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# Crystal structure of an unknown solvate of {2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]-diphenolato-$\kappa^4O,N,N',O'$}(*N*-ferrocenylisonicotinamide-$\kappa N^1$)cobalt(II): a $Co^{II}$–salen complex that forms hydrogen-bonded dimers

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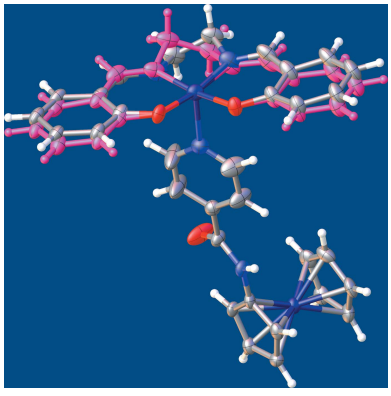
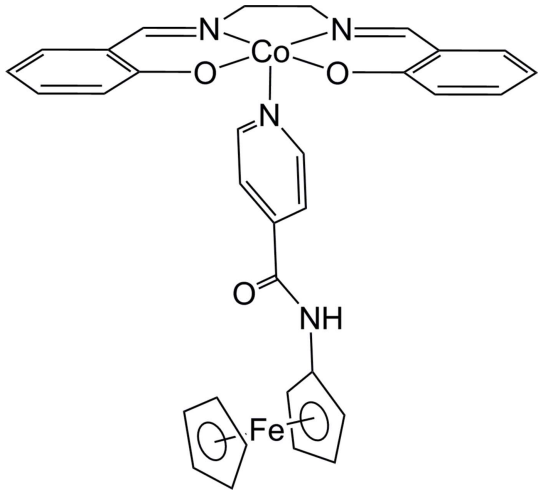
The title compound, $[CoFe(C_5H_5)(C_{16}H_{14}N_2O_2)(C_{11}H_9N_2O)]$, was prepared as an air-stable red–brown solid by mixing equimolar amounts of {2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}cobalt(II) and *N*-ferrocenylisonicotinamide in dry dichloromethane under nitrogen and was characterized by ESI–MS, IR, and single-crystal X-ray diffraction. The structure at 100 K has triclinic ($P\overline{1}$) symmetry and indicates that the complex crystallizes as a mixture of λ and δ conformers. It exhibits the expected square pyramidal geometry about Co, and forms hydrogen-bonded dimers through amide N—H groups and phenolate O atoms on an adjacent molecule. The involvement of only half of the salen ring structure in hydrogen-bonding interactions results in slight folding of the salen ring away from the pyridine coordination site in the δ conformer with an inter-salicylidene fold angle of 9.9 (7)°. In contrast, the λ conformer is nearly planar. The dimers pack into an open structure containing channels filled with highly disordered solvent molecules. These solvent molecules' contributions to the intensity data were removed with the SQUEEZE procedure [Spek (2015). *Acta Cryst.* C**71**, 9–18] available in *PLATON*.

## 1. Chemical context

Ferrocenes have been studied extensively on account of their stable sandwich structure, ability to undergo reversible one-electron oxidation, and, more recently, their potential utility in asymmetric catalysis applications (Stepnicka, 2008; Dai & Hou, 2010). *N*-Ferrocenylamides in particular have been investigated for their ability to form hydrogen bonds through the amide N—H group and carbonyl O atom. They have been employed to construct hydrogen-bonding scaffolds (Okamura *et al.*, 1998; Barisić *et al.*, 2006), perturb the redox properties of attached metal atoms (Okamura *et al.*, 2007), and form one-dimensional hydrogen-bonded chains that can support fast electron transfer (Okamura *et al.*, 2005). We recently demonstrated that the hydrogen-bond network in one of these systems, *N*-ferrocenylisonicotinamide, is able to support a mixed-valent state in the solid (Patterson *et al.*, 2015). Interestingly, the hydrogen bonds in *N*-ferrocenylisonicotinamide occur exclusively between the amide N—H group and the amide carbonyl O atom; the pyridyl N atom of the isonicotinoyl group is not involved. This suggested that it might be possible to use the pyridine N atom to coordinate metal atoms



while leaving the isonicotinamide amide group free to form hydrogen-bonded chains or otherwise engage in hydrogen-bonding interactions. To this end, a complex between *N*-ferrocenylisonicotinamide and {2,2′-[ethane-1,2-diylbis-(nitrilomethanylylidene)]diphenolato}cobalt(II) was prepared and its structure determined.




A cobalt complex of *N*,*N*′-bis(salicylidene)ethylenediamine (salen) was selected for this study since $Co^{II}$(salen), and its derivatives are known to function as oxygen carriers (Tsumaki, 1938; Calvin *et al.*, 1946; Chen *et al.*, 1989), both as solids and in solution. Complexes with pyridine-based ligands are of particular interest since the ability of $Co^{II}$(salen) to absorb oxygen in dichloromethane or chloroform solutions is dependent on the presence of pyridine or other co-ligands to complete the $d^6$ $Co^{III}$(salen)-superoxide complex's octahedral coordination sphere. The system also permits structural comparisons with reported crystal structures of oxygen-active (Schaefer and Marsh, 1969) and inactive (Holt *et al.*, 1971) forms of $Co^{II}$(salen) and with the products of its reaction with oxygen, $\kappa^1$-superoxido-complexes (Floriani & Calderazzo, 1969; Schaefer *et al.*, 1980) and peroxido-bridged dimers (Floriani & Calderazzo, 1969; Fritch *et al.*, 1973). Chiral and achiral salens and their derivatives are also of interest due to their ability to function as versatile catalysts for a variety of oxidation, ring opening, hydrolysis, and polymerization applications (Zhang *et al.*, 1990; Yoon & Jacobsen, 2003; Cozzi, 2004; Darensbourg, 2007; Gupta & Sutar, 2008; Ou & Wu, 2014). Cobalt–salen complexes in particular are used to catalyze the ring opening and hydrolysis of epoxides (Tokunaga *et al.*, 1997; Schaus *et al.*, 2002; Ford *et al.*, 2013; Crossley *et al.*, 2014; White *et al.*, 2014) and the oxidation of phenols (Van Dort & Geursen, 1967).

## 2. Structural commentary

The title compound crystallizes as a 58.3 (12)/41.7 (12)% mixture of its λ and δ chelate ring conformers. In both cases the coordination environment of the $Co^{II}$ ion is roughly square pyramidal (Fig. 1), although the $Co^{II}$ ion is displaced 0.15 Å away from the $N_2O_2$ plane of the salen and towards the axial N atom. A similar 0.20 Å displacement is observed in the structure of [$Co^{II}$(salen)(py)] (Calligaris *et al.*, 1970). The average $Co^{II}$–$N_{eq}$ and $Co^{II}$—O bond lengths in the present complex are 1.88 and 1.90 Å, both significantly shorter than the Co—$N_{ax}$ bond length of 2.159 (4) Å. The equatorial bond lengths are in good agreement with those observed for other pyridine complexes of Co(salen), although the axial Co—N bond length is more similar to the 2.10 (2) Å distance observed for [$Co^{II}$(salen)(py)] than the shorter 1.896 Å distance observed for the more highly oxidized [$Co^{III}$(salen)$(py)_2$]$^+$ (Shi *et al.*, 1995).

The axial py group in the present complex exhibits considerable librational mobility associated with its ability to rotate about the Co—N and C-amide bonds. In fact, the average twist angle between the pyridine and amide planes is 28.2 (2)°, suggesting that the two are not tightly coupled electronically; in contrast, the amide and Cp are tightly coupled with a N—C(Cp) distance of 1.395 (5) Å and an interplane twist angle of 4.83 (3)°. Similar behavior is observed in the structure of *N*-ferrocenylisonicotinamide itself (Patterson *et al.*, 2015).

## 3. Supramolecular Features

Molecules of the title compound form dimers in the solid state (Fig. 2). These are linked by hydrogen bonds between the amide N—H group and one of the phenolate O atoms on adjacent molecules. Interaction between these atoms is facilitated by twisting of the *N*-ferrocenylisonicotinamide

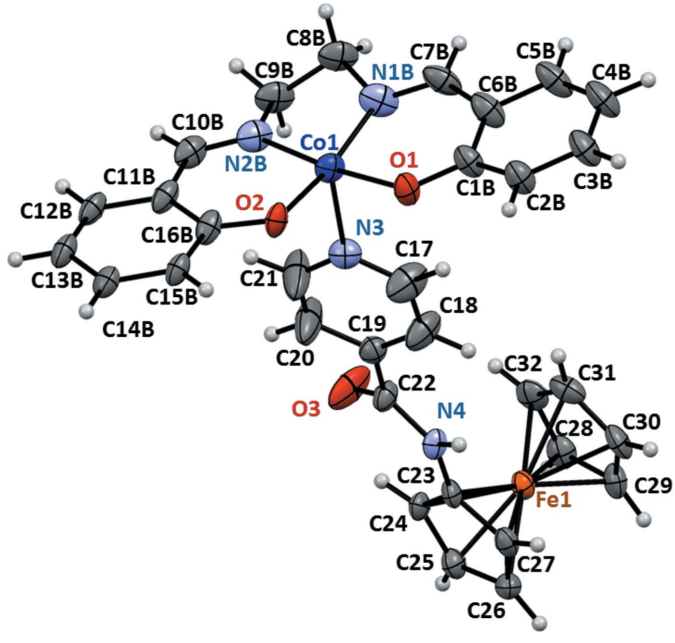



**Figure 1**
The asymmetric unit of the title compound, showing the atom-naming scheme. Only the δ conformer is depicted for clarity. The displacement ellipsoids are shown at the 50% probability level.

