

**{4-Chloro-2-[(*E*)-2-(dimethylamino)ethylimino-methyl]phenolato}thiocyanatocobalt(II)****San-Jun Peng<sup>a\*</sup> and Hai-Yun Hou<sup>b</sup>**<sup>a</sup>Department of Chemistry and Environmental Engineering, Changsha University of Science and Technology, Changsha 410076, People's Republic of China, and <sup>b</sup>College of Environment and Chemical Engineering, Xi'an University of Engineering Science and Technology, Xi'an 710048, People's Republic of China

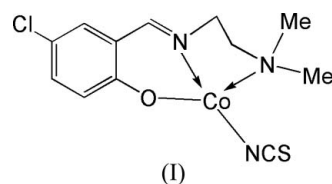
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**Key indicators**Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
Disorder in main residue  
*R* factor = 0.041  
*wR* factor = 0.114  
Data-to-parameter ratio = 16.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound,  $[\text{Co}(\text{C}_{11}\text{H}_{14}\text{ClN}_2\text{O})(\text{NCS})]$ , the  $\text{Co}^{\text{II}}$  atom, together with the Schiff base and the thiocyanate ligands, lie on a crystallographic mirror plane. The  $\text{Co}^{\text{II}}$  atom is four-coordinated by the imine N, amine N, and phenolate O atoms of the Schiff base ligand, and by the N atom of a thiocyanate anion, in a distorted square-planar coordination geometry.

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The design of *O/N*-donor multidentate ligands, their metallosupramolecular chemistry and the study of their physical properties have been of considerable recent interest (Robin & Fromm, 2006; Vicente & Arcas, 2005; Au-Yeung & Chan, 2004). A major goal in modern coordination chemistry is to synthesize molecules with a predefined geometry. Condensation of aromatic carbaldehydes with primary amines offers an easy and inexpensive way of forming a variety of polydentate Schiff base ligands, leading to the formation of a variety of complexes (Lewiński *et al.*, 2005; Salmon *et al.*, 2005; Xu *et al.*, 2005; Liu *et al.*, 2006). Pseudohalide anions ( $\text{N}_3^-$ ,  $\text{SCN}^-$ ,  $\text{CN}^-$ , *etc.*) are found to be versatile bridging ligands connecting several metal centres to form polynuclear complexes (Wang *et al.*, 2005; Muthiah *et al.*, 2005; Yu *et al.*, 2006; Zhang, Ai *et al.*, 2006; Peng *et al.*, 2006; Herres-Pawlis *et al.*, 2005; Vavra *et al.*, 2006; Pu *et al.*, 2005). These anions also act as terminal monodentate ligands in many cases (Zeng *et al.*, 2006; He *et al.*, 2004; Sun & Du, 2005; Ni *et al.*, 2005). We report here the synthesis and structure of the mononuclear cobalt(II) title complex, (I), in which 4-chloro-2-[(*E*)-2-(dimethylamino)ethyliminomethyl]phenolate acts as a tridentate Schiff base ligand, with the thiocyanate anion monodentate coordinating through nitrogen (Fig. 1 and Table 1).



In (I), the  $\text{Co}^{\text{II}}$  atom, together with the Schiff base and the thiocyanate ligands, lie on a crystallographic mirror plane. The  $\text{Co}^{\text{II}}$  atom is four-coordinated by the imine N, amine N, and phenolate O atoms of the Schiff base ligand, and by the N atom of the thiocyanate anion, forming a distorted square planar coordination geometry. The metal–ligand bond lengths are comparable to the values in other cobalt(II) complexes

(Zhou *et al.*, 2004; Iyere *et al.*, 2004; Zhang, Hu *et al.*, 2006; Yue *et al.*, 2005). In the crystal structure, molecules stack in columns down the *b* axis (Fig. 2).

### Experimental

5-Chloro-2-hydroxybenzaldehyde (0.5 mmol, 78.1 mg), *N,N*-dimethylethane-1,2-diamine (0.5 mmol, 44.2 mg), ammonium thiocyanate (0.5 mmol, 38.1 mg) and cobalt(II) acetate tetrahydrate (0.5 mmol, 12.4 mg) were stirred at 318 K in methanol (50 ml) for 30 min. The filtrate was kept in air for two weeks, depositing brown block-like crystals of (I). Analysis found: C 42.06, H 4.12, N 12.26%; calculated for C<sub>12</sub>H<sub>14</sub>ClCoN<sub>3</sub>OS: C 41.83, H 4.23, N 12.32%.

