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Bis[benzyl 2-(heptan-4-ylidene)hydrazine-1-carboxylate]bis(thiocyanato)cobalt(II)

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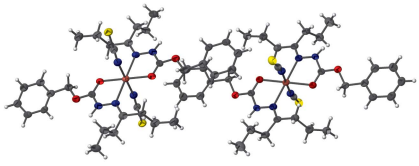
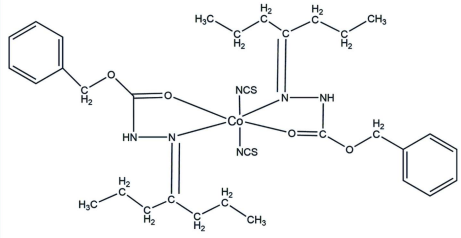
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Co(NCS)_2(C_{15}H_{22}N_2O_2)_2]$ or $C_{32}H_{44}CoN_6O_4S_2$, was prepared from cobalt(II) nitrate, benzyl carbazate and ammonium thiocyanate in the presence of 4-heptanone. The compound crystallizes with two centrosymmetric complexes in which the cobalt(II) atoms have a *trans*-CoO_2N_4 octahedral coordination geometry. In the crystal, N—H···S, C—H···S and C—H···π contacts stack the complex molecules along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Our previous work involving Schiff-base complexes derived from benzyl carbazate and carbonyl compounds was limited to short-chain dialkyl ketones (Nithya *et al.*, 2016, 2017). In order to investigate and compare the coordinating ability of benzyl carbazate Schiff bases derived from higher homologues, we have prepared the title cobalt complex from benzyl carbazate with 4-heptanone with thiocyanate as the charge-balancing anionic ligand. We report the molecular and crystal structure of the complex here. Neither the structure of the bidentate ligand used here, nor of its complexes, have been reported previously.

The title compound, $Co(C_{15}H_{22}N_2O_2)_2(NCS)_2$, crystallizes with two centrosymmetric, octahedral cobalt(II) complexes (1) and (2) in the monoclinic unit cell. These are differentiated in the numbering scheme by leading 1 and 2 characters, respectively (Fig. 1). The molecules overlay with an r.m.s. deviation of 0.602 Å (Fig. 2), with the greatest conformational differences in the vicinity of the *n*-propyl substituents on C12 and C22 (Macrae *et al.*, 2008). The benzyl-2-(heptan-4-ylidene)hydrazine-1-carboxylate ligand is *N*,*O*-bidentate with two such ligands in the equatorial plane, binding through the imine N and carbonyl O atoms. The N bound thiocyanato ligands occupy *trans*-axial positions and are slightly kinked, with N—C—S and Co—N—C bond angles of 177.3 (6)

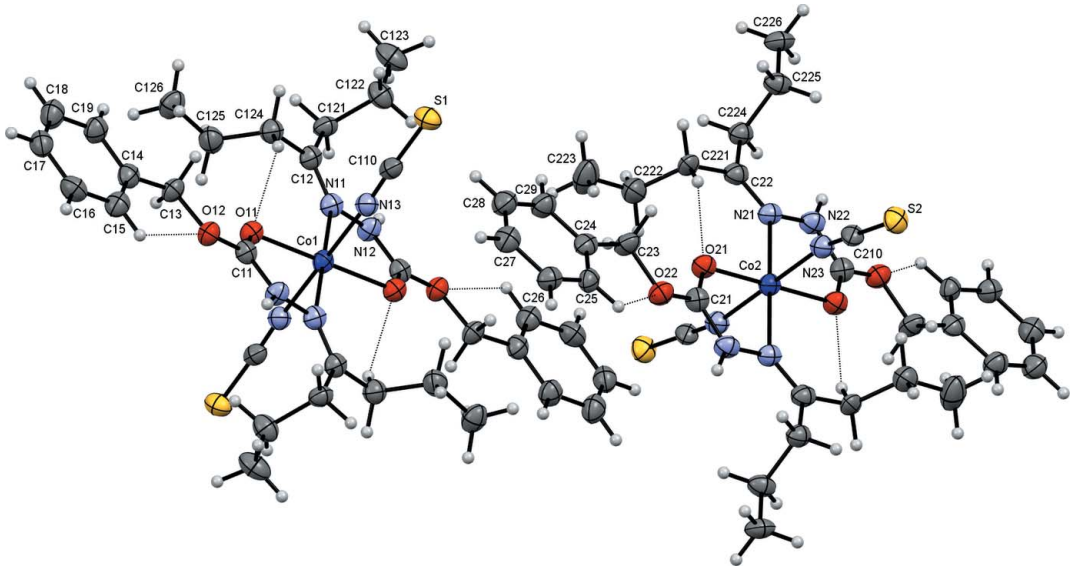


Figure 1
The molecular structure of the title compound with ellipsoids drawn at the 50% probability level. Intramolecular hydrogen bonds are drawn as dashed lines. Labelled atom are related to unlabelled atoms by the symmetry operations $-x, -y, -z$ for molecule (1) and $-x+1, -y, -z+1$ for molecule (2).

and 169.8 (5)°, respectively, in (1) and 178.9 (6) and 165.6 (6)°, respectively, in (2). With the exception of the di-*n*-propyl substituents on the C12 and C22 carbon atoms, the non-hydrogen atoms of the bidentate ligands lie close to the equatorial planes of both complexes with r.m.s. deviations from the best-fit plane through N11, N12, O11, C11, O12, C13···C19 of 0.079 Å for (1) and 0.094 Å for the corresponding plane in (2). Pairs of intramolecular C—H···O hydrogen bonds form in both molecules, Table 1, Fig. 1. In the crystal, N—H···S and weaker C—H···S hydrogen bonds combine with a C—H···π contact between molecules (1) and (2), Table 1, to stack the complexes along the *b*-axis direction, Fig. 3.