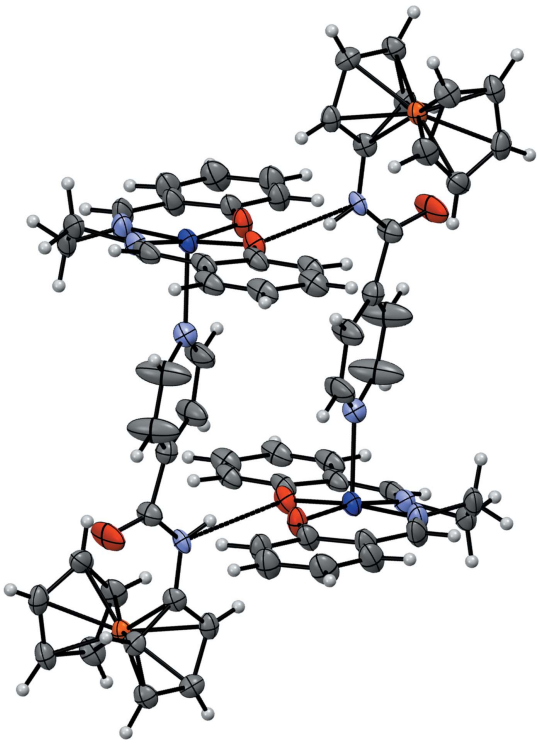


**Figure 2**
Hydrogen-bonded dimers of the title compound, showing the hydrogen bonds (dashed lines) formed between amide N—H groups and phenolate O atoms. Only the λ conformers are depicted for clarity. The displacement ellipsoids are shown at the 50% probability level.

amide group so that the amide plane (and presumably the amide N—H group) is oriented towards one of the two phenolate O atoms on the adjacent complex. The N···O distance for this interaction is 2.799 (4) Å, within the typical range for medium strength hydrogen bonds (Steiner, 2002) and shorter than the 2.969 (4) Å distance between the amide N and the other phenolate O atom. The Co—O distance to the hydrogen-bonded O atom, 1.908 (3) Å, is slightly longer than the 1.885 (3) Å distance between $Co^{II}$ and the other phenolate O atom. The amide N—H···O hydrogen-bond angle is 151.3°, smaller than the 164.0 (2)° angle observed in the structure of the *N*-ferrocenylisonicotinamide ligand (Patterson *et al.*, 2015) and within the range of those observed for aliphatic *N*-ferrocenylamides engaged in N—H···O=C hydrogen bonding (Okamura *et al.*, 2005).

The involvement of only half of the salen ring structure in hydrogen-bonding interactions means that the λ and δ conformers are diastereomeric. In the δ conformer, the salen ring is slightly folded away from the py coordination site (Fig. 3), with an intersalicylidene fold angle of 9.9 (7)°. In contrast, the λ conformer is nearly planar with an intersalicylidene fold angle of 2.3 (5)°. The discrepancy between the λ and δ fold angles is consistent with the known flexibility of salen complexes. The related complex [$Co^{II}$(salen)(py)], for instance, exhibits bending of the salen ring system away from the axial pyridine (py) ring with a fold angle of 28.8° (Calligaris *et al.*, 1970).

The dimers pack into a layered structure along the [100] direction and perpendicular to the Co—py bond. In the crystal, the open coordination site of each Co(salen)py subunit is blocked by the imine C—H group of an adjoining dimer, an observation consistent with the solid state complex's stability towards oxygen (in contrast dilute solutions of the complex react rapidly with oxygen). The structure contains large channels oriented along the [100] direction (Fig. 4). These channels are filled with highly-disordered solvent which we were unable to model. The *PLATON* (Spek, 2009) SQUEEZE (Spek, 2015) report indicated a solvent-accessible volume of 448.2 Å$^3$ per cell, corresponding to 26.1% of the unit-cell volume, that is occupied by 144.9 electrons. However, SQUEEZE slightly underestimates the actual void volume since it assumes simultaneous occupancy of both conformers of the title compound. The void volumes calculated for the λ and δ conformers using a 1.2 Å probe radius are 432 and 505 Å$^3$ per cell, corresponding to an occupancy-weighted average void volume of 462 Å$^3$ per cell. These void volumes and electron counts are both much larger than would be expected from the 0.3 $CH_2Cl_2$ and 1.5 $Et_2O$ solvent molecules per unit cell indicated by elemental analysis of the vacuum dried crystals. We suspect that 1.7 molecules of dichloromethane solvent per unit cell are lost when the crystals are dried prior to elemental analysis. If the undried crystals contained 2 $CH_2Cl_2$ and 1.5 $Et_2O$ solvent molecules per unit cell, a void volume and electron count of 470 Å$^3$ per cell and 147 electrons per cell are expected, consistent with the expected void volume and SQUEEZE electron count results.

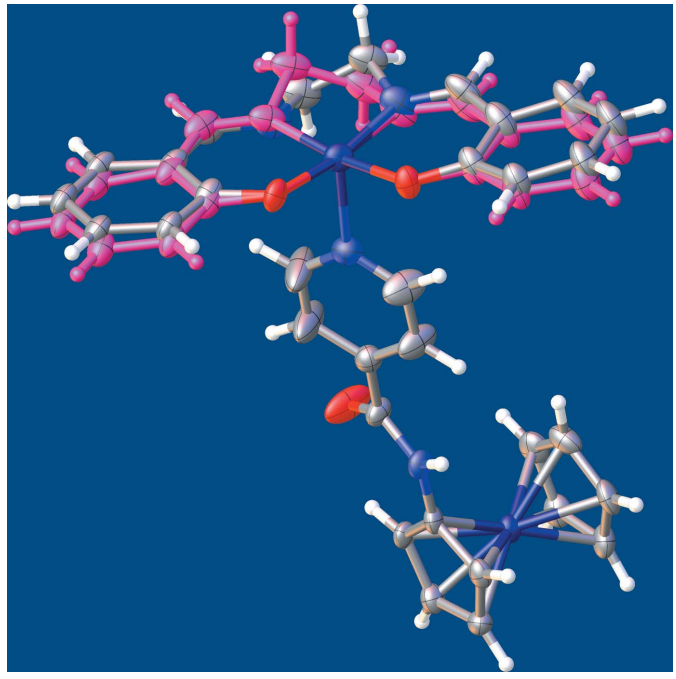


**Figure 3**
Comparison of the salen ring structure in the λ and δ conformers of the title compound, showing the greater bowing of salen in the latter. The salen ring system of the δ conformer is colored by element, while that of the λ conformer is shown in purple.

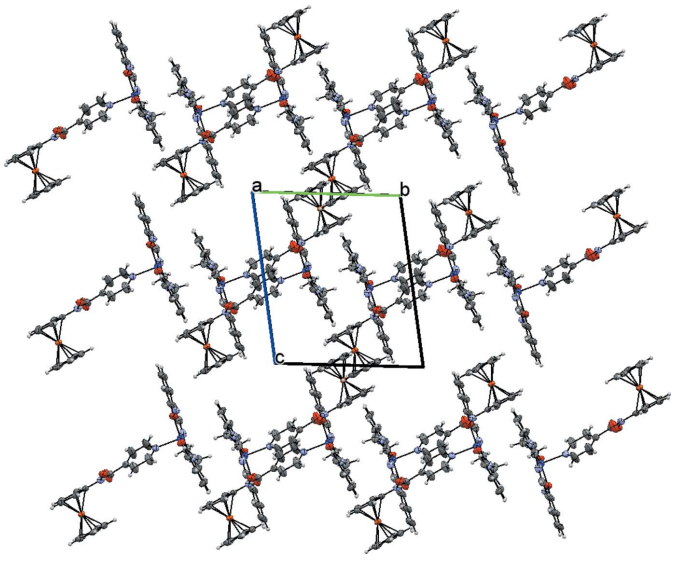



**Figure 4**
Packing structure view along the (100) axis of the crystal, showing the channels formed by packing of dimers of the title compound. Only the $\delta$ conformers are depicted for clarity.

## 4. Database survey

For structural studies of *N*-ferrocenylisonicotinamide, see: Patterson *et al.* (2015). For structural studies on hydrogen-bonded assemblies of *N*-ferrocenylamides and the use of *N*-ferrocenylamides, see: Okamura *et al.* (1998, 2005); Patterson *et al.* (2015). For complexes involving *N*-ferrocenylamide derivatives of thiolate ligands, see: Okamura *et al.* (2007). For structural studies on {2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}cobalt(II) and its pyridine derivatives, see: Brückner *et al.* (1969); Calligaris *et al.* (1970, 1972); Shi *et al.* (1995). For a summary of the basic features of the stereochemistry of metal salen systems, see: Yamada (1999).

## 5. Synthesis and crystallization

All syntheses and purification steps were conducted under a nitrogen atmosphere using degassed solvents. *N*-ferrocenylisonicotinamide was prepared as described previously (Patterson *et al.*, 2015). Acetonitrile, THF, and dichloromethane were purchased from VWR and purified using an HG Waters solvent purification system prior to use. All other reagents and solvents were obtained from VWR or Sigma–Aldrich in reagent grade or higher purity and used as received.

NMR spectra were obtained using either a Bruker Avance III 400MHz NMR spectrometer or a Bruker Avance 300MHz NMR spectrometer with gradient probe. All spectra were referenced relative to solvent peaks. Mass spectra were obtained on samples in HPLC grade MeOH using a Thermoelectron LCQ-Deca XP Mass Spectrometer. UV–Vis Spectra were obtained on anaerobic samples in quartz cuvettes using a Thermo Nicolet Evolution 300 UV–Vis spectrometer using the appropriate solvent as a blank. IR spectra were obtained using a Thermo Electron Nexus 470 FTIR.

