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Research Article

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Steric control over cobalt oxidation state and coordination geometry in Schiff base complexes: Synthesis, crystal structures, spectroscopic properties and urease inhibitory activity of tris-chelate Co(III) and bis-chelate Co(II) complexes

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Abstract

Two Schiff bases, 4-bromo-2-[(cyclopentylimino)methyl]phenol (HL¹) and 4-bromo-2-[(cyclohexylimino)methyl]phenol (HL²), derived from 4-bromosalicylaldehyde and cyclopentylamine or cyclohexylamine, have been used to prepare the cobalt complexes [Co(L¹)₃] (**1**) and [Co(L²)₂] (**2**). The compounds were characterized by IR and UV spectroscopy and single crystal X-ray diffraction. Although both complexes were prepared under the same air atmosphere, the steric demand of the *N*-alkyl substituent controls both the coordination chemistry and the oxidation state of the metal: the less hindered cyclopentyl group allows tris-chelation and gives a mononuclear octahedral Co(III) complex with three bidentate O,N-donor ligands, whereas the bulkier cyclohexyl group favors bis-chelation and affords a mononuclear tetrahedral Co(II) complex with two bidentate O,N-donor ligands. Complex **1** inhibits *jack bean* urease by 73% with an IC₅₀ of 32 μmol L⁻¹, while complex **2** exhibits 91% inhibition with an IC₅₀ of 8.2 μmol L⁻¹.

Keywords: Schiff base; Cobalt complex; Crystal structure; Steric effect; Urease inhibition

Introduction

Schiff bases are among the most versatile classes of organic ligands in coordination chemistry. They are readily prepared by condensation of primary amines with aldehydes or ketones and possess an azomethine (C=N) donor atom that can be combined with additional O-, N- or S-donor groups to generate chelating ligands with tunable steric and electronic properties. Schiff base ligands and their metal complexes have been widely investigated in catalysis, materials chemistry, molecular magnetism, chemical sensing and medicinal chemistry [1-3]. In particular, salicylaldehyde type Schiff bases, which are derived from salicylaldehyde and its substituted derivatives, form stable five- or six-membered chelate rings through the phenolic oxygen and the azomethine nitrogen and are therefore excellent building blocks for transition metal complexes with well-defined geometries [4-6]. Cobalt is especially attractive in this context because it readily adopts different oxidation states and coordination geometries. Cobalt(II) complexes are commonly four-, five- or six-coordinate and can be tetrahedral, square planar or octahedral, whereas cobalt(III) generally prefers six-coordinate octahedral geometry [7,8]. Schiff base cobalt complexes have shown antimicrobial, anticancer, antioxidant and enzyme-inhibitory activities [9,10]. The biological behavior of these complexes depends strongly on the metal center, the coordination environment, the lipophilicity of the ligand and the accessibility of the metal site to biological targets.

Urease is a nickel-containing metalloenzyme that catalyzes the hydrolysis of urea to ammonia and carbamate. The resulting increase in pH and release of ammonia are associated with several pathological conditions, including peptic ulcers, urinary stones, pyelonephritis and infections caused by *Helicobacter pylori* [11,12]. Urease inhibition is therefore an important therapeutic strategy, and a wide range of organic inhibitors, including hydroxamic acids, phosphorodiamidates and thiosemicarbazones, has been developed [13-15]. Metal complexes have emerged as promising alternatives because they can combine strong metal–ligand interactions with tunable redox and coordination properties. Schiff base cobalt complexes are particularly interesting in this context, since their coordination geometry and steric environment can be systematically modified by the ligand periphery [16].

In the present work, we exploit the different steric demands of cyclopentyl and cyclohexyl substituents to control the coordination chemistry of cobalt Schiff base complexes derived from 4-bromosalicylaldehyde. The less hindered cyclopentyl ligand gives the tris-chelate Co(III) complex $[\text{Co}(\text{L}^1)_3]$ (**1**), whereas the more hindered cyclohexyl ligand affords the bis-chelate Co(II) complex $[\text{Co}(\text{L}^2)_2]$ (**2**). Importantly, both syntheses were carried out under the same air atmosphere, yet the two products contain cobalt in different oxidation states. This observation identifies steric control of the metal oxidation state, rather than simple control of the metal-to-ligand ratio, as the central novelty of the present study. Their urease inhibitory activities were also measured.