Synthesis and crystallization

Cobalt(II) nitrate (0.146 g, 0.50 mmol) dissolved in 10 ml of doubly distilled water was added to a methanolic solution (10 ml) of benzyl carbazate (0.166 g, 1.00 mmol) and ammonium thiocyanate (0.076 g, 1.00 mmol). The solution was then layered with 4-heptanone (0.1 ml, 1 mmol) and the colour changed from pink to blue. The resulting mixture was retained for slow evaporation at room temperature, resulting in olive-green crystals, which were collected, washed with water and air-dried. Yield 81.5% (0.119 g) with respect to the metal.

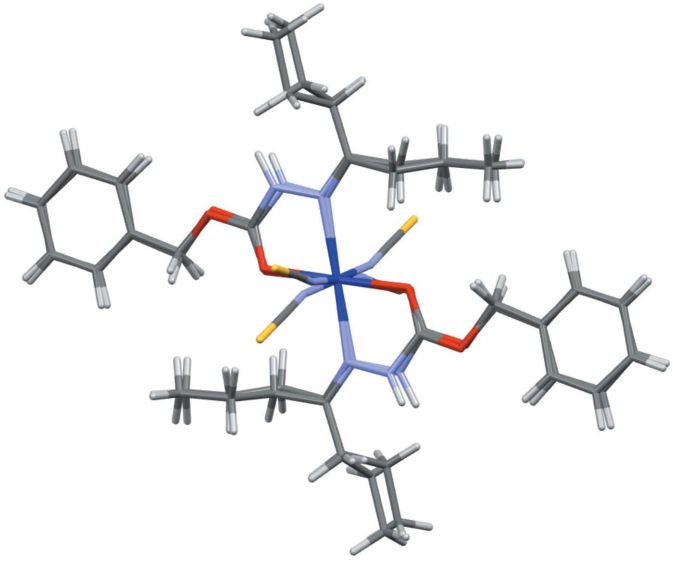


Figure 2
An overlay of the two unique molecules of the title compound (r.m.s. deviation = 0.602 Å).

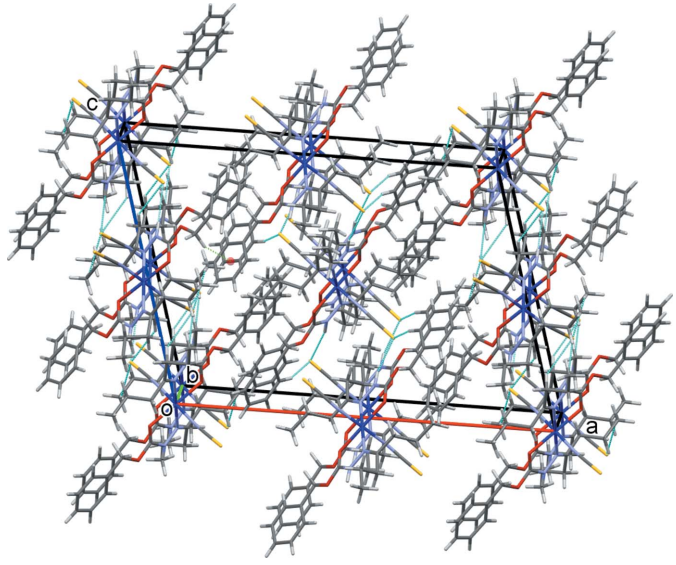


Figure 3
A view of the overall packing of the title compound along the *b*-axis direction. Hydrogen bonds are drawn as cyan dashed lines and a representative C—H···π(ring) contact is shown as a green dashed line, with a red sphere representing the ring centroid.