For the preparation of the title compound, *N*-ferrocenylisonicotinamide (48.39 mg, 0.1580 mmol) and {2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}cobalt(II) (52.10 mg, 0.1602 mmol) were mixed with dry dichloromethane (5 ml) under nitrogen. The resulting mixture was heated to 323 K for approximately 2 h, during which time the reactants dissolved to give a red solution. The reaction mixture was allowed to cool and then the solvent was removed using an oil-pump vacuum to give a waxy solid, which was washed with six 10 ml aliquots of dry diethyl ether, redissolved in 3 ml fresh dichloromethane, reprecipitated by the addition of diethyl ether (25 ml), and dried under vacuum for 18 h to give the product as a red–brown solid that is soluble in dichloromethane, acetonitrile, methanol, THF, acetone, DMF, and DMSO, but insoluble in water, ether, and hexanes. Yield: 60 mg (75.83%). $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ 2.427 (*br s*, 2H), 3.907 (*br s*), 4.013 (*br s*) (Note: the two preceding singlets were not fully resolved and integrated to a total of 6H), 4.714 (*br s*, 1H), 6.27 (*br s*, 1H), 6.966 (*br s*, 2H), 8.30 (*br s*, 2H), 14.422 (*br s*, 2H). ESI–MS (MeOH, positive ion): *m*/*z* 630.7, 325.1 and 307. Selected IR (KBr, cm$^{-1}$): 3249, 3215 (NH), 1670 (amide C=O stretch). UV–Vis, concentrated in $CH_2Cl_2$: [$\lambda_{max}$ ($\varepsilon$, $M^{-1}$ cm$^{-1}$)]: 336 (15109), 406 (17461), 482 (3674). Calculated for $C_{32}H_{28}CoFeN_4O_3{\cdot}0.75C_4H_{10}O{\cdot}0.15\ CH_2Cl_2$: C 60.34, H 5.16, N 8.01%; found: C 60.39, H 5.21, N 8.06%.

**Table 1**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $[CoFe(C_5H_5)(C_{16}H_{14}N_2O_2)(C_{11}H_9N_2O)]$ |
| $M_r$ | 631.36 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 100 |
| $a, b, c$ (Å) | 10.684 (2), 11.989 (3), 13.858 (3) |
| $\alpha, \beta, \gamma$ (°) | 80.220 (5), 85.234 (5), 80.047 (5) |
| $V$ (Å$^3$) | 1720.2 (7) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.94 |
| Crystal size (mm) | 0.2 × 0.2 × 0.1 |
| Data collection | |
| Diffractometer | Bruker SMART APEXII area detector |
| Absorption correction | Multi-scan (*SADABS*; Sheldrick, 2012) |
| $T_{min}$, $T_{max}$ | 0.639, 0.745 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 10667, 7295, 3968 |
| $R_{int}$ | 0.047 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.644 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.056, 0.136, 0.93 |
| No. of reflections | 7295 |
| No. of parameters | 521 |
| No. of restraints | 638 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.62, −0.58 |

Computer programs: *APEX2* (Bruker, 2005), *OLEX2.solve* (Bourhis *et al.*, 2015), *SHELXL2014* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

Crystals were grown as opaque pale-red–brown plates by vapor diffusion of ethyl ether into a concentrated dichloromethane solution at 233 K under a nitrogen atmosphere.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. H atoms were placed in idealized positions and refined as riding with bond lengths of 0.95 (CH), 0.98 ($CH_2$), and 0.88 Å (amide NH). $U_{iso}$(H) values were fixed at 1.2$U_{eq}$(C). Several restraints were used to model the disorder associated with cocrystallization of the λ and δ chelate ring conformers. All phenolate C—O bond lengths were set to be equal using the SADI command and the phenolate C—O and its adjacent C atoms were constrained to be coplanar using the FLAT command. The displacement parameters of atoms C1*A* and C16*A* were set equal to those of C1*B* and C16*B* using the EADP command. The displacement parameter of all other disordered atoms (C2–C15) were constrained using the SIMU command.

After attempts to model the highly disordered solvent proved unsuccessful, the SQUEEZE technique (Spek, 2015) operated under *PLATON* (Spek, 2009) was used to filter out the contributions of the disordered solvent molecules, none of which was near the open coordination site on the $Co^{II}$ atom, capable of forming hydrogen bonds with the N—H hydrogen or other O and N atoms in the structure, or otherwise within bonding distance to the molecular structure.

Hydrogen-bond parameters were calculated assuming an ideal N—H bond angle and an N—H bond length of 1.009 Å, the value determined by neutron diffraction (Allen *et al.*, 2006). The void volumes expected for unit cells containing only the λ or δ chelate ring conformers were calculated in *Mercury3.3* (Macrae *et al.*, 2006) using the default probe radius of 1.2Å. The expected void volume occupancies for ether and dichloromethane molecules were taken as 173 and 106 $Å^3$, respectively, the average molecular volume of each compound in the pure liquid at 293 K.

## Acknowledgements

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# supporting information

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# Crystal structure of an unknown solvate of {2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato-$\kappa^4O,N,N',O'$}(*N*-ferrocenylisonicotinamide-$\kappa N^1$)cobalt(II): a $Co^{II}$–salen complex that forms hydrogen-bonded dimers

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## Computing details

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2* (Bruker, 2005); data reduction: *APEX2* (Bruker, 2005); program(s) used to solve structure: olex2.solve (Bourhis *et al.*, 2015); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: OLEX2 (Dolomanov *et al.*, 2009); software used to prepare material for publication: OLEX2 (Dolomanov *et al.*, 2009).

**{2,2′-[Ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato-$\kappa^4O,N,N',O'$}(*N*-ferrocenylisonicotinamide-$\kappa N^1$)cobalt(II)**

*Crystal data*

| | |
|---|---|
| $[CoFe(C_5H_5)(C_{16}H_{14}N_2O_2)(C_{11}H_9N2O)]$ | $V$ = 1720.2 (7) Å$^3$ |
| $M_r$ = 631.36 | $Z$ = 2 |
| Triclinic, $P\overline{1}$ | $F(000)$ = 650 |
| $a$ = 10.684 (2) Å | $D_x$ = 1.219 Mg m$^{-3}$ |
| $b$ = 11.989 (3) Å | Mo $K\alpha$ radiation, $\lambda$ = 0.71069 Å |
| $c$ = 13.858 (3) Å | $\mu$ = 0.94 mm$^{-1}$ |
| $\alpha$ = 80.220 (5)° | $T$ = 100 K |
| $\beta$ = 85.234 (5)° | Plates, dull dark red |
| $\gamma$ = 80.047 (5)° | 0.2 × 0.2 × 0.1 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII area-detector diffractometer | $T_{min}$ = 0.639, $T_{max}$ = 0.745 |
| | 10667 measured reflections |
| Radiation source: microfocus sealed X-ray tube, Incoatec I$\mu$s | 7295 independent reflections |
| | 3968 reflections with $I > 2\sigma(I)$ |
| Mirror optics monochromator | $R_{int}$ = 0.047 |
| Detector resolution: 7.9 pixels mm$^{-1}$ | $\theta_{max}$ = 27.2°, $\theta_{min}$ = 1.5° |
| $\omega$ and $\varphi$ scans | $h$ = −13→11 |
| Absorption correction: multi-scan (SADABS2012; Sheldrick, 2012) | $k$ = −15→12 |
| | $l$ = −17→17 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $S$ = 0.93 |
| Least-squares matrix: full | 7295 reflections |
| $R[F^2 > 2\sigma(F^2)]$ = 0.056 | 521 parameters |
| $wR(F^2)$ = 0.136 | 638 restraints |

Primary atom site location: iterative
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å$^{-3}$
$\Delta\rho_{min} = -0.58$ e Å$^{-3}$