Experimental

Materials and physical measurements

4-Bromosalicylaldehyde, cyclopentylamine, cyclohexylamine, and cobalt nitrate hexahydrate were commercially available and used as received without further purification. All solvents were of analytical grade. Elemental analyses (C, H, N) were performed on a Perkin-Elmer 2400 analyzer. Infrared spectra were recorded from KBr pellets on a Bruker spectrometer in the 4000–400 cm^{-1} region. Solution UV–Vis spectra were recorded on a Shimadzu UV-2550 spectrophotometer. Single crystal X-ray diffraction data were collected on a Bruker SMART CCD diffractometer using graphite-monochromated Mo $\text{K}\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$).

Synthesis of the Schiff bases HL^1 and HL^2

HL^1 was prepared by condensation of 4-bromosalicylaldehyde (0.20 g, 1.0 mmol) with cyclopentylamine (0.085 g, 1.0 mmol) in methanol (30 mL) under reflux. HL^2 was obtained analogously from 4-bromosalicylaldehyde and cyclohexylamine (0.099 g, 1.0 mmol). The yellow Schiff bases were collected by filtration and used directly for complexation. The formulations of the ligands are consistent with the crystal structures of the corresponding cobalt complexes: $\text{HL}^1 = \text{C}_{12}\text{H}_{14}\text{BrNO}$, $\text{HL}^2 = \text{C}_{13}\text{H}_{16}\text{BrNO}$.

Synthesis of $[\text{Co}(\text{L}^1)_3]$ (**1**) and $[\text{Co}(\text{L}^2)_2]$ (**2**)

Complex **1** was synthesized by reaction of $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (29 mg, 0.10 mmol) with HL^1 (27 mg, 0.10 mmol) in methanol (15 mL) under reflux in air. After cooling, the solution was filtered and left to evaporate slowly at room temperature. Brown block crystals of **1** suitable for X-ray diffraction were obtained. Complex **2** was prepared in the same manner

using HL² (28 mg, 0.10 mmol) in place of HL¹, also in air, affording brown block crystals of **2**.

Complex 1: Yield 71% based on HL¹. Anal. calcd for C₃₆H₃₉Br₃CoN₃O₃: C 50.26, H 4.57, N 4.88%. Found: C 50.05, H 4.63, N 4.81%. IR data (KBr, cm⁻¹): 2953 (aliphatic ν_{C-H}), 1622 ($\nu_{C=N}$), 1582, 1512 ($\nu_{C=C}$), 1452, 1425 (δ_{C-H}), 1393, 1333, 1292, 1244 (ν_{C-O}), 1177 (ν_{C-N}), 1128, 1059, 920, 852, 775, 604, 534, 459. UV-Vis (λ_{max} , nm): 203, 223, 251, 321, 346, 378.

Complex 2: Yield 63% based on HL². Anal. calcd for C₂₆H₃₀Br₂CoN₂O₂: C 50.26, H 4.87, N 4.51%. Found: C 50.38, H 4.82; N 4.43%. IR data (KBr, cm⁻¹): 2878 (aliphatic ν_{C-H}), 1643 ($\nu_{C=N}$), 1591, 1506 ($\nu_{C=C}$), 1456, 1422 (δ_{C-H}), 1339, 1292, 1240 (ν_{C-O}), 1177 (ν_{C-N}), 1128, 1065, 920, 851, 806, 779, 604, 536, 500, 447. UV-Vis (λ_{max} , nm): 222, 250, 266, 324, 375.