#### Crystal data

[Co(C <sub>11</sub> H <sub>14</sub> ClN <sub>2</sub> O)(NCS)]	Z = 4
<i>M<sub>r</sub></i> = 342.70	<i>D<sub>x</sub></i> = 1.562 Mg m <sup>-3</sup>
Orthorhombic, <i>Pnma</i>	Mo <i>K</i> α radiation
<i>a</i> = 19.145 (1) Å	<i>μ</i> = 1.50 mm <sup>-1</sup>
<i>b</i> = 6.732 (1) Å	<i>T</i> = 293 (2) K
<i>c</i> = 11.310 (2) Å	Block, brown
<i>V</i> = 1457.7 (3) Å <sup>3</sup>	0.16 × 0.11 × 0.08 mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer	12369 measured reflections
<i>ω</i> scans	1930 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	1516 reflections with <i>I</i> > 2σ( <i>I</i> )
<i>T<sub>min</sub></i> = 0.796, <i>T<sub>max</sub></i> = 0.890	<i>R<sub>int</sub></i> = 0.035
	<i>θ<sub>max</sub></i> = 28.5°

#### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.8561P]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.114$	( $\Delta/\sigma$ ) <sub>max</sub> < 0.001
<i>S</i> = 1.05	$\Delta\rho_{max} = 0.54 \text{ e \AA}^{-3}$
1930 reflections	$\Delta\rho_{min} = -0.78 \text{ e \AA}^{-3}$
115 parameters	
H-atom parameters constrained	

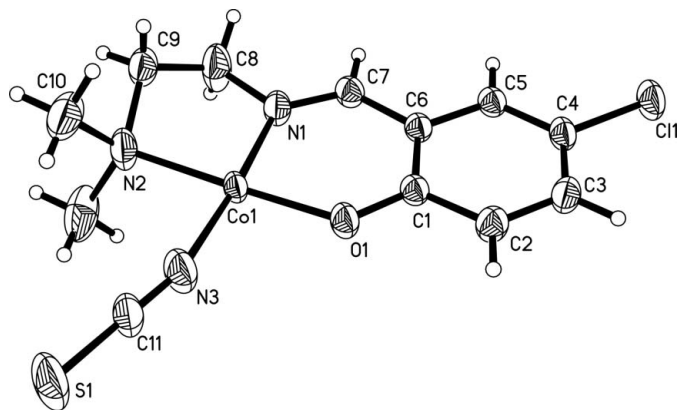
**Table 1**

Selected geometric parameters (Å, °).

Co1—O1	1.903 (3)	Co1—N3	1.929 (4)
Co1—N1	1.915 (3)	Co1—N2	2.060 (4)
O1—Co1—N1	93.20 (12)	O1—Co1—N2	177.91 (13)
O1—Co1—N3	91.45 (14)	N1—Co1—N2	84.72 (14)
N1—Co1—N3	175.36 (14)	N3—Co1—N2	90.64 (15)

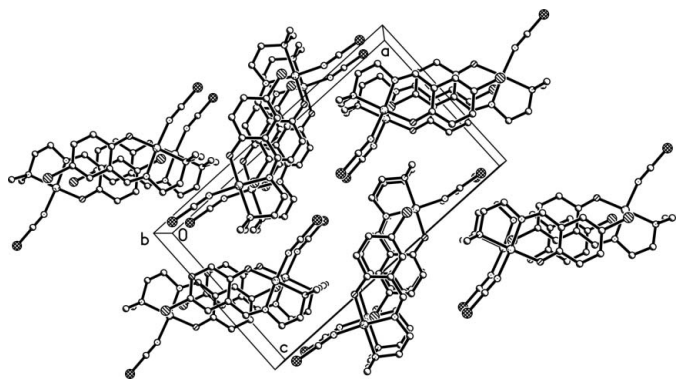
All H atoms bound to carbon were refined using a riding model, with C—H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for aromatic H atoms, and C—H = 0.96 Å and *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C) for methyl H atoms. The H atoms bound to C8 and C9 were also refined as riding, with C—H close to 0.96 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). Atoms C8 and C9 atoms are disordered across the mirror plane and their occupancy factors were fixed at 0.50.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.



**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms are shown as spheres of arbitrary radii.



**Figure 2**

Packing diagram for (I). H atoms have been omitted.

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