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STRUCTURE AND PROPERTIES OF N,N-DI-n-BUTYLDITHIOCARBAMATO-1, 2-DICYANOETHENE-1, 2-DITHIOLATO-GOLD(III)

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The crystal and molecular structure and some spectral data of the compound N,N-di-n-butylthiocarbamato-1, 2-dicyanoethene-1, 2-dithiolato-gold(III), Au₅S₂CN(C₄H₉)₂S₂C₂(CN)₂, are reported. The crystal structure has been determined from a three-dimensional single-crystal X-ray diffraction study. The orthorhombic cell, space group Pbcα, with a = 14.066(3), b = 28.980(2) and c = 9.192(2) Å, contains eight formula units. Intensity data were collected on an automatic diffractometer. The structural parameters were refined by full-matrix least-squares methods to a conventional R-factor of 0.047 for 1587 independent non-zero reflections. The structure determination proved the compound to be a mixed dithiocarbamato-dithiolato complex, Au(dtc)(mnt), (dtc = N,N-di-n-butyl-dithiocarbamate, mnt = maleonitriledithiolate = 1,2-dicyanoethene-1, 2-dithiolate), as expected from spectral data. The gold atom is in approximately square-planar coordination, however, deviations from mm₂ (C₂ᵥ) symmetry are considerable. Au—S bond distances in the dtc-moiety (2.329(5) and 2.324(5) Å) are significantly longer than those in the mnt-moiety (2.303(5) and 2.284(5) Å). The molecules are packed pairwise around inversion centres with relatively short intermolecular S–S distances.

INTRODUCTION

Recently the structure of the ionic compound Au(dtc)₂⁺Au(mnt)₂⁻ (dtc = N,N-di-n-butylthiocarbamate, mnt = maleonitriledithiolate = 1,2-dicyanoethene-1,2-dithiolate) has been reported. In the present paper we report the crystal structure and some spectral data of the isomeric mixed-ligand complex Au(dtc)(mnt). This complex belongs to a class of complexes of the type M(R₂dtc)(mnt)⁺ (z = 0, M = Ni, Cu, Au: z = —1, M = Ni, Cu, Pd, Pt: R₂dtc = N,N-di-alkylthiocarbamate = R₂NCS₂⁻) of which the given members have recently been synthesized and characterized. The structure determination presents the first X-ray analysis of a bis-complex involving both a 1,1- and a 1,2-dithiolato ligand.

EXPERIMENTAL

X-ray Crystal Structure Analysis

The compound Au(dtc)(mnt) was prepared as reported previously, and crystallizes as well-formed green plate-shaped crystals. Preliminary oscillation, rotation and Weissenberg photographs taken with Cu Kα radiation showed that the crystals belonged to the orthorhombic system. The systematic absences were found to be h0l absent for l = 2n + 1; 0kl absent for k = 2n + 1; hkl absent for h = 2n + 1; space group Pbcα. The unit cell dimensions were obtained from Pt-calibrated Weissenberg photographs. Least-squares adjustment of observed θ-values for 146 hkl and 84 h0l reflections (56° < Θ < 81°) resulted in a = 14.066(3) Å, b = 28.980(2) Å, c = 9.192(2) Å and Vc = 3747(1) Å³.

The calculated density of 1.92 g cm⁻³ for F.W. = 541.52 and Z = 8, agrees well with the value of 1.93(1) g cm⁻³ measured by flotation in a tetrachloromethane/iodomethane mixture. Intensity data were collected on an automatic diffractometer using the moving-counter moving-crystal method. Three series of intensity data were collected for a crystal of approximate dimensions 0.20 × 0.08 × 0.30 mm³ that was mounted with c along the φ-axis.

I. The octant hkl (all indices positive), scan speed 0.3°/min.
II. The octant hkl (all indices positive), scan speed 1.2°/min.
III. The octant hkl (h and k indices negative, l index positive), scan speed 0.3°/min.
For each of the series of measurements reciprocal
space was explored up to \( \sin \theta / \lambda = 0.60 \text{Å}^{-1} \) using
Zr-filtered Mo-radiation (\( \lambda = 0.71069 \text{Å}, \) linear
absorption coefficient \( \mu = 85.6 \text{cm}^{-1} \)). After every
fifteen reflections a reference reflection was measured
to detect and allow corrections to be made for slow
fluctuations in the primary beam. (Differences
between the intensities of the reference reflections
did not exceed 3\%). The intensity data were
corrected in the usual way for Lorentz and polariza-
tion effects and absorption. The latter correction
was calculated according to the Busing and Levy\(^5\)
scheme: \( 11 X_1 4 X_1 3 \) volume elements and \( 16 \)
accurately located boundary planes were taken into
account. (The maximum and minimum values of
the absorption factor in the intensities are 4.55 and
1.83 respectively). After absorption correction the
three series of intensity data were brought to a
common scale.