*Special details*

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

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Co1 | 0.08639 (5) | 0.29271 (5) | 0.45247 (4) | 0.03107 (18) | |
| Fe1 | 0.24831 (5) | −0.44739 (5) | 0.91168 (4) | 0.02567 (17) | |
| O1 | −0.0897 (2) | 0.2936 (2) | 0.4787 (2) | 0.0326 (7) | |
| O2 | 0.0587 (2) | 0.2644 (2) | 0.3252 (2) | 0.0312 (7) | |
| N4 | 0.1996 (3) | −0.2891 (3) | 0.7102 (2) | 0.0255 (8) | |
| H4 | 0.1182 | −0.2654 | 0.7009 | 0.033* | |
| N3 | 0.1421 (4) | 0.1144 (3) | 0.5130 (3) | 0.0346 (9) | |
| O3 | 0.3940 (3) | −0.2369 (3) | 0.6831 (3) | 0.0619 (12) | |
| C1A | −0.1586 (16) | 0.3192 (14) | 0.5562 (10) | 0.0333 (12) | 0.583 (12) |
| C2A | −0.2883 (16) | 0.3127 (16) | 0.5624 (13) | 0.036 (2) | 0.583 (12) |
| H2A | −0.3230 | 0.2914 | 0.5085 | 0.047* | 0.583 (12) |
| C3A | −0.3684 (14) | 0.3352 (11) | 0.6418 (11) | 0.044 (2) | 0.583 (12) |
| H3A | −0.4560 | 0.3294 | 0.6421 | 0.057* | 0.583 (12) |
| C4A | −0.3204 (12) | 0.3668 (11) | 0.7221 (10) | 0.048 (3) | 0.583 (12) |
| H4A | −0.3750 | 0.3847 | 0.7770 | 0.062* | 0.583 (12) |
| C5A | −0.1939 (12) | 0.3714 (11) | 0.7203 (10) | 0.046 (3) | 0.583 (12) |
| H5A | −0.1607 | 0.3888 | 0.7765 | 0.060* | 0.583 (12) |
| C6A | −0.1090 (13) | 0.3515 (17) | 0.6382 (12) | 0.039 (2) | 0.583 (12) |
| C7A | 0.0225 (12) | 0.3585 (14) | 0.6398 (13) | 0.044 (3) | 0.583 (12) |
| H7A | 0.0495 | 0.3784 | 0.6973 | 0.053* | 0.583 (12) |
| N1A | 0.1100 (12) | 0.340 (2) | 0.5693 (16) | 0.043 (3) | 0.583 (12) |
| C8A | 0.2460 (9) | 0.3394 (10) | 0.5832 (7) | 0.044 (2) | 0.583 (12) |
| H8AA | 0.2872 | 0.2613 | 0.6108 | 0.053* | 0.583 (12) |
| H8AB | 0.2546 | 0.3924 | 0.6290 | 0.053* | 0.583 (12) |
| C9A | 0.3079 (9) | 0.3779 (10) | 0.4829 (7) | 0.043 (2) | 0.583 (12) |
| H9AA | 0.2891 | 0.4624 | 0.4650 | 0.052* | 0.583 (12) |
| H9AB | 0.4014 | 0.3540 | 0.4827 | 0.052* | 0.583 (12) |
| N2A | 0.2519 (17) | 0.321 (2) | 0.4131 (10) | 0.038 (2) | 0.583 (12) |
| C10A | 0.3152 (18) | 0.3082 (18) | 0.3311 (9) | 0.040 (2) | 0.583 (12) |
| H10A | 0.3973 | 0.3298 | 0.3220 | 0.048* | 0.583 (12) |
| C11A | 0.2709 (18) | 0.264 (3) | 0.2535 (13) | 0.0325 (19) | 0.583 (12) |
| C12A | 0.3569 (16) | 0.2361 (13) | 0.1739 (11) | 0.038 (3) | 0.583 (12) |
| H12A | 0.4439 | 0.2423 | 0.1769 | 0.046* | 0.583 (12) |

| | | | | | |
|---|---|---|---|---|---|
| C13A | 0.3206 (15) | 0.2009 (11) | 0.0939 (10) | 0.039 (3) | 0.583 (12) |
| H13A | 0.3801 | 0.1850 | 0.0412 | 0.050* | 0.583 (12) |
| C14A | 0.1927 (16) | 0.1888 (12) | 0.0914 (11) | 0.040 (3) | 0.583 (12) |
| H14A | 0.1648 | 0.1665 | 0.0352 | 0.052* | 0.583 (12) |
| C15A | 0.1061 (16) | 0.2088 (15) | 0.1694 (13) | 0.033 (3) | 0.583 (12) |
| H15A | 0.0207 | 0.1977 | 0.1664 | 0.043* | 0.583 (12) |
| C16A | 0.1422 (16) | 0.245 (2) | 0.2527 (13) | 0.0322 (16) | 0.583 (12) |
| C1B | −0.160 (2) | 0.329 (2) | 0.5527 (13) | 0.0333 (12) | 0.417 (12) |
| C2B | −0.293 (2) | 0.334 (2) | 0.5589 (18) | 0.037 (3) | 0.417 (12) |
| H2B | −0.3323 | 0.3116 | 0.5079 | 0.048* | 0.417 (12) |
| C3B | −0.3678 (19) | 0.3715 (16) | 0.6359 (16) | 0.043 (3) | 0.417 (12) |
| H3B | −0.4570 | 0.3722 | 0.6381 | 0.056* | 0.417 (12) |
| C4B | −0.3151 (17) | 0.4085 (15) | 0.7113 (14) | 0.046 (3) | 0.417 (12) |
| H4B | −0.3676 | 0.4328 | 0.7651 | 0.060* | 0.417 (12) |
| C5B | −0.1880 (17) | 0.4094 (15) | 0.7069 (14) | 0.044 (3) | 0.417 (12) |
| H5B | −0.1516 | 0.4369 | 0.7568 | 0.058* | 0.417 (12) |
| C6B | −0.1098 (18) | 0.370 (3) | 0.6290 (17) | 0.041 (3) | 0.417 (12) |
| C7B | 0.0179 (17) | 0.3844 (19) | 0.6309 (18) | 0.042 (3) | 0.417 (12) |
| H7B | 0.0406 | 0.4186 | 0.6826 | 0.050* | 0.417 (12) |
| N1B | 0.1056 (16) | 0.354 (3) | 0.567 (2) | 0.043 (3) | 0.417 (12) |
| C8B | 0.2280 (12) | 0.3908 (14) | 0.5762 (11) | 0.042 (2) | 0.417 (12) |
| H8BA | 0.2520 | 0.3734 | 0.6453 | 0.050* | 0.417 (12) |
| H8BB | 0.2234 | 0.4741 | 0.5531 | 0.050* | 0.417 (12) |
| C9B | 0.3209 (11) | 0.3236 (14) | 0.5133 (11) | 0.042 (2) | 0.417 (12) |
| H9BA | 0.3946 | 0.3637 | 0.4927 | 0.050* | 0.417 (12) |
| H9BB | 0.3523 | 0.2470 | 0.5504 | 0.050* | 0.417 (12) |
| N2B | 0.256 (2) | 0.311 (3) | 0.4260 (13) | 0.039 (3) | 0.417 (12) |
| C10B | 0.323 (3) | 0.298 (3) | 0.3468 (13) | 0.036 (3) | 0.417 (12) |
| H10B | 0.4096 | 0.3080 | 0.3443 | 0.044* | 0.417 (12) |
| C11B | 0.277 (3) | 0.271 (4) | 0.2613 (19) | 0.033 (2) | 0.417 (12) |
| C12B | 0.362 (2) | 0.2614 (19) | 0.1778 (14) | 0.033 (3) | 0.417 (12) |
| H12B | 0.4465 | 0.2746 | 0.1805 | 0.040* | 0.417 (12) |
| C13B | 0.326 (2) | 0.2343 (16) | 0.0944 (14) | 0.035 (3) | 0.417 (12) |
| H13B | 0.3862 | 0.2256 | 0.0407 | 0.046* | 0.417 (12) |
| C14B | 0.200 (2) | 0.2192 (17) | 0.0869 (16) | 0.033 (3) | 0.417 (12) |
| H14B | 0.1751 | 0.2004 | 0.0283 | 0.043* | 0.417 (12) |
| C15B | 0.112 (2) | 0.232 (2) | 0.1659 (17) | 0.030 (3) | 0.417 (12) |
| H15B | 0.0262 | 0.2232 | 0.1599 | 0.040* | 0.417 (12) |
| C16B | 0.148 (2) | 0.257 (4) | 0.2543 (18) | 0.0322 (16) | 0.417 (12) |
| C17 | 0.0672 (5) | 0.0607 (4) | 0.5791 (4) | 0.0554 (16) | |
| H17 | −0.0165 | 0.0991 | 0.5918 | 0.072* | |
| C18 | 0.1031 (4) | −0.0478 (4) | 0.6307 (4) | 0.0505 (15) | |
| H18 | 0.0448 | −0.0828 | 0.6765 | 0.066* | |
| C19 | 0.2235 (4) | −0.1038 (4) | 0.6149 (3) | 0.0305 (10) | |
| C20 | 0.2989 (5) | −0.0493 (5) | 0.5444 (4) | 0.074 (2) | |
| H20 | 0.3826 | −0.0861 | 0.5294 | 0.096* | |
| C21 | 0.2560 (6) | 0.0567 (5) | 0.4953 (4) | 0.078 (2) | |
| H21 | 0.3109 | 0.0910 | 0.4459 | 0.093* | |

