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Cocrystal of (2-guanidinobenzimidazole-κ^2N,N')-[hydridotris(3,5-methylphenylpyrazolyl)borato-κ^3N,N',N'']cobalt(II) perchlorate and (2-guanidinobenzimidazolato-κ^2N,N')[hydridotris(3,5-methylphenylpyrazolyl)borato-κ^3N,N',N'']cobalt(II) methanol solvate monohydrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
H-atom completeness 98%
R factor = 0.062
wR factor = 0.198
Data-to-parameter ratio = 14.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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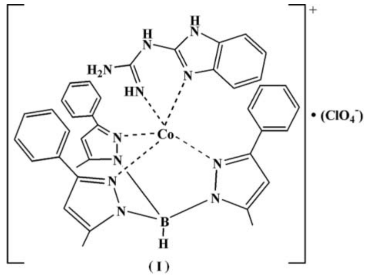
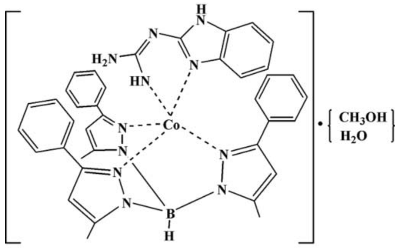
In the title cocrystal, $\{[Co(C_8H_9N_5)(C_{30}H_{28}BN_6)]ClO_4\}\cdot[Co(C_8H_9N_5)(C_{30}H_{27}BN_6)]\cdot CH_3OH\cdot H_2O$, two independent complexes co-crystallize in the asymmetric unit, together with methanol and water solvent molecules and a perchlorate anion. Each Co^{2+} ion is five-coordinated by three N atoms from a hydridotris(3,5-methylphenyl)borate group and two N atoms from a 2-guanidinobenzimidazolyl (GBI) ligand. In one molecule, GBI binds to Co^{2+} in the neutral form with perchlorate as counter-ion, whereas in the other molecule, it ligates to Co^{2+} in the anionic form after deprotonation. The coordination geometry can be best described as distorted trigonal bipyramidal.

Comment

Previously, Jacobsen *et al.* (2006, 2007) reported the substitution reactions between [$Tp^{Me,Ph}$Co–Cl] and HL under basic conditions, where $Tp^{Me,Ph}$ is the hydridotris(3,5-methylphenyl-1-pyrazolyl)borate anion and HL are pyrone derivatives. In the resulting complexes, the Co^{2+} ions are exclusively five-coordinate with distorted square-pyramidal geometry. Reported here is the crystal structure of the title complex that was obtained from the direct interaction of [$Tp^{Me,Ph}$Co–solvent](ClO_4) with 2-guanidinobenzimidazole (GBI).



(I)



(II)

The compound crystallizes in the triclinic system with space group $P\bar{1}$. There are two independent complexes in each asymmetric unit, together with methanol and water solvent

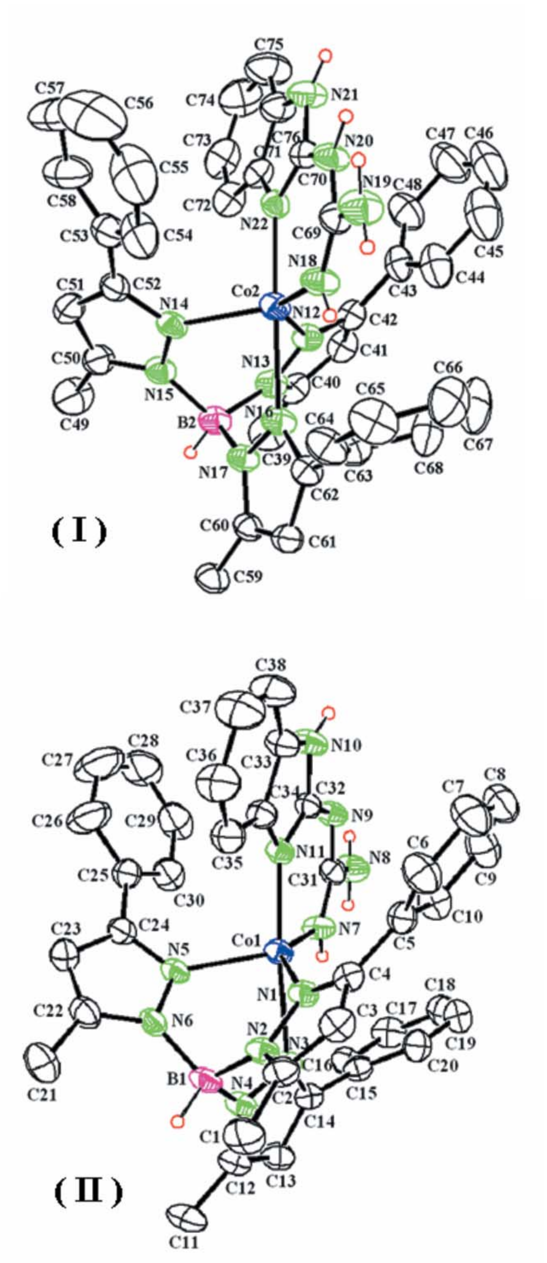


Figure 1

A view of the structures of molecule (I) and cation (II), with displacement ellipsoids drawn at the 30% probability level. H atoms on C atoms, counter-ions and solvent molecules have been omitted for clarity.

molecules and a perchlorate anion. One complex, (I), is cationic, with perchlorate as counter-ion, and the other, (II), is a neutral compound with deprotonated GBI coordination.

