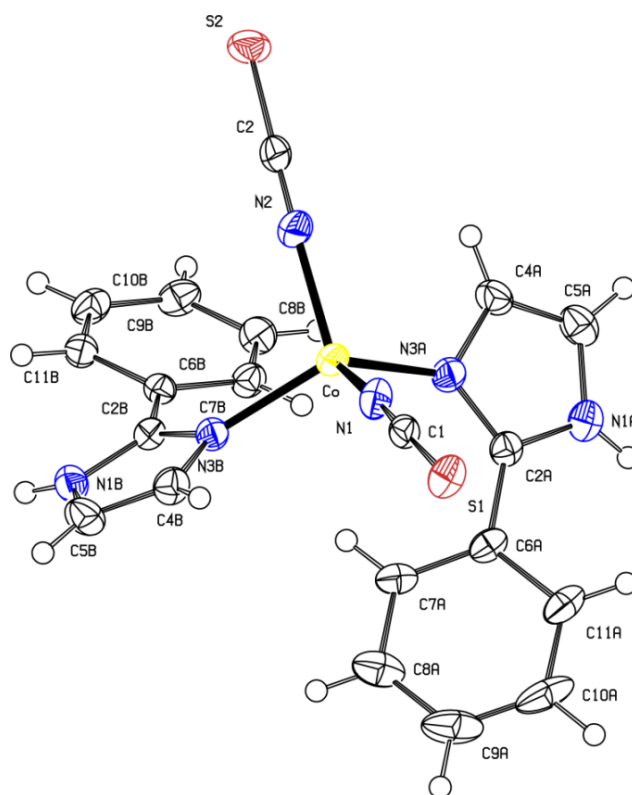


Figure S4 A view of the structure of compound **4** with atom labelling and displacement ellipsoids drawn at the 50% probability level.

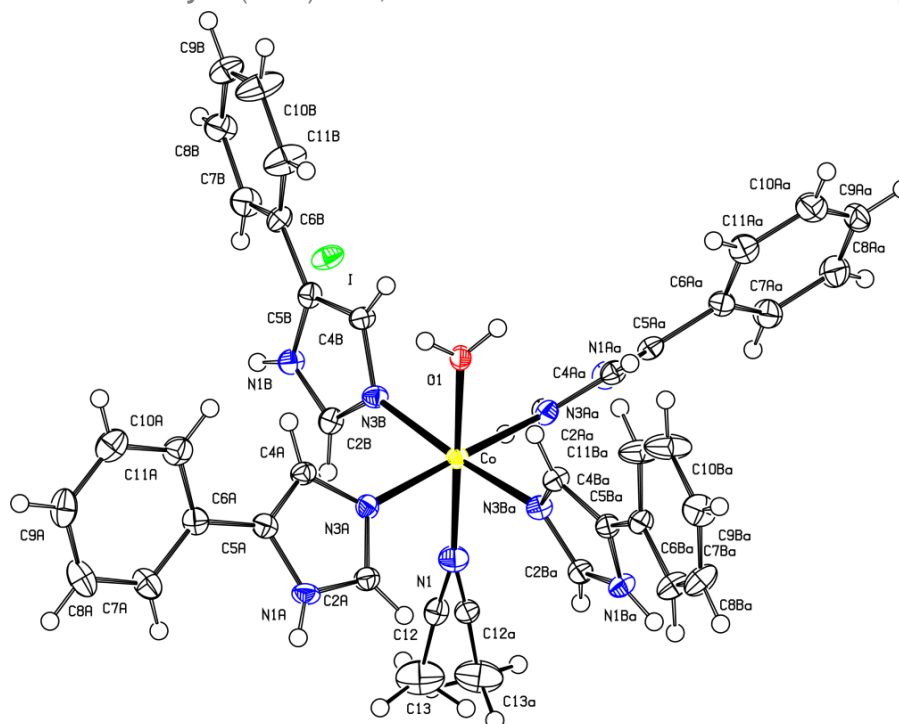


Figure S5 A view of the structure of compound **5** with atom labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (a) $1 - x, 1 - y, z$. The disordered acetonitrile solvent molecule is shown with both orientations.