| | | | | |
|---|---|---|---|---|
| C22 | 0.2794 (4) | −0.2170 (4) | 0.6734 (3) | 0.0311 (11) |
| C23 | 0.2335 (4) | −0.3992 (4) | 0.7623 (3) | 0.0258 (10) |
| C24 | 0.3578 (4) | −0.4609 (4) | 0.7841 (3) | 0.0276 (10) |
| H24 | 0.4360 | −0.4331 | 0.7670 | 0.036* |
| C25 | 0.3430 (4) | −0.5707 (4) | 0.8356 (3) | 0.0302 (10) |
| H25 | 0.4101 | −0.6298 | 0.8583 | 0.039* |
| C26 | 0.2107 (4) | −0.5779 (4) | 0.8478 (3) | 0.0293 (10) |
| H26 | 0.1739 | −0.6420 | 0.8799 | 0.038* |
| C27 | 0.1441 (4) | −0.4710 (4) | 0.8029 (3) | 0.0281 (10) |
| H27 | 0.0542 | −0.4511 | 0.8006 | 0.036* |
| C28 | 0.3275 (4) | −0.4656 (4) | 1.0441 (3) | 0.0337 (11) |
| H28 | 0.4000 | −0.5191 | 1.0659 | 0.044* |
| C29 | 0.1990 (4) | −0.4846 (4) | 1.0571 (3) | 0.0347 (11) |
| H29 | 0.1703 | −0.5529 | 1.0891 | 0.045* |
| C30 | 0.1218 (4) | −0.3836 (4) | 1.0140 (3) | 0.0363 (11) |
| H30 | 0.0317 | −0.3720 | 1.0124 | 0.047* |
| C31 | 0.2011 (4) | −0.3030 (4) | 0.9739 (3) | 0.0371 (11) |
| H31 | 0.1738 | −0.2280 | 0.9401 | 0.048* |
| C32 | 0.3285 (4) | −0.3527 (4) | 0.9927 (3) | 0.0371 (11) |
| H32 | 0.4015 | −0.3169 | 0.9742 | 0.048* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Co1 | 0.0191 (3) | 0.0351 (4) | 0.0402 (4) | −0.0031 (3) | −0.0074 (3) | −0.0078 (3) |
| Fe1 | 0.0189 (3) | 0.0331 (4) | 0.0253 (3) | −0.0017 (3) | −0.0004 (3) | −0.0086 (3) |
| O1 | 0.0198 (15) | 0.0488 (19) | 0.0320 (16) | −0.0056 (13) | −0.0019 (13) | −0.0138 (15) |
| O2 | 0.0155 (15) | 0.0455 (19) | 0.0311 (16) | −0.0072 (13) | 0.0018 (12) | −0.0009 (14) |
| N4 | 0.0130 (17) | 0.035 (2) | 0.0276 (19) | −0.0022 (15) | −0.0042 (14) | −0.0027 (16) |
| N3 | 0.034 (2) | 0.034 (2) | 0.035 (2) | −0.0041 (18) | −0.0082 (18) | −0.0044 (18) |
| O3 | 0.0157 (18) | 0.052 (2) | 0.108 (3) | −0.0075 (15) | −0.0101 (19) | 0.021 (2) |
| C1A | 0.027 (2) | 0.043 (3) | 0.030 (2) | 0.004 (2) | −0.0060 (18) | −0.014 (2) |
| C2A | 0.028 (3) | 0.048 (6) | 0.035 (4) | 0.001 (4) | −0.004 (3) | −0.020 (4) |
| C3A | 0.031 (3) | 0.058 (6) | 0.044 (4) | 0.001 (4) | −0.003 (3) | −0.021 (5) |
| C4A | 0.039 (4) | 0.061 (6) | 0.042 (4) | 0.008 (5) | −0.001 (3) | −0.021 (5) |
| C5A | 0.039 (4) | 0.057 (6) | 0.042 (4) | 0.010 (4) | −0.009 (3) | −0.026 (4) |
| C6A | 0.030 (3) | 0.050 (5) | 0.038 (4) | 0.007 (3) | −0.009 (3) | −0.021 (4) |
| C7A | 0.039 (4) | 0.052 (6) | 0.047 (4) | 0.008 (4) | −0.019 (3) | −0.028 (4) |
| N1A | 0.028 (3) | 0.048 (6) | 0.057 (4) | 0.003 (3) | −0.016 (3) | −0.024 (4) |
| C8A | 0.028 (4) | 0.048 (5) | 0.064 (4) | 0.003 (4) | −0.020 (3) | −0.028 (4) |
| C9A | 0.026 (3) | 0.035 (5) | 0.072 (4) | −0.001 (3) | −0.019 (3) | −0.015 (4) |
| N2A | 0.022 (3) | 0.032 (4) | 0.061 (4) | −0.001 (3) | −0.012 (3) | −0.012 (4) |
| C10A | 0.019 (4) | 0.036 (4) | 0.059 (4) | −0.001 (3) | −0.005 (4) | 0.007 (4) |
| C11A | 0.019 (3) | 0.033 (4) | 0.040 (4) | −0.003 (3) | −0.002 (3) | 0.009 (3) |
| C12A | 0.020 (3) | 0.040 (6) | 0.046 (4) | −0.001 (4) | 0.004 (3) | 0.011 (4) |
| C13A | 0.024 (3) | 0.042 (6) | 0.041 (3) | −0.001 (5) | 0.007 (3) | 0.010 (4) |
| C14A | 0.031 (4) | 0.045 (6) | 0.037 (4) | −0.002 (5) | 0.003 (3) | 0.005 (4) |
| C15A | 0.021 (3) | 0.039 (6) | 0.033 (3) | −0.002 (4) | 0.001 (3) | 0.006 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C16A | 0.019 (2) | 0.037 (4) | 0.035 (2) | −0.002 (2) | −0.0026 (18) | 0.007 (2) |
| C1B | 0.027 (2) | 0.043 (3) | 0.030 (2) | 0.004 (2) | −0.0060 (18) | −0.014 (2) |
| C2B | 0.027 (4) | 0.051 (6) | 0.035 (4) | 0.000 (4) | −0.006 (4) | −0.018 (5) |
| C3B | 0.034 (4) | 0.054 (7) | 0.041 (4) | 0.009 (5) | −0.001 (4) | −0.021 (5) |
| C4B | 0.041 (4) | 0.055 (7) | 0.042 (4) | 0.011 (5) | −0.003 (4) | −0.027 (5) |
| C5B | 0.041 (4) | 0.053 (6) | 0.040 (5) | 0.013 (5) | −0.014 (4) | −0.025 (5) |
| C6B | 0.033 (4) | 0.051 (5) | 0.040 (4) | 0.010 (4) | −0.011 (3) | −0.021 (4) |
| C7B | 0.038 (4) | 0.044 (6) | 0.047 (4) | 0.005 (4) | −0.017 (4) | −0.025 (5) |
| N1B | 0.028 (4) | 0.047 (6) | 0.056 (4) | 0.002 (4) | −0.019 (4) | −0.017 (4) |
| C8B | 0.029 (4) | 0.042 (5) | 0.060 (4) | −0.005 (4) | −0.019 (4) | −0.015 (5) |
| C9B | 0.025 (4) | 0.043 (5) | 0.062 (5) | −0.005 (4) | −0.018 (4) | −0.012 (4) |
| N2B | 0.022 (4) | 0.036 (5) | 0.058 (5) | 0.001 (4) | −0.012 (4) | −0.006 (5) |
| C10B | 0.017 (4) | 0.035 (5) | 0.054 (5) | −0.001 (4) | −0.008 (4) | 0.001 (5) |
| C11B | 0.017 (4) | 0.034 (4) | 0.042 (4) | −0.004 (3) | −0.002 (4) | 0.008 (4) |
| C12B | 0.017 (4) | 0.034 (6) | 0.044 (4) | −0.006 (4) | 0.000 (4) | 0.007 (4) |
| C13B | 0.023 (4) | 0.037 (6) | 0.041 (4) | −0.007 (5) | 0.005 (4) | 0.007 (5) |
| C14B | 0.028 (4) | 0.034 (6) | 0.035 (4) | −0.009 (5) | 0.002 (4) | 0.004 (5) |
| C15B | 0.019 (4) | 0.036 (6) | 0.032 (4) | −0.007 (4) | 0.001 (4) | 0.005 (4) |
| C16B | 0.019 (2) | 0.037 (4) | 0.035 (2) | −0.002 (2) | −0.0026 (18) | 0.007 (2) |
| C17 | 0.024 (3) | 0.046 (3) | 0.089 (4) | 0.000 (2) | −0.015 (3) | 0.010 (3) |
| C18 | 0.021 (3) | 0.045 (3) | 0.078 (4) | −0.005 (2) | −0.003 (2) | 0.012 (3) |
| C19 | 0.028 (2) | 0.033 (3) | 0.032 (2) | −0.007 (2) | −0.0021 (19) | −0.006 (2) |
| C20 | 0.053 (4) | 0.046 (4) | 0.097 (5) | 0.014 (3) | 0.044 (3) | 0.017 (3) |
| C21 | 0.071 (4) | 0.050 (4) | 0.080 (4) | 0.020 (3) | 0.045 (3) | 0.026 (3) |
| C22 | 0.021 (2) | 0.033 (3) | 0.037 (3) | −0.0040 (19) | 0.0037 (19) | 0.001 (2) |
| C23 | 0.019 (2) | 0.032 (3) | 0.025 (2) | −0.0010 (18) | 0.0054 (17) | −0.0078 (19) |
| C24 | 0.016 (2) | 0.033 (3) | 0.034 (2) | −0.0064 (18) | 0.0063 (18) | −0.008 (2) |
| C25 | 0.023 (2) | 0.036 (3) | 0.031 (2) | 0.0001 (19) | 0.0014 (19) | −0.008 (2) |
| C26 | 0.032 (3) | 0.027 (2) | 0.029 (2) | −0.0067 (19) | 0.0036 (19) | −0.006 (2) |
| C27 | 0.023 (2) | 0.039 (3) | 0.025 (2) | −0.0036 (19) | −0.0009 (18) | −0.013 (2) |
| C28 | 0.028 (3) | 0.047 (3) | 0.027 (2) | −0.003 (2) | −0.0073 (19) | −0.010 (2) |
| C29 | 0.032 (3) | 0.048 (3) | 0.022 (2) | −0.003 (2) | 0.0039 (19) | −0.006 (2) |
| C30 | 0.027 (3) | 0.048 (3) | 0.033 (3) | 0.007 (2) | 0.003 (2) | −0.019 (2) |
| C31 | 0.045 (3) | 0.032 (3) | 0.034 (3) | 0.004 (2) | −0.012 (2) | −0.013 (2) |
| C32 | 0.037 (3) | 0.048 (3) | 0.032 (3) | −0.009 (2) | −0.007 (2) | −0.018 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Co1—O1 | 1.885 (3) | C1B—C6B | 1.421 (12) |
| Co1—O2 | 1.908 (3) | C2B—H2B | 0.9500 |
| Co1—N3 | 2.159 (4) | C2B—C3B | 1.369 (13) |
| Co1—N1A | 1.854 (18) | C3B—H3B | 0.9500 |
| Co1—N2A | 1.877 (17) | C3B—C4B | 1.396 (13) |
| Co1—N1B | 1.89 (3) | C4B—H4B | 0.9500 |
| Co1—N2B | 1.87 (2) | C4B—C5B | 1.356 (13) |
| Fe1—C23 | 2.064 (4) | C5B—H5B | 0.9500 |
| Fe1—C24 | 2.052 (4) | C5B—C6B | 1.406 (13) |
| Fe1—C25 | 2.039 (4) | C6B—C7B | 1.408 (12) |

