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Dichlorido{(*E*)-1-[1-(pyridin-2-yl)ethylidene]-thiosemicarbazonato-κ^3N,N',S}gallium(III)

Ying-Ju Fan,[a]* Jian-Ping Ma[b] and Zhong-Xi Sun[a]

[a]School of Chemistry and Chemical Engineering, Jinan University, Jinan 250022, People's Republic of China, and [b]Department of Chemistry, Shandong Normal University, Jinan 250014, People's Republic of China

Correspondence e-mail: wangle0315@mail.sdu.edu.cn

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Key indicators

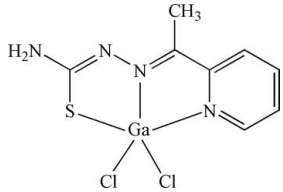
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.060
Data-to-parameter ratio = 14.8

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

Reaction of $GaCl_3$ with *E*)-1-[1-(pyridin-2-yl)ethylidene]thiosemicarbazide (petc) gives the title compound, $[Ga(C_8H_9N_4S)Cl_2]$. The petc ligand resembles a deprotonated enol, coordinated to Ga^{III} through one S and two N atoms. Two Cl atoms complete a distorted trigonal–bipyramidal coordination geometry around the Ga^{III} atom.

Comment

Schiff base ligands are currently being investigated as complexing agents (Dong, Wang, Ma & Huang, 2006). Coordination polymers with novel network connectivities can be synthesized by reaction of these ligands with transition metals (Dong, Wang, Ma, Zhao *et al.*, 2006). Reaction of the Schiff base ligand (*E*)-1-[1-(pyridin-2-yl)ethylidene]thiosemicarbazide (petc) with $GaCl_3$ forms the title compound, (I).



(I)

Compound (I) consists of Ga^{III} coordinated by one deprotonated petc ligand and two Cl atoms in a distorted trigonal-bipyramidal geometry (Fig. 1). In the petc ligand, the C6—N2 bond distance of 1.292 (3) Å shows clearly the C=N double-bond character of the Schiff base. The C8—N3 bond [1.320 (3) Å] is also short, while the C8—S1 bond [1.730 (2) Å] is relatively long, indicating that the coordinated petc ligand resembles a deprotonated enol (Sonja *et al.*, 1998). In the crystal structure, molecules of (I) are linked by N—H···N and N—H···S hydrogen bonds (Table 1).

Experimental

A methanol solution (10 ml) of $GaCl_3$ (17.7 mg, 0.10 mmol) was slowly diffused into an ethanol solution (10 ml) of (*E*)-1-[1-(pyridin-2-yl)ethylidene]thiosemicarbazide (19.4 mg, 0.10 mmol). Yellow single crystals of (I) were obtained after the solution was left to stand at room temperature for two weeks.

Crystal data

$[Ga(C_8H_9N_4S)Cl_2]$
M_r = 333.87
Monoclinic, $C2/c$
a = 16.248 (2) Å
b = 10.2777 (14) Å
c = 16.327 (2) Å
β = 118.871 (2)°
V = 2387.7 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.90 mm^{-1}
T = 298 (2) K
0.34 × 0.24 × 0.15 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.429, T_{max} = 0.647
6023 measured reflections
2159 independent reflections
1963 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.060
S = 1.04
2159 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···N3^{i}	0.86	2.23	3.083 (3)	173
N4—H4B···S1^{ii}	0.86	2.73	3.534 (2)	157

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

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and the group was allowed to rotate about its local threefold axis, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 Å or N—H = 0.86 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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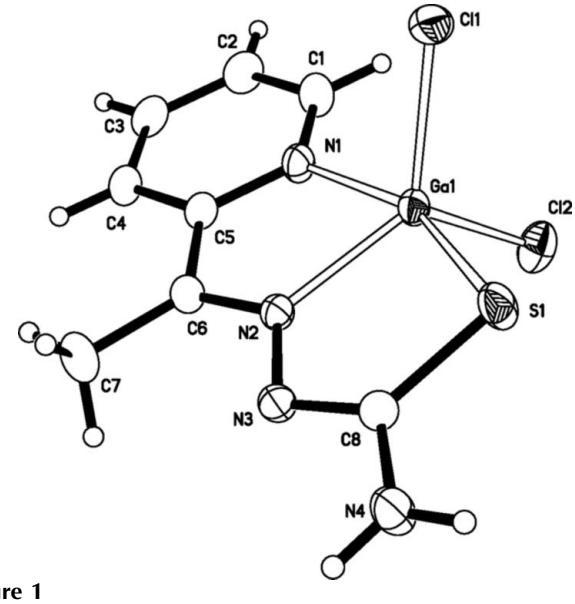

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

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