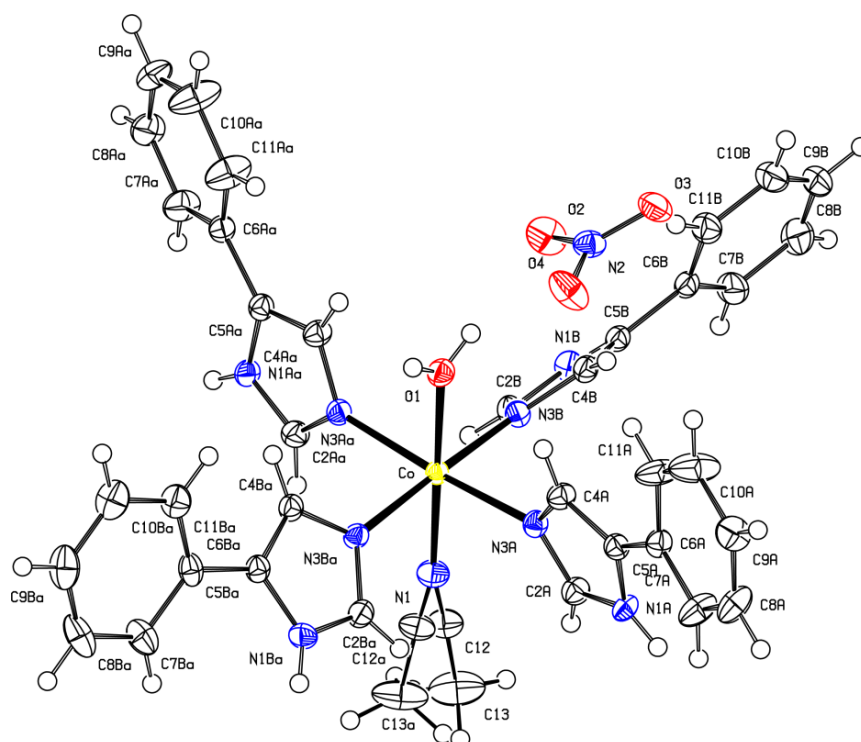


Figure S6 A view of the structure of compound **6** with atom labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (a) $1 - x, -y, z$. The disordered acetonitrile solvent molecule is shown with both orientations.