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| Fe1—C26 | 2.035 (4) | C7B—H7B | 0.9500 |
| Fe1—C27 | 2.031 (4) | C7B—N1B | 1.289 (13) |
| Fe1—C28 | 2.046 (4) | N1B—C8B | 1.473 (14) |
| Fe1—C29 | 2.034 (4) | C8B—H8BA | 0.9900 |
| Fe1—C30 | 2.029 (4) | C8B—H8BB | 0.9900 |
| Fe1—C31 | 2.032 (4) | C8B—C9B | 1.487 (13) |
| Fe1—C32 | 2.052 (4) | C9B—H9BA | 0.9900 |
| O1—C1A | 1.300 (9) | C9B—H9BB | 0.9900 |
| O1—C1B | 1.306 (12) | C9B—N2B | 1.482 (14) |
| O2—C16A | 1.311 (9) | N2B—C10B | 1.275 (13) |
| O2—C16B | 1.312 (12) | C10B—H10B | 0.9500 |
| N4—H4 | 0.8800 | C10B—C11B | 1.429 (13) |
| N4—C22 | 1.330 (5) | C11B—C12B | 1.419 (13) |
| N4—C23 | 1.396 (5) | C11B—C16B | 1.429 (12) |
| N3—C17 | 1.323 (6) | C12B—H12B | 0.9500 |
| N3—C21 | 1.317 (6) | C12B—C13B | 1.354 (13) |
| O3—C22 | 1.220 (5) | C13B—H13B | 0.9500 |
| C1A—C2A | 1.396 (10) | C13B—C14B | 1.401 (13) |
| C1A—C6A | 1.429 (10) | C14B—H14B | 0.9500 |
| C2A—H2A | 0.9500 | C14B—C15B | 1.395 (12) |
| C2A—C3A | 1.372 (10) | C15B—H15B | 0.9500 |
| C3A—H3A | 0.9500 | C15B—C16B | 1.407 (13) |
| C3A—C4A | 1.397 (11) | C17—H17 | 0.9500 |
| C4A—H4A | 0.9500 | C17—C18 | 1.381 (6) |
| C4A—C5A | 1.360 (10) | C18—H18 | 0.9500 |
| C5A—H5A | 0.9500 | C18—C19 | 1.363 (6) |
| C5A—C6A | 1.421 (10) | C19—C20 | 1.366 (6) |
| C6A—C7A | 1.423 (10) | C19—C22 | 1.510 (6) |
| C7A—H7A | 0.9500 | C20—H20 | 0.9500 |
| C7A—N1A | 1.314 (10) | C20—C21 | 1.358 (7) |
| N1A—C8A | 1.480 (11) | C21—H21 | 0.9500 |
| C8A—H8AA | 0.9900 | C23—C24 | 1.432 (5) |
| C8A—H8AB | 0.9900 | C23—C27 | 1.415 (6) |
| C8A—C9A | 1.523 (11) | C24—H24 | 0.9500 |
| C9A—H9AA | 0.9900 | C24—C25 | 1.414 (5) |
| C9A—H9AB | 0.9900 | C25—H25 | 0.9500 |
| C9A—N2A | 1.490 (12) | C25—C26 | 1.425 (6) |
| N2A—C10A | 1.292 (10) | C26—H26 | 0.9500 |
| C10A—H10A | 0.9500 | C26—C27 | 1.422 (5) |
| C10A—C11A | 1.424 (11) | C27—H27 | 0.9500 |
| C11A—C12A | 1.422 (10) | C28—H28 | 0.9500 |
| C11A—C16A | 1.432 (10) | C28—C29 | 1.422 (6) |
| C12A—H12A | 0.9500 | C28—C32 | 1.420 (6) |
| C12A—C13A | 1.358 (11) | C29—H29 | 0.9500 |
| C13A—H13A | 0.9500 | C29—C30 | 1.412 (6) |
| C13A—C14A | 1.402 (10) | C30—H30 | 0.9500 |
| C14A—H14A | 0.9500 | C30—C31 | 1.408 (6) |
| C14A—C15A | 1.389 (10) | C31—H31 | 0.9500 |

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|---|---|---|---|
| C15A—H15A | 0.9500 | C31—C32 | 1.414 (6) |
| C15A—C16A | 1.404 (10) | C32—H32 | 0.9500 |
| C1B—C2B | 1.403 (12) | | |

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| O1—Co1—O2 | 85.79 (12) | C1B—C2B—H2B | 118.9 |
| O1—Co1—N3 | 95.43 (13) | C3B—C2B—C1B | 122.1 (14) |
| O1—Co1—N1B | 93.8 (4) | C3B—C2B—H2B | 118.9 |
| O2—Co1—N3 | 95.16 (13) | C2B—C3B—H3B | 119.5 |
| N1A—Co1—O1 | 94.4 (3) | C2B—C3B—C4B | 121.1 (14) |
| N1A—Co1—O2 | 172.6 (9) | C4B—C3B—H3B | 119.5 |
| N1A—Co1—N3 | 92.2 (9) | C3B—C4B—H4B | 120.4 |
| N1A—Co1—N2A | 86.5 (4) | C5B—C4B—C3B | 119.2 (12) |
| N2A—Co1—O1 | 168.7 (8) | C5B—C4B—H4B | 120.4 |
| N2A—Co1—O2 | 91.8 (3) | C4B—C5B—H5B | 119.9 |
| N2A—Co1—N3 | 95.8 (8) | C4B—C5B—C6B | 120.3 (13) |
| N1B—Co1—O2 | 167.8 (13) | C6B—C5B—H5B | 119.9 |
| N1B—Co1—N3 | 97.0 (13) | C5B—C6B—C1B | 121.7 (11) |
| N2B—Co1—O1 | 173.1 (11) | C5B—C6B—C7B | 113.4 (13) |
| N2B—Co1—O2 | 96.2 (4) | C7B—C6B—C1B | 124.8 (13) |
| N2B—Co1—N3 | 91.0 (11) | C6B—C7B—H7B | 118.2 |
| N2B—Co1—N1B | 82.9 (6) | N1B—C7B—C6B | 123.7 (16) |
| C24—Fe1—C23 | 40.72 (15) | N1B—C7B—H7B | 118.2 |
| C24—Fe1—C32 | 108.71 (18) | C7B—N1B—Co1 | 127.4 (14) |
| C25—Fe1—C23 | 68.13 (16) | C7B—N1B—C8B | 114.0 (17) |
| C25—Fe1—C24 | 40.46 (15) | C8B—N1B—Co1 | 117.7 (11) |
| C25—Fe1—C28 | 108.90 (17) | N1B—C8B—H8BA | 110.8 |
| C25—Fe1—C32 | 126.39 (18) | N1B—C8B—H8BB | 110.8 |
| C26—Fe1—C23 | 68.49 (16) | N1B—C8B—C9B | 104.6 (12) |
| C26—Fe1—C24 | 68.76 (16) | H8BA—C8B—H8BB | 108.9 |
| C26—Fe1—C25 | 40.96 (16) | C9B—C8B—H8BA | 110.8 |
| C26—Fe1—C28 | 125.45 (17) | C9B—C8B—H8BB | 110.8 |
| C26—Fe1—C32 | 163.07 (17) | C8B—C9B—H9BA | 110.0 |
| C27—Fe1—C23 | 40.42 (16) | C8B—C9B—H9BB | 110.0 |
| C27—Fe1—C24 | 68.50 (16) | H9BA—C9B—H9BB | 108.4 |
| C27—Fe1—C25 | 68.50 (17) | N2B—C9B—C8B | 108.5 (12) |
| C27—Fe1—C26 | 40.93 (16) | N2B—C9B—H9BA | 110.0 |
| C27—Fe1—C28 | 162.01 (17) | N2B—C9B—H9BB | 110.0 |
| C27—Fe1—C29 | 124.10 (18) | C9B—N2B—Co1 | 113.7 (12) |
| C27—Fe1—C31 | 119.63 (17) | C10B—N2B—Co1 | 126.7 (14) |
| C27—Fe1—C32 | 155.19 (17) | C10B—N2B—C9B | 118.9 (16) |
| C28—Fe1—C23 | 156.71 (17) | N2B—C10B—H10B | 117.6 |
| C28—Fe1—C24 | 121.89 (17) | N2B—C10B—C11B | 124.8 (16) |
| C28—Fe1—C32 | 40.55 (17) | C11B—C10B—H10B | 117.6 |
| C29—Fe1—C23 | 160.94 (16) | C12B—C11B—C10B | 118.3 (14) |
| C29—Fe1—C24 | 156.65 (16) | C12B—C11B—C16B | 118.3 (12) |
| C29—Fe1—C25 | 121.28 (17) | C16B—C11B—C10B | 123.3 (14) |
| C29—Fe1—C26 | 106.84 (18) | C11B—C12B—H12B | 119.0 |
| C29—Fe1—C28 | 40.80 (16) | C13B—C12B—C11B | 122.0 (13) |