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*6 is the centroid of the C24–C29 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12···S1^{i}	0.85 (8)	2.47 (8)	3.298 (6)	166 (7)
C121—H12*B*···S1^{i}	0.99	2.93	3.786 (7)	146
N22—H22···S2^{ii}	0.96 (8)	2.55 (8)	3.480 (6)	164 (6)
C25—H25···S2^{ii}	0.95	2.94	3.811 (7)	153
C124—H12*I*···O11^{iii}	0.99	2.48	3.259 (9)	135
C221—H22*A*···O21^{iv}	0.99	2.38	3.229 (8)	144
C13—H13*B*···*Cg*6	0.99	2.60	3.464 (7)	145

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, -y, -z$; (iv) $-x+1, -y, -z+1$.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Crystals of this compound were not of good quality and, despite several data collections on different samples with both Cu and Mo radiation, the residuals reported here were the best that could be obtained.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Co(NCS)_2(C_{15}H_{22}N_2O_2)_2]$
M_r	699.78
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	23.194 (3), 9.825 (1), 16.475 (2)
β (°)	106.154 (13)
V (Å^3)	3606.1 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	5.16
Crystal size (mm)	0.21 × 0.15 × 0.11
Data collection	
Diffractometer	Agilent SuperNova, Dual, Cu at zero, Atlas
Absorption correction	Gaussian (*CrysAlis PRO*; Agilent, 2014)
T_{min}, T_{max}	0.839, 0.912
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34985, 7198, 4299
R_{int}	0.153
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.094, 0.263, 1.07
No. of reflections	7198
No. of parameters	419
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.19, −0.62

Computer programs: *CrysAlis PRO* (Agilent, 2014), *SIR2011* (Burla *et al.*, 2012), *SHELXL2018* (Sheldrick, 2015) and *TITAN* (Hunter & Simpson, 1999), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014* (Sheldrick, 2015), *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009) and *publCIF* (Westrip 2010).

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full crystallographic data

IUCrData (2019). **4**, x190812 [https://doi.org/10.1107/S2414314619008125]

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Crystal data

$[Co(NCS)_2(C_{15}H_{22}N_2O_2)_2]$
M_r = 699.78
Monoclinic, $P2_1/c$
a = 23.194 (3) Å
b = 9.825 (1) Å
c = 16.475 (2) Å
β = 106.154 (13)°
V = 3606.1 (8) Å^3
Z = 4
$F(000)$ = 1476
D_x = 1.289 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 2699 reflections
θ = 3.9–72.7°
μ = 5.16 mm^{-1}
T = 100 K
Block, olive green
0.21 × 0.15 × 0.11 mm

Data collection

Agilent SuperNova, Dual, Cu at zero, Atlas diffractometer
Radiation source: sealed X-ray tube, SuperNova (Cu) X-ray Source
Detector resolution: 5.1725 pixels mm^{-1}
ω scans
Absorption correction: gaussian (CrysAlis PRO; Agilent, 2014)
T_{min} = 0.839, T_{max} = 0.912
34985 measured reflections
7198 independent reflections
4299 reflections with $I > 2\sigma(I)$
R_{int} = 0.153
θ_{max} = 74.4°, θ_{min} = 4.0°
h = −28→28
k = −11→12
l = −19→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.094
$wR(F^2)$ = 0.263
S = 1.07
7198 reflections
419 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 14.0183P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. l reflection with Fo >>> Fc was omitted from the final refinement cycles.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co1	0.000000	0.000000	0.000000	0.0298 (4)
N11	0.0137 (2)	−0.1536 (6)	0.1013 (3)	0.0322 (12)
C12	−0.0084 (3)	−0.2731 (7)	0.1072 (4)	0.0323 (15)
C121	0.0110 (3)	−0.3609 (7)	0.1846 (4)	0.0341 (15)
H12A	−0.021053	−0.427640	0.184426	0.041*
H12B	0.016911	−0.303327	0.235640	0.041*
C122	0.0698 (3)	−0.4373 (8)	0.1883 (5)	0.0419 (17)
H12C	0.065812	−0.483492	0.133592	0.050*
H12D	0.103087	−0.370939	0.197190	0.050*
C123	0.0847 (4)	−0.5416 (9)	0.2586 (5)	0.052 (2)
H12E	0.083817	−0.498159	0.311823	0.078*
H12F	0.124762	−0.578869	0.264194	0.078*
H12G	0.055024	−0.615241	0.245368	0.078*
C124	−0.0538 (3)	−0.3287 (8)	0.0323 (4)	0.0364 (15)
H12H	−0.045942	−0.426947	0.027124	0.044*
H12I	−0.049392	−0.282823	−0.019149	0.044*
C125	−0.1180 (3)	−0.3104 (8)	0.0371 (5)	0.0441 (18)
H12J	−0.128347	−0.212379	0.032133	0.053*
H12K	−0.120808	−0.342201	0.092904	0.053*
C126	−0.1631 (3)	−0.3887 (8)	−0.0324 (5)	0.0448 (18)
H12L	−0.157943	−0.363491	−0.087509	0.067*
H12M	−0.203926	−0.366375	−0.030912	0.067*
H12N	−0.156212	−0.486701	−0.023340	0.067*
N12	0.0573 (3)	−0.1037 (6)	0.1712 (4)	0.0327 (12)
H12	0.070 (3)	−0.136 (8)	0.221 (5)	0.039*
O11	0.0806 (2)	0.0600 (5)	0.0883 (3)	0.0323 (10)
C11	0.0897 (3)	0.0026 (7)	0.1561 (4)	0.0298 (14)
O12	0.1327 (2)	0.0389 (5)	0.2253 (3)	0.0330 (10)
C13	0.1703 (3)	0.1503 (7)	0.2106 (4)	0.0333 (15)
H13A	0.145852	0.234005	0.196051	0.040*
H13B	0.186039	0.127334	0.162198	0.040*
C14	0.2213 (3)	0.1757 (7)	0.2867 (4)	0.0347 (15)
C15	0.2366 (3)	0.0952 (8)	0.3578 (5)	0.0392 (16)
H15	0.212777	0.017778	0.360963	0.047*
C16	0.2865 (3)	0.1251 (8)	0.4254 (5)	0.0438 (18)
H16	0.296721	0.068016	0.473807	0.053*
C17	0.3209 (3)	0.2383 (8)	0.4212 (5)	0.0408 (17)
H17	0.355073	0.258792	0.466877	0.049*
C18	0.3058 (3)	0.3213 (9)	0.3514 (5)	0.0468 (19)
H18	0.329365	0.399711	0.349200	0.056*
C19	0.2563 (3)	0.2911 (8)	0.2838 (5)	0.0402 (17)
H19	0.246196	0.348720	0.235564	0.048*
N13	−0.0433 (2)	0.1289 (6)	0.0627 (4)	0.0333 (12)
C110	−0.0677 (3)	0.2137 (7)	0.0880 (4)	0.0323 (14)
S1	−0.10507 (8)	0.33019 (19)	0.12477 (11)	0.0400 (4)