X-ray crystallography

Single crystals of the complexes suitable for X-ray diffraction analysis were selected and mounted on a Bruker Apex II CCD area-detector diffractometer equipped with Mo K α radiation ($\lambda = 0.71073$ Å). Diffraction data were collected at room temperature and corrected for Lorentz and polarization effects as well as for linear decay. A multi-scan absorption correction based on ω -scans was applied. Data collection and reduction were performed using the SMART and SAINT programs, respectively [17]. The crystal structures were solved by direct methods using SHELXT and subsequently refined by full-matrix least-squares methods on F^2 using SHELXL, with successive difference Fourier syntheses [18]. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed at calculated positions and refined using a riding model. Crystallographic data and selected structure refinement parameters are summarized in Table 1.

Urease inhibition assay

The assay mixture containing 75 μ L of *jack bean* urease (EC 3.5.1.5, *Canavalia ensiformis*) and 75 μ L of tested compounds with various concentrations (100, 50, 25, 12.5, 6.25, 3.12, 1.56, 0.78, 0.39, 0.20, 0.10, 0.05 μ mol L⁻¹; dissolved in 1 mL DMSO,

then diluted by water) was preincubated for 15 min on a 96-well assay plate. Acetohydroxamic acid was used as a reference, and VO(acac)₂ was assayed as comparison. Both compounds were carried out at the same concentration and with the same procedure as the above-mentioned compounds. Then 75 μ L of phosphate buffer at pH 6.8 containing phenol red (0.18 mmol L⁻¹) and urea (400 mmol L⁻¹) were added and incubated at 25 °C. The reaction time required for enough ammonium carbonate to form to raise the pH of the phosphate buffer from 6.8 to 7.7 was measured by a BioTek Synergy HT microplate reader (560 nm) with the end-point being determined by the color change of phenol-red indicator.

Results and discussion

Synthesis and general characterization

The Schiff bases HL¹ and HL² were prepared by condensation of 4-bromosalicylaldehyde with cyclopentylamine and cyclohexylamine, respectively. Reaction of these ligands with Co(NO₃)₂·6H₂O in methanol under air afforded the cobalt complexes **1** and **2** as brown block crystals. The molecular structures determined by X-ray diffraction show that both complexes are mononuclear and that the Schiff base ligands coordinate in their monoanionic bidentate O,N-chelating form through the phenolic oxygen and the azomethine nitrogen. However, the metal-to-ligand ratio and the oxidation state of the metal are different in the two complexes: **1** contains three Schiff base ligands around a Co(III) center, while **2** contains only two Schiff base ligands around a Co(II) center. This difference originates from the steric demand of the *N*-alkyl substituent and is the key structural feature discussed below.

Crystal structure of [Co(L¹)₃] (**1**)

Molecular structure of complex **1** is shown in Fig. 1. Selected bond lengths and angles are summarized in Table 2. The compound crystallizes in the monoclinic space group *P*2₁/*n* with *Z* = 4. The cobalt center is coordinated by three bidentate Schiff base ligands, each bound through one phenolate oxygen atom and one azomethine nitrogen atom, giving a CoN₃O₃ donor set and a distorted octahedral geometry. The three chelate rings adopt a meridional arrangement, as indicated by the *trans* angles O1–Co1–O3 = 172.97(18)°, O2–Co1–N1 = 175.6(2)° and N3–Co1–N2 = 175.5(2)°, which are close to

linear. The Co–O bond lengths in **1** are 1.883(4), 1.885(4) and 1.888(4) Å for Co1–O2, Co1–O1 and Co1–O3, respectively. The Co–N bond lengths are 1.926(5), 1.950(5) and 1.954(5) Å for Co1–N1, Co1–N3 and Co1–N2, respectively, which are comparable with those observed in Schiff base cobalt(III) complexes [19,20]. These values are typical of low-spin Co(III) in an octahedral N/O environment and indicate that the cobalt center has been oxidized from Co(II) to Co(III) during the reaction. The azomethine C=N bond lengths [C7=N1 1.293(8) Å, C19=N2 1.287(8) Å, C31=N3 1.287(7) Å] and the phenolate C–O bond lengths [O1–C2 1.303(7) Å, O2–C14 1.309(7) Å, O3–C26 1.303(7) Å] are consistent with the deprotonated, delocalized salicylaldimine form of the ligands.