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| C29—Fe1—C32 | 68.46 (19) | C13B—C12B—H12B | 119.0 |
| C30—Fe1—C23 | 124.19 (17) | C12B—C13B—H13B | 119.9 |
| C30—Fe1—C24 | 161.74 (17) | C12B—C13B—C14B | 120.2 (13) |
| C30—Fe1—C25 | 155.71 (18) | C14B—C13B—H13B | 119.9 |
| C30—Fe1—C26 | 119.56 (19) | C13B—C14B—H14B | 120.1 |
| C30—Fe1—C27 | 106.31 (18) | C15B—C14B—C13B | 119.8 (13) |
| C30—Fe1—C28 | 68.32 (17) | C15B—C14B—H14B | 120.1 |
| C30—Fe1—C29 | 40.66 (16) | C14B—C15B—H15B | 119.5 |
| C30—Fe1—C31 | 40.59 (18) | C14B—C15B—C16B | 121.0 (13) |
| C30—Fe1—C32 | 68.22 (19) | C16B—C15B—H15B | 119.5 |
| C31—Fe1—C23 | 107.38 (17) | O2—C16B—C11B | 124.8 (19) |
| C31—Fe1—C24 | 125.44 (18) | O2—C16B—C15B | 116.6 (18) |
| C31—Fe1—C25 | 162.81 (18) | C15B—C16B—C11B | 118.6 (12) |
| C31—Fe1—C26 | 154.61 (18) | N3—C17—H17 | 117.9 |
| C31—Fe1—C28 | 68.24 (18) | N3—C17—C18 | 124.1 (5) |
| C31—Fe1—C29 | 68.44 (18) | C18—C17—H17 | 117.9 |
| C31—Fe1—C32 | 40.50 (17) | C17—C18—H18 | 120.5 |
| C32—Fe1—C23 | 121.27 (18) | C19—C18—C17 | 119.0 (4) |
| C1A—O1—Co1 | 128.0 (9) | C19—C18—H18 | 120.5 |
| C1B—O1—Co1 | 127.7 (12) | C18—C19—C20 | 116.5 (4) |
| C16A—O2—Co1 | 128.8 (9) | C18—C19—C22 | 124.5 (4) |
| C16B—O2—Co1 | 124.0 (12) | C20—C19—C22 | 119.0 (4) |
| C22—N4—H4 | 117.1 | C19—C20—H20 | 119.5 |
| C22—N4—C23 | 125.8 (3) | C21—C20—C19 | 121.1 (5) |
| C23—N4—H4 | 117.1 | C21—C20—H20 | 119.5 |
| C17—N3—Co1 | 120.8 (3) | N3—C21—C20 | 123.2 (5) |
| C21—N3—Co1 | 122.8 (3) | N3—C21—H21 | 118.4 |
| C21—N3—C17 | 116.0 (4) | C20—C21—H21 | 118.4 |
| O1—C1A—C2A | 119.2 (13) | N4—C22—C19 | 117.3 (4) |
| O1—C1A—C6A | 123.9 (13) | O3—C22—N4 | 124.3 (4) |
| C2A—C1A—C6A | 116.9 (9) | O3—C22—C19 | 118.4 (4) |
| C1A—C2A—H2A | 118.1 | N4—C23—Fe1 | 128.1 (3) |
| C3A—C2A—C1A | 123.7 (10) | N4—C23—C24 | 128.9 (4) |
| C3A—C2A—H2A | 118.1 | N4—C23—C27 | 123.4 (4) |
| C2A—C3A—H3A | 120.2 | C24—C23—Fe1 | 69.2 (2) |
| C2A—C3A—C4A | 119.6 (10) | C27—C23—Fe1 | 68.5 (2) |
| C4A—C3A—H3A | 120.2 | C27—C23—C24 | 107.6 (4) |
| C3A—C4A—H4A | 120.7 | Fe1—C24—H24 | 126.0 |
| C5A—C4A—C3A | 118.7 (9) | C23—C24—Fe1 | 70.1 (2) |
| C5A—C4A—H4A | 120.7 | C23—C24—H24 | 126.2 |
| C4A—C5A—H5A | 118.4 | C25—C24—Fe1 | 69.3 (2) |
| C4A—C5A—C6A | 123.1 (10) | C25—C24—C23 | 107.7 (4) |
| C6A—C5A—H5A | 118.4 | C25—C24—H24 | 126.2 |
| C5A—C6A—C1A | 117.9 (8) | Fe1—C25—H25 | 126.3 |
| C5A—C6A—C7A | 120.8 (10) | C24—C25—Fe1 | 70.3 (2) |
| C7A—C6A—C1A | 121.3 (10) | C24—C25—H25 | 125.6 |
| C6A—C7A—H7A | 116.9 | C24—C25—C26 | 108.7 (3) |
| N1A—C7A—C6A | 126.2 (12) | C26—C25—Fe1 | 69.4 (2) |

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| N1A—C7A—H7A | 116.9 | C26—C25—H25 | 125.6 |
| C7A—N1A—Co1 | 126.2 (10) | Fe1—C26—H26 | 126.1 |
| C7A—N1A—C8A | 121.2 (13) | C25—C26—Fe1 | 69.7 (2) |
| C8A—N1A—Co1 | 112.1 (8) | C25—C26—H26 | 126.4 |
| N1A—C8A—H8AA | 110.3 | C27—C26—Fe1 | 69.4 (2) |
| N1A—C8A—H8AB | 110.3 | C27—C26—C25 | 107.1 (4) |
| N1A—C8A—C9A | 107.2 (10) | C27—C26—H26 | 126.4 |
| H8AA—C8A—H8AB | 108.5 | Fe1—C27—H27 | 125.3 |
| C9A—C8A—H8AA | 110.3 | C23—C27—Fe1 | 71.1 (2) |
| C9A—C8A—H8AB | 110.3 | C23—C27—C26 | 108.8 (4) |
| C8A—C9A—H9AA | 110.6 | C23—C27—H27 | 125.6 |
| C8A—C9A—H9AB | 110.6 | C26—C27—Fe1 | 69.7 (2) |
| H9AA—C9A—H9AB | 108.8 | C26—C27—H27 | 125.6 |
| N2A—C9A—C8A | 105.5 (9) | Fe1—C28—H28 | 126.4 |
| N2A—C9A—H9AA | 110.6 | C29—C28—Fe1 | 69.1 (2) |
| N2A—C9A—H9AB | 110.6 | C29—C28—H28 | 126.0 |
| C9A—N2A—Co1 | 113.5 (8) | C32—C28—Fe1 | 69.9 (2) |
| C10A—N2A—Co1 | 128.4 (10) | C32—C28—H28 | 126.0 |
| C10A—N2A—C9A | 117.7 (12) | C32—C28—C29 | 107.9 (4) |
| N2A—C10A—H10A | 117.6 | Fe1—C29—H29 | 125.9 |
| N2A—C10A—C11A | 124.8 (12) | C28—C29—Fe1 | 70.1 (2) |
| C11A—C10A—H10A | 117.6 | C28—C29—H29 | 126.2 |
| C10A—C11A—C16A | 122.4 (10) | C30—C29—Fe1 | 69.5 (2) |
| C12A—C11A—C10A | 119.4 (10) | C30—C29—C28 | 107.7 (4) |
| C12A—C11A—C16A | 118.2 (9) | C30—C29—H29 | 126.2 |
| C11A—C12A—H12A | 118.4 | Fe1—C30—H30 | 126.1 |
| C13A—C12A—C11A | 123.1 (10) | C29—C30—Fe1 | 69.9 (2) |
| C13A—C12A—H12A | 118.4 | C29—C30—H30 | 125.8 |
| C12A—C13A—H13A | 121.0 | C31—C30—Fe1 | 69.8 (2) |
| C12A—C13A—C14A | 118.1 (10) | C31—C30—C29 | 108.4 (4) |
| C14A—C13A—H13A | 121.0 | C31—C30—H30 | 125.8 |
| C13A—C14A—H14A | 119.4 | Fe1—C31—H31 | 125.7 |
| C15A—C14A—C13A | 121.2 (10) | C30—C31—Fe1 | 69.6 (3) |
| C15A—C14A—H14A | 119.4 | C30—C31—H31 | 125.8 |
| C14A—C15A—H15A | 119.3 | C30—C31—C32 | 108.4 (4) |
| C14A—C15A—C16A | 121.4 (10) | C32—C31—Fe1 | 70.5 (3) |
| C16A—C15A—H15A | 119.3 | C32—C31—H31 | 125.8 |
| O2—C16A—C11A | 121.8 (13) | Fe1—C32—H32 | 126.9 |
| O2—C16A—C15A | 120.3 (13) | C28—C32—Fe1 | 69.5 (2) |
| C15A—C16A—C11A | 117.8 (9) | C28—C32—H32 | 126.2 |
| O1—C1B—C2B | 121.9 (17) | C31—C32—Fe1 | 69.0 (3) |
| O1—C1B—C6B | 122.5 (18) | C31—C32—C28 | 107.6 (4) |
| C2B—C1B—C6B | 115.5 (12) | C31—C32—H32 | 126.2 |