Co2	0.500000	0.000000	0.500000	0.0305 (4)
N21	0.4960 (2)	0.1867 (6)	0.4197 (3)	0.0317 (12)
C22	0.5324 (3)	0.2874 (7)	0.4219 (5)	0.0362 (16)
C221	0.5867 (3)	0.2997 (7)	0.4961 (5)	0.0353 (15)
H22A	0.579237	0.251136	0.544811	0.042*
H22B	0.593417	0.396932	0.511629	0.042*
C222	0.6438 (3)	0.2414 (8)	0.4786 (5)	0.0474 (19)
H22C	0.638771	0.142286	0.468111	0.057*
H22D	0.649752	0.284469	0.427178	0.057*
C223	0.6985 (4)	0.2666 (11)	0.5525 (6)	0.065 (3)
H22E	0.703882	0.364756	0.562330	0.097*
H22F	0.734119	0.228732	0.539771	0.097*
H22G	0.692954	0.222654	0.603170	0.097*
C224	0.5242 (3)	0.3964 (7)	0.3546 (5)	0.0363 (15)
H22H	0.504172	0.356725	0.298601	0.044*
H22I	0.563979	0.431013	0.353031	0.044*
C225	0.4860 (3)	0.5153 (7)	0.3730 (5)	0.0381 (16)
H22J	0.445356	0.481693	0.370723	0.046*
H22K	0.504616	0.550544	0.430677	0.046*
C226	0.4811 (4)	0.6303 (7)	0.3089 (5)	0.0420 (17)
H22L	0.521319	0.664875	0.311985	0.063*
H22M	0.456602	0.704064	0.321719	0.063*
H22N	0.462331	0.595675	0.251870	0.063*
N22	0.4473 (3)	0.1744 (6)	0.3494 (4)	0.0353 (13)
H22	0.435 (3)	0.238 (8)	0.304 (5)	0.042*
O21	0.4248 (2)	−0.0321 (5)	0.3958 (3)	0.0343 (11)
C21	0.4151 (3)	0.0578 (7)	0.3420 (4)	0.0327 (14)
O22	0.3730 (2)	0.0517 (5)	0.2689 (3)	0.0371 (11)
C23	0.3364 (3)	−0.0692 (7)	0.2566 (5)	0.0393 (16)
H23A	0.317866	−0.079440	0.303634	0.047*
H23B	0.361459	−0.150441	0.255731	0.047*
C24	0.2882 (3)	−0.0577 (7)	0.1742 (4)	0.0351 (15)
C25	0.2887 (3)	0.0403 (7)	0.1141 (4)	0.0339 (15)
H25	0.320617	0.104275	0.124184	0.041*
C26	0.2432 (3)	0.0459 (7)	0.0395 (4)	0.0363 (15)
H26	0.243128	0.115637	−0.000417	0.044*
C27	0.1972 (3)	−0.0505 (8)	0.0226 (5)	0.0415 (17)
H27	0.166382	−0.048600	−0.029316	0.050*
C28	0.1970 (3)	−0.1493 (8)	0.0828 (5)	0.0430 (17)
H28	0.165563	−0.214556	0.072367	0.052*
C29	0.2422 (3)	−0.1534 (8)	0.1576 (5)	0.0410 (17)
H29	0.241882	−0.222004	0.198078	0.049*
N23	0.5525 (3)	−0.0819 (6)	0.4321 (4)	0.0357 (13)
C210	0.5825 (3)	−0.1012 (7)	0.3862 (4)	0.0320 (14)
S2	0.62538 (8)	−0.1277 (2)	0.32411 (12)	0.0406 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0294 (7)	0.0330 (9)	0.0297 (8)	−0.0011 (7)	0.0125 (6)	0.0001 (7)
N11	0.035 (3)	0.035 (3)	0.031 (3)	−0.001 (2)	0.015 (2)	−0.001 (2)
C12	0.034 (3)	0.036 (4)	0.032 (3)	−0.002 (3)	0.018 (3)	−0.002 (3)
C121	0.040 (4)	0.027 (4)	0.039 (4)	−0.006 (3)	0.018 (3)	−0.002 (3)
C122	0.043 (4)	0.048 (5)	0.038 (4)	0.009 (3)	0.016 (3)	−0.001 (3)
C123	0.064 (5)	0.050 (5)	0.046 (5)	0.021 (4)	0.021 (4)	0.000 (4)
C124	0.037 (4)	0.037 (4)	0.039 (4)	−0.001 (3)	0.016 (3)	−0.001 (3)