Crystal structure of [Co(L²)₂] (**2**)

Molecular structure of complex **2** is shown in Fig. 2. Selected bond lengths and angles are summarized in Table 2. The compound also crystallizes in the monoclinic space group *P*2₁/*n* with *Z* = 4. Two bidentate Schiff base ligands coordinate to the cobalt center through their phenolate oxygen and azomethine nitrogen atoms, giving a CoN₂O₂ donor set. The coordination geometry is best described as distorted tetrahedral. The largest angles around cobalt are O2–Co1–O1 = 120.97(13)° and N2–Co1–N1 = 121.94(14)°, while the remaining angles lie in the range 96.58(13)–111.52(13)°. The calculated τ_4 parameter of 0.83 confirms a geometry close to tetrahedral but noticeably distorted [20]. The Co–O bond lengths in **2** are 1.897(3) and 1.917(3) Å for Co1–O2 and Co1–O1, respectively, and the Co–N bond lengths are 1.979(3) and 1.987(3) Å for Co1–N2 and Co1–N1, respectively, which are comparable with those observed in Schiff base cobalt(III) complexes [21,22]. These distances are slightly longer than those in **1**, consistent with the presence of Co(II) rather than Co(III). The azomethine C=N distances [C7=N1 1.288(5) Å and C20=N2 1.299(5) Å] and the phenolate C–O distances [O1–C2 1.309(5) Å and O2–C15 1.311(5) Å] again confirm the monoanionic bidentate coordination mode of the Schiff base ligands.

Steric effects and structural comparison

The most important difference between the two complexes is the number of coordinated Schiff base ligands and the resulting oxidation state of the cobalt center. In **1**, the cyclopentyl substituent is relatively compact and allows three bidentate ligands to coordinate, producing a six-coordinate CoN₃O₃ octahedron. In **2**, the cyclohexyl

substituent is sterically more demanding, and the formation of a third chelate ring is disfavored. The bis-chelate product is therefore obtained instead, giving a four-coordinate CoN_2O_2 center with a distorted tetrahedral geometry. Notably, both reactions were performed in air, so the different oxidation states are not caused by a change in the reaction atmosphere. The tris-chelate Co(III) complex **1** is obtained with the less hindered cyclopentyl ligand, whereas the bis-chelate Co(II) complex **2** is obtained with the more hindered cyclohexyl ligand. Similar coordination modes can be observed in the cobalt(II/III) complexes with Schiff base ligands containing cyclopentyl or cyclohexyl groups [23-26]. Thus, steric control of the metal oxidation state is therefore a key outcome of this work.

The structural differences are also reflected in the bond lengths. The Co–O and Co–N distances in **1** are shorter than those in **2**, in line with the higher oxidation state of cobalt in **1**. In addition, the octahedral tris-chelate arrangement in **1** leads to a more regular coordination sphere than the tetrahedral bis-chelate arrangement in **2**, as shown by the near-linear *trans* angles in **1** and the wider angular spread in **2**.

IR and UV-vis spectra

The IR spectra of **1** and **2** are consistent with the crystallographic results. Both complexes show strong bands in the 1622–1643 cm^{-1} region, which are assigned to the azomethine C=N stretching vibration [27]. The absence of a strong O–H stretching band in the expected 3300–3500 cm^{-1} region is consistent with deprotonation of the phenolic oxygen and formation of the monoanionic Schiff base ligands. The absorptions at 1292, 1177 and 1128 cm^{-1} in both spectra arise from C–O and C–N stretching and ring vibrations. The low-energy regions contain several bands associated with the metal–ligand skeleton: 604, 534 and 459 cm^{-1} for **1** and 604, 536, 500 and 447 cm^{-1} for **2** are assigned to Co–O and Co–N stretching vibrations. The presence of these bands confirms that the Schiff base ligands are coordinated to the cobalt center through the phenolate oxygen and azomethine nitrogen atoms.