As shown in Fig. 1, the Co^{2+} in (I) is five-coordinated by atoms N1, N3 and N5 from the tripodal ligand and atoms N7 and N11 from the bidentate GBI anion. Atoms N1, N5 and N7 are in equatorial positions and atoms N3 and N11 in axial positions. The geometry can be described as distorted trigonal bipyramidal. The bond lengths between atom Co1 and the equatorial N atoms are very similar, whereas those between atom Co1 and the two axial N atoms are quite different (Table 1).

The Co^{2+} ion in (II) is also five-coordinate, with GBI binding to the central metal ion in the neutral form. Atoms N12, N14 and N18 are in equatorial positions and atoms N16 and N22 in axial positions.

One major difference between complexes (I) and (II) is the angle between the least-squares GBI plane and its head-on phenyl plane in the pyrazolyl group. These angles are 58.54 (18)° for (I) and 71.06 (18)° for (II).

The hydrogen-bond geometry of the title co-crystal is listed in Table 2.

Experimental

Equimolar quantities of potassium hydridotris(3,5-methylphenyl-1-pyrazolyl)borate (0.52 g, 1 mmol) and cobalt(II) perchlorate hexahydrate (0.37 g, 1 mmol) in methanol–dichloromethane (1:1 *v*/*v*) (10 ml and 2 ml, respectively) were mixed and stirred at room temperature for 24 h. The solid was removed by filtration and 2-guanidinobenzimidazole (0.21 g, 1 mmol) in methanol (5 ml) was added. The reulting solution was stirred for another 12 h. After filtration, the clear filtrate was kept at room temperature. Dark-red crystals were obtained after two weeks (yield 0.62 g, 79%).

Crystal data

$\{[Co(C_8H_9N_5)(C_{30}H_{28}BN_6)]ClO_4\}\cdot[Co(C_8H_9N_5)(C_{30}H_{27}BN_6)]\cdot CH_4O\cdot H_2O$
$M_r = 1583.55$
Triclinic, $P\bar{1}$
$a = 12.208$ (2) Å
$b = 17.727$ (4) Å
$c = 20.295$ (4) Å
$\alpha = 106.31$ (3)°
$\beta = 99.30$ (3)°
$\gamma = 103.14$ (3)°
$V = 3983.7$ (18) Å^3
$Z = 2$
Mo *Kα* radiation
$\mu = 0.52$ mm^{-1}
$T = 293$ (2) K
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART 1 K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.861$, $T_{max} = 0.904$
56246 measured reflections
14765 independent reflections
7850 reflections with $I > 2\sigma(I)$
$R_{int} = 0.081$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.198$
$S = 1.02$
14765 reflections
1019 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.73$ e Å^{-3}
$\Delta\rho_{min} = -0.62$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Co1—N1	2.084 (4)	Co2—N12	2.052 (4)
Co1—N3	2.299 (4)	Co2—N14	2.062 (4)
Co1—N5	2.076 (4)	Co2—N16	2.235 (4)
Co1—N7	1.963 (4)	Co2—N18	1.972 (4)
Co1—N11	2.018 (4)	Co2—N22	2.047 (4)
N1—Co1—N5	95.0 (1)	N12—Co2—N14	95.8 (2)
N1—Co1—N11	98.8 (1)	N14—Co2—N18	126.8 (2)
N3—Co1—N11	174.8 (1)	N12—Co2—N22	95.9 (2)
N5—Co1—N11	100.0 (1)	N14—Co2—N22	97.7 (2)
N7—Co1—N11	87.5 (2)	N16—Co2—N22	177.2 (1)
N5—Co1—N7	121.4 (2)	N18—Co2—N22	88.0 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N19—H84A···O3$^{\rm i}$	0.89	2.15	3.007 (11)	161
N20—H85···O2$^{\rm i}$	0.88 (5)	1.98 (5)	2.832 (9)	162 (5)
N21—H86···O6$^{\rm i}$	0.88	2.31	3.086 (12)	146
O5—H5···N9$^{\rm ii}$	0.84	1.91	2.734 (5)	167

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+1, -y, -z$.

H atoms on N8, N10, N18, N19 and N20 were refined. H atoms on aqua O could not be located in a difference map and were therefore not included. Other H atoms were geometrically positioned and refined in riding mode as follows: for methyl H, C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C); for aromatic H, C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C); for amino H, N—H = 0.86 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N); for hydroxy H, O—H = 0.84 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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