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|---|---|---|---|
| Co1—O1—C1A—C2A | −178.9 (8) | N2A—C10A—C11A—C16A | 10 (4) |
| Co1—O1—C1A—C6A | −0.5 (16) | C10A—C11A—C12A—C13A | −175 (2) |
| Co1—O1—C1B—C2B | 174.0 (12) | C10A—C11A—C16A—O2 | −2 (4) |
| Co1—O1—C1B—C6B | −2 (2) | C10A—C11A—C16A—C15A | 176 (3) |

| | | | |
|---|---|---|---|
| Co1—O2—C16A—C11A | −12 (3) | C11A—C12A—C13A—C14A | −2 (2) |
| Co1—O2—C16A—C15A | 170.3 (12) | C12A—C11A—C16A—O2 | 177 (2) |
| Co1—O2—C16B—C11B | −1 (5) | C12A—C11A—C16A—C15A | −5 (4) |
| Co1—O2—C16B—C15B | 177.9 (16) | C12A—C13A—C14A—C15A | −1.8 (16) |
| Co1—N3—C17—C18 | −170.8 (4) | C13A—C14A—C15A—C16A | 2 (2) |
| Co1—N3—C21—C20 | 169.5 (5) | C14A—C15A—C16A—O2 | 179.4 (18) |
| Co1—N1A—C8A—C9A | 37.0 (19) | C14A—C15A—C16A—C11A | 2 (3) |
| Co1—N2A—C10A—C11A | −3 (3) | C16A—C11A—C12A—C13A | 5 (4) |
| Co1—N1B—C8B—C9B | −24 (3) | C1B—C2B—C3B—C4B | 2 (3) |
| Co1—N2B—C10B—C11B | 2 (5) | C1B—C6B—C7B—N1B | −5 (3) |
| Fe1—C23—C24—C25 | 59.3 (3) | C2B—C1B—C6B—C5B | 2 (2) |
| Fe1—C23—C27—C26 | −59.7 (3) | C2B—C1B—C6B—C7B | −172 (2) |
| Fe1—C24—C25—C26 | 58.9 (3) | C2B—C3B—C4B—C5B | 1 (2) |
| Fe1—C25—C26—C27 | 59.5 (3) | C3B—C4B—C5B—C6B | −2 (2) |
| Fe1—C26—C27—C23 | 60.5 (3) | C4B—C5B—C6B—C1B | 0 (3) |
| Fe1—C28—C29—C30 | −59.5 (3) | C4B—C5B—C6B—C7B | 175.4 (16) |
| Fe1—C28—C32—C31 | 58.6 (3) | C5B—C6B—C7B—N1B | 180 (2) |
| Fe1—C29—C30—C31 | −59.4 (3) | C6B—C1B—C2B—C3B | −3 (2) |
| Fe1—C30—C31—C32 | −60.1 (3) | C6B—C7B—N1B—Co1 | 4 (4) |
| Fe1—C31—C32—C28 | −58.9 (3) | C6B—C7B—N1B—C8B | 173 (2) |
| O1—Co1—N1A—C7A | 3 (2) | C7B—N1B—C8B—C9B | 166 (2) |
| O1—Co1—N1A—C8A | 174.1 (15) | N1B—Co1—O1—C1B | 0.7 (16) |
| O1—Co1—N2A—C9A | 87.6 (18) | N1B—Co1—N2B—C9B | 18 (2) |
| O1—Co1—N2A—C10A | −85 (3) | N1B—Co1—N2B—C10B | −172 (3) |
| O1—Co1—N1B—C7B | −2 (3) | N1B—C8B—C9B—N2B | 36 (3) |
| O1—Co1—N1B—C8B | −170 (2) | C8B—C9B—N2B—Co1 | −36 (3) |
| O1—C1A—C2A—C3A | 178.4 (15) | C8B—C9B—N2B—C10B | 153 (2) |
| O1—C1A—C6A—C5A | −176.7 (15) | C9B—N2B—C10B—C11B | 172 (4) |
| O1—C1A—C6A—C7A | 0.4 (19) | N2B—Co1—N1B—C7B | 172 (3) |
| O1—C1B—C2B—C3B | −180 (2) | N2B—Co1—N1B—C8B | 4 (3) |
| O1—C1B—C6B—C5B | 179 (2) | N2B—C10B—C11B—C12B | 179 (3) |
| O1—C1B—C6B—C7B | 4 (3) | N2B—C10B—C11B—C16B | 2 (6) |
| O2—Co1—O1—C1A | −173.3 (10) | C10B—C11B—C12B—C13B | 179 (3) |
| O2—Co1—O1—C1B | −167.0 (13) | C10B—C11B—C16B—O2 | −2 (6) |
| O2—Co1—N2A—C9A | 165.3 (14) | C10B—C11B—C16B—C15B | 179 (4) |
| O2—Co1—N2A—C10A | −7.2 (19) | C11B—C12B—C13B—C14B | 3 (3) |
| O2—Co1—N1B—C7B | 86 (4) | C12B—C11B—C16B—O2 | −179 (3) |
| O2—Co1—N1B—C8B | −83 (3) | C12B—C11B—C16B—C15B | 2 (5) |
| O2—Co1—N2B—C9B | −174 (2) | C12B—C13B—C14B—C15B | 0 (2) |
| O2—Co1—N2B—C10B | −4 (3) | C13B—C14B—C15B—C16B | −2 (3) |
| N4—C23—C24—Fe1 | 122.8 (4) | C14B—C15B—C16B—O2 | −178 (2) |
| N4—C23—C24—C25 | −177.9 (4) | C14B—C15B—C16B—C11B | 1 (4) |
| N4—C23—C27—Fe1 | −122.3 (4) | C16B—C11B—C12B—C13B | −3 (5) |
| N4—C23—C27—C26 | 178.0 (4) | C17—N3—C21—C20 | −3.2 (10) |
| N3—Co1—O1—C1A | 91.9 (10) | C17—C18—C19—C20 | −3.0 (8) |
| N3—Co1—O1—C1B | 98.2 (13) | C17—C18—C19—C22 | 173.5 (5) |
| N3—Co1—N1A—C7A | −93 (2) | C18—C19—C20—C21 | 2.0 (9) |
| N3—Co1—N1A—C8A | 78.5 (16) | C18—C19—C22—N4 | 30.4 (7) |

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| N3—Co1—N2A—C9A | −99.3 (14) | C18—C19—C22—O3 | −150.3 (5) |
| N3—Co1—N2A—C10A | 88.1 (19) | C19—C20—C21—N3 | 1.3 (11) |
| N3—Co1—N1B—C7B | −98 (3) | C20—C19—C22—N4 | −153.2 (5) |
| N3—Co1—N1B—C8B | 94 (3) | C20—C19—C22—O3 | 26.1 (7) |
| N3—Co1—N2B—C9B | −79 (2) | C21—N3—C17—C18 | 2.0 (8) |
| N3—Co1—N2B—C10B | 91 (3) | C22—N4—C23—Fe1 | 90.0 (5) |
| N3—C17—C18—C19 | 1.1 (9) | C22—N4—C23—C24 | −3.0 (7) |
| C1A—C2A—C3A—C4A | 0.0 (18) | C22—N4—C23—C27 | 177.7 (4) |
| C1A—C6A—C7A—N1A | 2 (2) | C22—C19—C20—C21 | −174.7 (6) |
| C2A—C1A—C6A—C5A | 1.6 (17) | C23—N4—C22—O3 | −2.3 (7) |
| C2A—C1A—C6A—C7A | 178.8 (13) | C23—N4—C22—C19 | 177.0 (4) |
| C2A—C3A—C4A—C5A | −1.7 (16) | C23—C24—C25—Fe1 | −59.8 (3) |
| C3A—C4A—C5A—C6A | 3.4 (16) | C23—C24—C25—C26 | −0.9 (5) |
| C4A—C5A—C6A—C1A | −3.4 (18) | C24—C23—C27—Fe1 | 58.3 (3) |
| C4A—C5A—C6A—C7A | 179.4 (12) | C24—C23—C27—C26 | −1.4 (5) |
| C5A—C6A—C7A—N1A | 178.8 (16) | C24—C25—C26—Fe1 | −59.5 (3) |
| C6A—C1A—C2A—C3A | −0.1 (17) | C24—C25—C26—C27 | 0.1 (5) |
| C6A—C7A—N1A—Co1 | −3 (3) | C25—C26—C27—Fe1 | −59.7 (3) |
| C6A—C7A—N1A—C8A | −174.3 (16) | C25—C26—C27—C23 | 0.8 (5) |
| C7A—N1A—C8A—C9A | −151.1 (19) | C27—C23—C24—Fe1 | −57.9 (3) |
| N1A—Co1—O1—C1A | −0.7 (12) | C27—C23—C24—C25 | 1.4 (5) |
| N1A—Co1—N2A—C9A | −7.5 (15) | C28—C29—C30—Fe1 | 59.9 (3) |
| N1A—Co1—N2A—C10A | 180 (2) | C28—C29—C30—C31 | 0.5 (5) |
| N1A—C8A—C9A—N2A | −40.5 (17) | C29—C28—C32—Fe1 | −58.9 (3) |
| C8A—C9A—N2A—Co1 | 28.8 (17) | C29—C28—C32—C31 | −0.3 (5) |
| C8A—C9A—N2A—C10A | −157.9 (16) | C29—C30—C31—Fe1 | 59.5 (3) |
| C9A—N2A—C10A—C11A | −175 (2) | C29—C30—C31—C32 | −0.6 (5) |
| N2A—Co1—O1—C1A | −95.1 (19) | C30—C31—C32—Fe1 | 59.5 (3) |
| N2A—Co1—N1A—C7A | 171 (2) | C30—C31—C32—C28 | 0.6 (5) |
| N2A—Co1—N1A—C8A | −17.2 (16) | C32—C28—C29—Fe1 | 59.4 (3) |
| N2A—C10A—C11A—C12A | −170 (2) | C32—C28—C29—C30 | −0.1 (5) |