The UV-vis spectra of **1** and **2** are dominated by intense absorptions in the ultraviolet region. Complex **1** exhibits absorption bands at 203, 223, 251, 321, 346 and 378 nm, while complex **2** shows bands at 222, 250, 266, 324 and 375 nm. The high-energy bands below 270 nm are attributed to $\pi \rightarrow \pi^*$ transitions of the aromatic rings and

the azomethine chromophore of the Schiff base ligands. The bands in the 320–380 nm region are assigned to $n \rightarrow \pi^*$ transitions of the azomethine groups and to ligand-to-metal charge-transfer (LMCT) transitions from the phenolate oxygen atoms to the cobalt center [28].

The spectra of the two complexes are qualitatively similar because both contain the same 4-bromosalicylaldehyde chromophore. However, the positions and relative intensities of the bands differ slightly, reflecting the different coordination environments and metal oxidation states. In particular, the higher-energy LMCT band of **1** is consistent with the higher charge of the Co(III) center, whereas the tetrahedral Co(II) center in **2** gives a somewhat different charge-transfer profile. No well-resolved $d-d$ transitions were observed in the visible region, probably because they are weak and obscured by the tail of the more intense charge-transfer bands.

Urease inhibitory activity

The urease inhibitory activities of the free Schiff bases and both complexes were evaluated against *jack bean* urease using the phenol red method. The two Schiff bases have very weak activity, with inhibition lower than 15%. However, both complexes have higher activity than the free Schiff bases. Complex **1** showed $73 \pm 3\%$ inhibition with $IC_{50} = 32 \pm 2 \mu\text{mol L}^{-1}$, whereas complex **2** showed $91 \pm 2\%$ inhibition with $IC_{50} = 8.2 \pm 1.3 \mu\text{mol L}^{-1}$. Complex **2** is therefore about four times more potent than complex **1** under the same assay conditions. The higher activity of **2** correlates with its tetrahedral Co(II) center, lower coordination number and more open metal environment, which may facilitate interaction with the dinuclear nickel active site of urease. The tris-chelate octahedral Co(III) complex **1** is more sterically shielded and less accessible, consistent with its higher IC_{50} value. These results suggest that the steric bulk of the Schiff base ligand can be used not only to control the coordination geometry and oxidation state of cobalt, but also to tune urease inhibitory potency.

Conclusion

Two new cobalt Schiff base complexes derived from 4-bromosalicylaldehyde have been synthesized and structurally characterized. The cyclopentyl-substituted ligand gives the tris-chelate octahedral Co(III) complex, whereas the more sterically demanding

cyclohexyl-substituted ligand affords the bis-chelate tetrahedral Co(II) complex. Because both complexes were prepared in air, the different metal oxidation states demonstrate that the steric bulk of the *N*-alkyl substituent controls not only the metal-to-ligand ratio and coordination geometry but also the oxidation state of the cobalt center. Complex **1** inhibits urease with $IC_{50} = 32 \pm 2 \mu\text{mol L}^{-1}$, while complex **2** is more active, with $IC_{50} = 8.2 \pm 1.3 \mu\text{mol L}^{-1}$. These results provide a useful structural basis for the design of cobalt-based Schiff base complexes as urease inhibitors.

Supplementary material

CCDC 2581256 and 2581257 contain the supplementary crystallographic data for the complexes. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44)1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

Funding Declaration

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Table 1. Crystallographic and experimental data for the complexes

Parameter	1	2
Empirical formula	C ₃₆ H ₃₉ Br ₃ CoN ₃ O ₃	C ₂₆ H ₃₀ Br ₂ CoN ₂ O ₂
Formula weight	860.36	621.27
Temperature (K)	298(2)	298(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> (Å)	11.7410(10)	9.8516(11)
<i>b</i> (Å)	20.3070(11)	27.1077(13)
<i>c</i> (Å)	15.4249(12)	9.9828(10)
α (°)	90	90
β (°)	107.2670(10)	98.7350(10)
γ (°)	90	90
Volume (Å ³)	3511.9(4)	2635.0(4)
<i>Z</i>	4	4
<i>D</i> _{calc} (g cm ⁻³)	1.627	1.566
μ (mm ⁻¹)	3.941	3.709
<i>F</i> (000)	1728	1252
Crystal size (mm)	0.20 × 0.18 × 0.17	0.17 × 0.15 × 0.15
θ range (°)	1.708–25.500	2.197–25.491
Reflections collected / unique	18583 / 6534	14009 / 4890
<i>R</i> _{int}	0.0784	0.0521
Data / restraints / parameters	6534 / 0 / 415	4890 / 0 / 298
Goodness-of-fit on <i>F</i> ²	1.012	1.009
<i>R</i> ₁ , <i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.0594, 0.1242	0.0473, 0.0898
<i>R</i> ₁ , <i>wR</i> ₂ (all data)	0.1364, 0.1562	0.0946, 0.1059
Largest diff. peak / hole (e Å ⁻³)	0.964 / -0.593	0.623 / -0.563