C125	0.037 (4)	0.045 (5)	0.052 (5)	0.003 (3)	0.015 (3)	0.007 (4)
C126	0.043 (4)	0.048 (5)	0.043 (4)	−0.009 (4)	0.012 (3)	0.009 (4)
N12	0.034 (3)	0.035 (3)	0.028 (3)	−0.004 (2)	0.008 (2)	0.006 (2)
O11	0.035 (2)	0.034 (3)	0.030 (2)	−0.003 (2)	0.0119 (19)	−0.001 (2)
C11	0.031 (3)	0.035 (4)	0.026 (3)	0.002 (3)	0.013 (3)	0.000 (3)
O12	0.032 (2)	0.036 (3)	0.032 (2)	−0.0044 (19)	0.0096 (19)	0.000 (2)
C13	0.032 (3)	0.035 (4)	0.035 (4)	−0.007 (3)	0.013 (3)	0.001 (3)
C14	0.032 (3)	0.039 (4)	0.038 (4)	−0.001 (3)	0.017 (3)	−0.006 (3)
C15	0.039 (4)	0.043 (4)	0.038 (4)	−0.005 (3)	0.014 (3)	−0.007 (3)
C16	0.046 (4)	0.040 (4)	0.045 (4)	0.008 (3)	0.012 (3)	0.005 (3)
C17	0.033 (3)	0.047 (5)	0.042 (4)	0.002 (3)	0.009 (3)	−0.005 (3)
C18	0.036 (4)	0.055 (5)	0.052 (5)	−0.005 (4)	0.017 (3)	−0.006 (4)
C19	0.036 (4)	0.044 (4)	0.043 (4)	−0.003 (3)	0.016 (3)	0.004 (3)
N13	0.034 (3)	0.032 (3)	0.036 (3)	0.000 (2)	0.013 (2)	0.000 (2)
C110	0.035 (3)	0.028 (4)	0.031 (3)	−0.005 (3)	0.005 (3)	0.001 (3)
S1	0.0469 (10)	0.0344 (10)	0.0380 (9)	0.0061 (8)	0.0108 (8)	−0.0038 (7)
Co2	0.0319 (8)	0.0302 (8)	0.0331 (8)	−0.0011 (7)	0.0152 (6)	0.0002 (7)
N21	0.038 (3)	0.028 (3)	0.033 (3)	−0.001 (2)	0.017 (2)	0.000 (2)
C22	0.041 (4)	0.030 (4)	0.042 (4)	0.000 (3)	0.020 (3)	−0.003 (3)
C221	0.031 (3)	0.027 (4)	0.052 (4)	−0.005 (3)	0.019 (3)	0.006 (3)
C222	0.042 (4)	0.040 (5)	0.063 (5)	−0.001 (3)	0.021 (4)	0.003 (4)
C223	0.044 (5)	0.073 (7)	0.076 (7)	−0.012 (5)	0.016 (4)	0.023 (5)
C224	0.041 (4)	0.031 (4)	0.044 (4)	−0.002 (3)	0.021 (3)	−0.001 (3)
C225	0.050 (4)	0.030 (4)	0.041 (4)	0.003 (3)	0.023 (3)	0.004 (3)
C226	0.060 (5)	0.024 (4)	0.047 (4)	−0.005 (3)	0.024 (4)	−0.002 (3)
N22	0.041 (3)	0.031 (3)	0.036 (3)	0.000 (3)	0.015 (3)	0.006 (3)
O21	0.038 (3)	0.034 (3)	0.033 (3)	−0.001 (2)	0.014 (2)	0.005 (2)
C21	0.035 (3)	0.036 (4)	0.028 (3)	0.000 (3)	0.011 (3)	0.001 (3)
O22	0.040 (3)	0.036 (3)	0.037 (3)	−0.005 (2)	0.013 (2)	0.001 (2)
C23	0.044 (4)	0.030 (4)	0.044 (4)	−0.009 (3)	0.012 (3)	0.004 (3)
C24	0.038 (4)	0.033 (4)	0.040 (4)	−0.002 (3)	0.021 (3)	−0.009 (3)
C25	0.028 (3)	0.038 (4)	0.040 (4)	−0.003 (3)	0.015 (3)	−0.004 (3)
C26	0.042 (4)	0.035 (4)	0.037 (4)	−0.003 (3)	0.019 (3)	−0.001 (3)
C27	0.043 (4)	0.046 (5)	0.037 (4)	−0.003 (3)	0.014 (3)	−0.005 (3)
C28	0.042 (4)	0.041 (4)	0.047 (4)	−0.006 (3)	0.013 (3)	−0.005 (3)
C29	0.042 (4)	0.037 (4)	0.046 (4)	−0.006 (3)	0.016 (3)	0.002 (3)
N23	0.037 (3)	0.032 (3)	0.039 (3)	0.000 (2)	0.013 (3)	−0.001 (2)
C210	0.033 (3)	0.031 (4)	0.035 (4)	0.000 (3)	0.013 (3)	−0.009 (3)