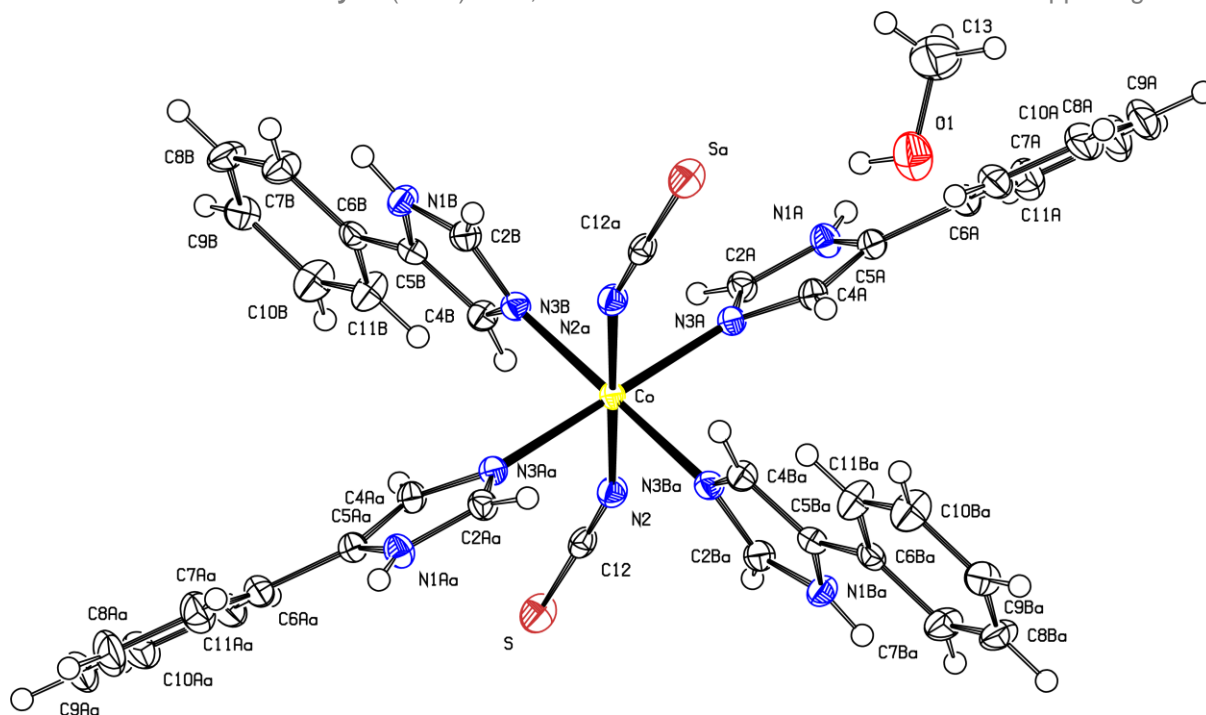


Figure S7 A view of the structure of compound 7·MeOH with atom labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (a) $1 - x, -y, -z$.

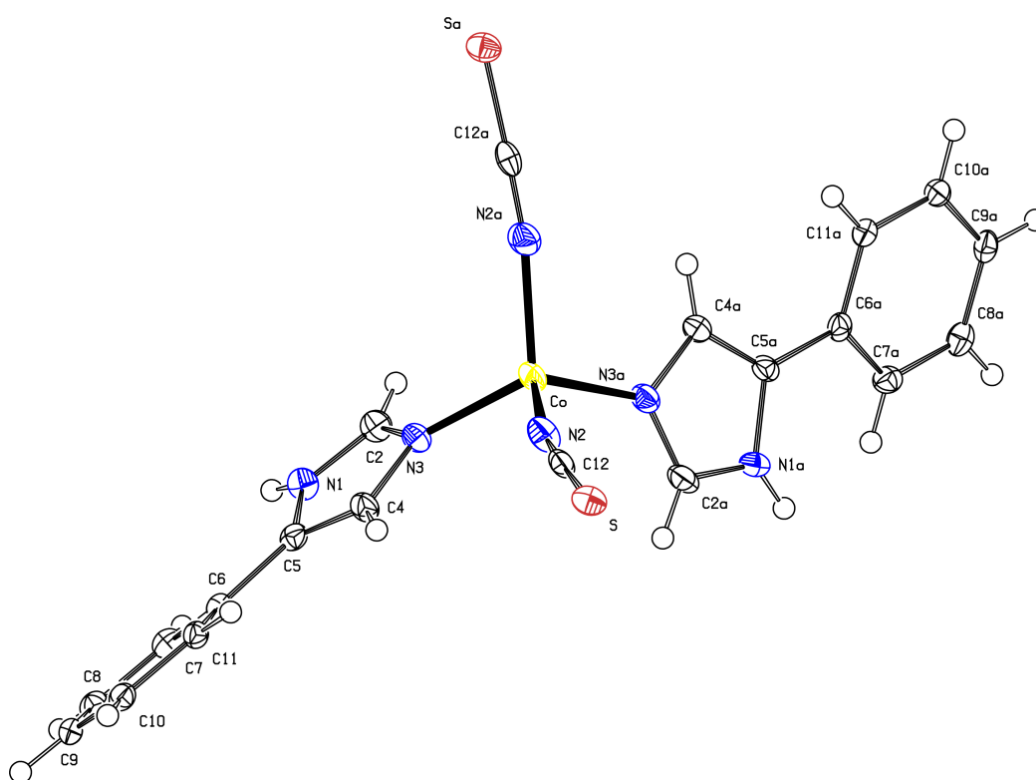


Figure S8 A view of the structure of compound 8 with atom labelling and displacement ellipsoids drawn at the 50% probability level. Symmetry code: (a) $1 - x, y, 3/2 - z$.