Table 2. Selected bond lengths (Å) and angles (°) for the complexes

Bond / angle	1	2
Co1–O1	1.885(4)	1.917(3)
Co1–O2	1.883(4)	1.897(3)
Co1–O3	1.888(4)	—
Co1–N1	1.926(5)	1.987(3)
Co1–N2	1.954(5)	1.979(3)
Co1–N3	1.950(5)	—
O1–C2 / O2–C14 or C15	1.303(7) / 1.309(7)	1.309(5) / 1.311(5)
N1=C7 / N2=C19 or C20	1.293(8) / 1.287(8)	1.288(5) / 1.299(5)
O1–Co1–O2	87.53(19)	120.97(13)
O1–Co1–O3	172.97(18)	—
O2–Co1–N1	175.6(2)	111.52(13)
N2–Co1–N1	93.5(2)	121.94(14)
N3–Co1–N2	175.5(2)	—
O2–Co1–N2	90.9(2)	97.24(14)
O1–Co1–N2	88.4(2)	110.41(13)

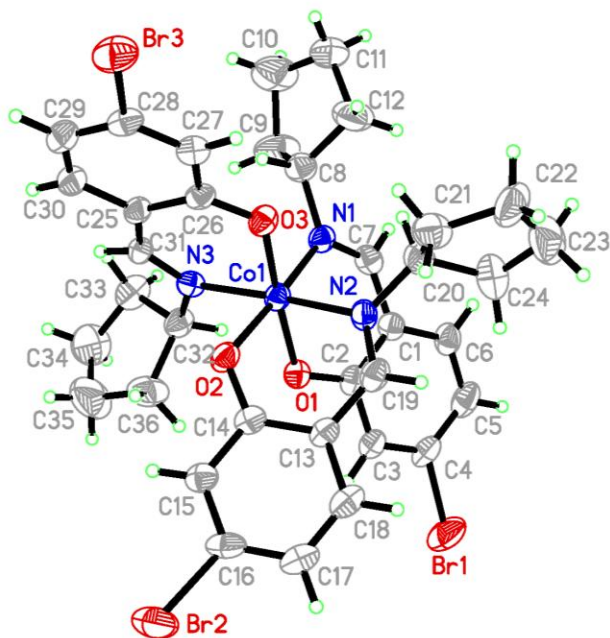


Figure 1. Molecular structure of complex 1. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

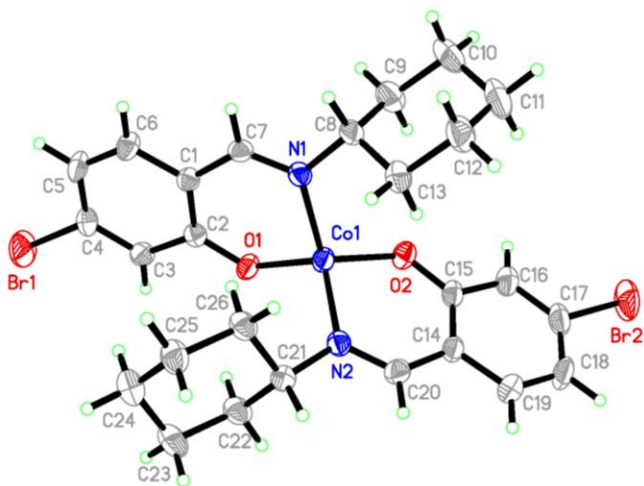


Figure 2. Molecular structure of complex 2. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.