S2	0.0397 (9)	0.0462 (11)	0.0409 (10)	0.0002 (8)	0.0193 (8)	−0.0053 (8)

Geometric parameters (Å, º)

Co1—N13	2.064 (6)	Co2—N23	2.036 (6)
Co1—N13^{i}	2.064 (6)	Co2—N23^{ii}	2.036 (6)
Co1—O11	2.109 (5)	Co2—O21	2.103 (5)
Co1—O11^{i}	2.109 (5)	Co2—O21^{ii}	2.103 (5)
Co1—N11	2.206 (6)	Co2—N21	2.248 (6)
Co1—N11^{i}	2.206 (6)	Co2—N21^{ii}	2.248 (6)
N11—C12	1.295 (9)	N21—C22	1.293 (9)
N11—N12	1.393 (8)	N21—N22	1.380 (8)
C12—C124	1.486 (10)	C22—C221	1.496 (10)
C12—C121	1.501 (9)	C22—C224	1.515 (10)
C121—C122	1.544 (9)	C221—C222	1.542 (9)
C121—H12A	0.9900	C221—H22A	0.9900
C121—H12B	0.9900	C221—H22B	0.9900
C122—C123	1.513 (11)	C222—C223	1.515 (12)
C122—H12C	0.9900	C222—H22C	0.9900
C122—H12D	0.9900	C222—H22D	0.9900
C123—H12E	0.9800	C223—H22E	0.9800
C123—H12F	0.9800	C223—H22F	0.9800
C123—H12G	0.9800	C223—H22G	0.9800
C124—C125	1.524 (9)	C224—C225	1.546 (9)
C124—H12H	0.9900	C224—H22H	0.9900
C124—H12I	0.9900	C224—H22I	0.9900
C125—C126	1.527 (11)	C225—C226	1.530 (9)
C125—H12J	0.9900	C225—H22J	0.9900
C125—H12K	0.9900	C225—H22K	0.9900
C126—H12L	0.9800	C226—H22L	0.9800
C126—H12M	0.9800	C226—H22M	0.9800
C126—H12N	0.9800	C226—H22N	0.9800
N12—C11	1.350 (9)	N22—C21	1.354 (9)
N12—H12	0.85 (8)	N22—H22	0.96 (8)
O11—C11	1.216 (8)	O21—C21	1.227 (8)
C11—O12	1.338 (8)	C21—O22	1.325 (8)
O12—C13	1.462 (8)	O22—C23	1.442 (8)
C13—C14	1.487 (9)	C23—C24	1.503 (10)
C13—H13A	0.9900	C23—H23A	0.9900
C13—H13B	0.9900	C23—H23B	0.9900
C14—C15	1.375 (10)	C24—C25	1.383 (10)
C14—C19	1.403 (10)	C24—C29	1.392 (10)
C15—C16	1.395 (11)	C25—C26	1.380 (10)
C15—H15	0.9500	C25—H25	0.9500
C16—C17	1.381 (11)	C26—C27	1.396 (10)
C16—H16	0.9500	C26—H26	0.9500
C17—C18	1.375 (11)	C27—C28	1.388 (11)
C17—H17	0.9500	C27—H27	0.9500

C18—C19	1.391 (11)	C28—C29	1.378 (11)
C18—H18	0.9500	C28—H28	0.9500
C19—H19	0.9500	C29—H29	0.9500
N13—C110	1.148 (9)	N23—C210	1.176 (8)
C110—S1	1.649 (7)	C210—S2	1.634 (6)
N13—Co1—N13^{i}	180.0	N23—Co2—N23^{ii}	180.0
N13—Co1—O11	86.8 (2)	N23—Co2—O21	88.8 (2)
N13^{i}—Co1—O11	93.2 (2)	N23^{ii}—Co2—O21	91.2 (2)
N13—Co1—O11^{i}	93.2 (2)	N23—Co2—O21^{ii}	91.2 (2)
N13^{i}—Co1—O11^{i}	86.8 (2)	N23^{ii}—Co2—O21^{ii}	88.8 (2)
O11—Co1—O11^{i}	180.0 (3)	O21—Co2—O21^{ii}	180.0
N13—Co1—N11	91.7 (2)	N23—Co2—N21	86.1 (2)
N13^{i}—Co1—N11	88.4 (2)	N23^{ii}—Co2—N21	93.9 (2)
O11—Co1—N11	75.87 (19)	O21—Co2—N21	75.71 (19)
O11^{i}—Co1—N11	104.13 (19)	O21^{ii}—Co2—N21	104.29 (19)
N13—Co1—N11^{i}	88.3 (2)	N23—Co2—N21^{ii}	93.9 (2)
N13^{i}—Co1—N11^{i}	91.6 (2)	N23^{ii}—Co2—N21^{ii}	86.1 (2)
O11—Co1—N11^{i}	104.13 (19)	O21—Co2—N21^{ii}	104.29 (19)
O11^{i}—Co1—N11^{i}	75.87 (19)	O21^{ii}—Co2—N21^{ii}	75.71 (19)
N11—Co1—N11^{i}	180.0	N21—Co2—N21^{ii}	180.0
C12—N11—N12	117.9 (6)	C22—N21—N22	117.7 (6)
C12—N11—Co1	134.5 (5)	C22—N21—Co2	133.5 (5)
N12—N11—Co1	107.7 (4)	N22—N21—Co2	108.2 (4)
N11—C12—C124	118.3 (6)	N21—C22—C221	118.6 (6)
N11—C12—C121	123.6 (6)	N21—C22—C224	124.9 (7)
C124—C12—C121	118.0 (6)	C221—C22—C224	116.5 (6)
C12—C121—C122	111.3 (5)	C22—C221—C222	112.9 (6)
C12—C121—H12A	109.4	C22—C221—H22A	109.0
C122—C121—H12A	109.4	C222—C221—H22A	109.0
C12—C121—H12B	109.4	C22—C221—H22B	109.0
C122—C121—H12B	109.4	C222—C221—H22B	109.0
H12A—C121—H12B	108.0	H22A—C221—H22B	107.8
C123—C122—C121	111.7 (6)	C223—C222—C221	111.1 (7)
C123—C122—H12C	109.3	C223—C222—H22C	109.4
C121—C122—H12C	109.3	C221—C222—H22C	109.4
C123—C122—H12D	109.3	C223—C222—H22D	109.4
C121—C122—H12D	109.3	C221—C222—H22D	109.4
H12C—C122—H12D	107.9	H22C—C222—H22D	108.0
C122—C123—H12E	109.5	C222—C223—H22E	109.5
C122—C123—H12F	109.5	C222—C223—H22F	109.5
H12E—C123—H12F	109.5	H22E—C223—H22F	109.5
C122—C123—H12G	109.5	C222—C223—H22G	109.5
H12E—C123—H12G	109.5	H22E—C223—H22G	109.5
H12F—C123—H12G	109.5	H22F—C223—H22G	109.5
C12—C124—C125	113.0 (6)	C22—C224—C225	110.6 (5)
C12—C124—H12H	109.0	C22—C224—H22H	109.5
C125—C124—H12H	109.0	C225—C224—H22H	109.5

C12—C124—H12I	109.0	C22—C224—H22I	109.5
C125—C124—H12I	109.0	C225—C224—H22I	109.5
H12H—C124—H12I	107.8	H22H—C224—H22I	108.1
C124—C125—C126	112.1 (6)	C226—C225—C224	111.0 (6)
C124—C125—H12J	109.2	C226—C225—H22J	109.4
C126—C125—H12J	109.2	C224—C225—H22J	109.4
C124—C125—H12K	109.2	C226—C225—H22K	109.4
C126—C125—H12K	109.2	C224—C225—H22K	109.4
H12J—C125—H12K	107.9	H22J—C225—H22K	108.0
C125—C126—H12L	109.5	C225—C226—H22L	109.5
C125—C126—H12M	109.5	C225—C226—H22M	109.5
H12L—C126—H12M	109.5	H22L—C226—H22M	109.5
C125—C126—H12N	109.5	C225—C226—H22N	109.5
H12L—C126—H12N	109.5	H22L—C226—H22N	109.5
H12M—C126—H12N	109.5	H22M—C226—H22N	109.5
C11—N12—N11	115.7 (5)	C21—N22—N21	116.8 (6)
C11—N12—H12	114 (5)	C21—N22—H22	117 (5)
N11—N12—H12	130 (5)	N21—N22—H22	127 (5)
C11—O11—Co1	113.4 (4)	C21—O21—Co2	115.2 (4)
O11—C11—O12	123.8 (6)	O21—C21—O22	124.4 (7)
O11—C11—N12	124.4 (6)	O21—C21—N22	123.9 (6)
O12—C11—N12	111.7 (5)	O22—C21—N22	111.6 (6)
C11—O12—C13	113.3 (5)	C21—O22—C23	114.9 (5)
O12—C13—C14	110.9 (5)	O22—C23—C24	109.0 (6)
O12—C13—H13A	109.5	O22—C23—H23A	109.9
C14—C13—H13A	109.5	C24—C23—H23A	109.9
O12—C13—H13B	109.5	O22—C23—H23B	109.9
C14—C13—H13B	109.5	C24—C23—H23B	109.9
H13A—C13—H13B	108.0	H23A—C23—H23B	108.3
C15—C14—C19	118.7 (7)	C25—C24—C29	119.2 (7)
C15—C14—C13	125.3 (6)	C25—C24—C23	123.2 (6)
C19—C14—C13	116.0 (6)	C29—C24—C23	117.6 (7)
C14—C15—C16	121.2 (7)	C26—C25—C24	120.5 (7)
C14—C15—H15	119.4	C26—C25—H25	119.7
C16—C15—H15	119.4	C24—C25—H25	119.7
C17—C16—C15	119.5 (7)	C25—C26—C27	120.2 (7)
C17—C16—H16	120.2	C25—C26—H26	119.9
C15—C16—H16	120.2	C27—C26—H26	119.9
C18—C17—C16	120.2 (7)	C28—C27—C26	119.1 (7)
C18—C17—H17	119.9	C28—C27—H27	120.5
C16—C17—H17	119.9	C26—C27—H27	120.5
C17—C18—C19	120.3 (8)	C29—C28—C27	120.4 (7)
C17—C18—H18	119.9	C29—C28—H28	119.8
C19—C18—H18	119.9	C27—C28—H28	119.8
C18—C19—C14	120.1 (7)	C28—C29—C24	120.5 (7)
C18—C19—H19	120.0	C28—C29—H29	119.8
C14—C19—H19	120.0	C24—C29—H29	119.8
C110—N13—Co1	169.8 (5)	C210—N23—Co2	165.6 (6)

N13—C110—S1	177.3 (6)	N23—C210—S2	178.9 (6)
N12—N11—C12—C124	−178.5 (5)	N22—N21—C22—C221	−177.7 (6)
Co1—N11—C12—C124	−0.2 (9)	Co2—N21—C22—C221	−8.0 (9)
N12—N11—C12—C121	−0.8 (9)	N22—N21—C22—C224	2.6 (10)
Co1—N11—C12—C121	177.6 (4)	Co2—N21—C22—C224	172.3 (5)
N11—C12—C121—C122	−81.0 (8)	N21—C22—C221—C222	97.9 (7)
C124—C12—C121—C122	96.8 (7)	C224—C22—C221—C222	−82.4 (8)
C12—C121—C122—C123	−171.4 (6)	C22—C221—C222—C223	175.2 (7)
N11—C12—C124—C125	−98.8 (7)	N21—C22—C224—C225	88.3 (8)
C121—C12—C124—C125	83.3 (8)	C221—C22—C224—C225	−91.4 (7)
C12—C124—C125—C126	−170.3 (6)	C22—C224—C225—C226	176.1 (6)
C12—N11—N12—C11	163.7 (6)	C22—N21—N22—C21	170.0 (6)
Co1—N11—N12—C11	−15.0 (6)	Co2—N21—N22—C21	−2.1 (6)
Co1—O11—C11—O12	−169.3 (5)	Co2—O21—C21—O22	174.5 (5)
Co1—O11—C11—N12	9.6 (8)	Co2—O21—C21—N22	−3.8 (8)
N11—N12—C11—O11	4.6 (10)	N21—N22—C21—O21	4.1 (10)
N11—N12—C11—O12	−176.3 (5)	N21—N22—C21—O22	−174.3 (5)
O11—C11—O12—C13	−3.3 (9)	O21—C21—O22—C23	2.1 (10)
N12—C11—O12—C13	177.7 (5)	N22—C21—O22—C23	−179.5 (6)
C11—O12—C13—C14	−173.5 (5)	C21—O22—C23—C24	176.2 (6)
O12—C13—C14—C15	8.2 (9)	O22—C23—C24—C25	12.5 (9)
O12—C13—C14—C19	−172.4 (6)	O22—C23—C24—C29	−169.4 (6)
C19—C14—C15—C16	−1.3 (10)	C29—C24—C25—C26	1.9 (10)
C13—C14—C15—C16	178.1 (7)	C23—C24—C25—C26	−180.0 (7)
C14—C15—C16—C17	0.6 (11)	C24—C25—C26—C27	−2.3 (10)
C15—C16—C17—C18	0.4 (11)	C25—C26—C27—C28	1.8 (11)
C16—C17—C18—C19	−0.8 (11)	C26—C27—C28—C29	−1.0 (11)
C17—C18—C19—C14	0.2 (11)	C27—C28—C29—C24	0.7 (12)
C15—C14—C19—C18	0.9 (10)	C25—C24—C29—C28	−1.1 (11)
C13—C14—C19—C18	−178.5 (7)	C23—C24—C29—C28	−179.3 (7)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

*Cg*6 is the centroid of the C24–C29 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N12—H12···S1^{iii}	0.85 (8)	2.47 (8)	3.298 (6)	166 (7)
C121—H12*B*···S1^{iii}	0.99	2.93	3.786 (7)	146
N22—H22···S2^{iv}	0.96 (8)	2.55 (8)	3.480 (6)	164 (6)
C25—H25···S2^{iv}	0.95	2.94	3.811 (7)	153
C124—H12*I*···O11^{i}	0.99	2.48	3.259 (9)	135
C221—H22*A*···O21^{ii}	0.99	2.38	3.229 (8)	144
C13—H13*B*···*Cg*6	0.99	2.60	3.464 (7)	145

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*+1, −*y*, −*z*+1; (iii) −*x*, *y*−1/2, −*z*+1/2; (iv) −*x*+1, *y*+1/2, −*z*+1/2.