Comparison of the three series of intensity data
resulted in
\[ R_{it}^n = 0.040, \quad R_{it}^m = 0.048 \quad \text{and} \quad R_{it}^i = 0.059 \]
where \( \Sigma_{ij} \) being the square root of the intensity as
obtained from the \( ith \) measurement. \( \Sigma \) denotes the
summation over all reflections measured with non-
zero intensity. From an analysis of the deviations
between the observations of reflections that are in
common in the series I, II and III, variances for
individual reflections were calculated according to
the semi-empirical formula:
\[ \sigma_i = \sigma_c^2 + a_1 + a_2 \cdot I^1 + a_3 \cdot I + a_4 \cdot I^2 + a_5 \cdot \sin^2 \theta + a_6 \cdot \sin^4 \theta + a_7 \cdot I \cdot \sin^2 \theta + a_8 \cdot I \cdot \sin^4 \theta + a_9 \cdot I^1 \cdot \sin^2 \theta + a_{10} \cdot I \cdot \sin^2 \theta \]
where \( \sigma_c^2 \) is the vari-
ance as obtained from counting statistics and where
the constants \( a_i \) have the following values:
\(-43.10^{-2}, -51.10^{-3}, 20.10^{-4}, -20.10^{-9},
-17.10^0, 27.10^1, 30.10^{-1}, 57.10^0, 28.10^0 \quad \text{and} \quad 72.10^{-3}. \) (We do not attach a physical meaning to
the individual values of these constants.)

For the solution and the refinement of the
structure average intensity data were used. From the
1637 symmetry-independent reflections that had been measured above threshold, 50 reflections
were excluded from the structure refinement be-
cause they showed differences between the three
intensity measurements that exceeded 2.5 \( \sigma \).

Physical measurements
\(^1\)H NMR spectra of Au(dtc)(mnt) were recorded
at various temperatures ranging from 20°C to
-60°C, in CDC\(_1\)\(_3\) solution using a Varian HA-100
spectrometer operating at 100 MHz.

UV-spectra were measured in methylene chloride
solutions using a Unicam SP 700C spectropho-
tometer.

Structure determination and refinement
The positions of the gold and sulfur atoms were determined
from a three-dimensional Patterson-
synthesis. Three cycles of full-matrix least-squares
refinement of the positional parameters and iso-
tropic temperature factors of these atoms resulted
in a conventional \( R \)-factor of 0.135. From a gold
and sulfur atom phased Fourier-synthesis all
remaining non-hydrogen atoms were found. Least-
squares refinement of all non-hydrogen atoms with
anisotropic temperature factors reduced \( R \) to 0.050.

A difference-Fourier-synthesis computed at this
stage (using only terms for which \( \sin \theta / \lambda < 0.30 \text{Å}^{-1} \)
showed significant residual electron density (0.3 to
0.6 \( e \text{Å}^{-3} \)) in the neighbourhood of the carbon
atoms of the butyl chains. Since the difference-
synthesis did not allow accurate location of the
hydrogen atoms, they were placed at calculated
positions in such a way that the best fit with the
difference-synthesis was obtained. Several more
cycles of full-matrix least-squares refinement with
fixed hydrogen parameters reduced \( R \) to a final
value of 0.047. (According to Hamilton's test,\(^15\)
the improvement of the model after addition of
the hydrogen atoms is highly significant). In the
last refinement cycle (using 1587 reflections),
changes in parameters did not exceed 0.2 e.s.d.
The atomic scattering factors used in the least-
squares refinement were those of Au\(^+, \) S, \( ^{12} \)C and H. The Au\(^+\) and S scattering curves were
corrected for the anomalous scattering term \( \Delta f' \).

All pertinent data were taken from the Inter-
national Tables for X-ray Crystallography.\(^6\)

RESULTS AND DISCUSSION
Crystal Structure of Au(dtc)(mnt)
The atomic parameters are given in Tables I and
II. Bond distances and angles are presented in
Figure 1. Projections of the structure along the \( b \)
and \( c \) axes are given in Figures 2 and 3.

As is clearly shown in Figure 3, the structure
consists of distinct layers of molecules perpendicu-
lar to the \( b \)-axis. Neighbouring layers are separated
by van der Waals distances. Figure 2 illustrates the
pairwise packing of the molecules around inversion centres, within such layers. The shortest sulfur-sulfur contacts between one molecule and its neighbours are also shown in Figure 2 and tabulated in Table III. At least one of these contacts is short as compared with the normal S-S van der Waals distance of 3.70 Å, however, not so short that the Au(dtc)(mnt) structure can be interpreted as a clear case of ‘inter-donor atom bonding'.12,13 Nevertheless the Au(dtc)(mnt) structure is interesting in view of this suggestion.

Within one molecule, the gold atom is in approximately square-planar coordination, however, the deviations from mm2 (C2) symmetry are considerable. The interligand S-Au-S angles differ by 4.1° (95.0° and 99.1°) and the central part of the molecule deviates significantly from planarity. The dihedral angle between the weighted least-squares planes through the atoms of the dtc-ligand and the atoms of the mnt-ligand is 8.5°. Moreover, the gold atom is neither situated in one of these planes nor in the plane through the four sulfur atoms, but at distances of 0.084 Å, 0.102 Å and 0.035 Å from these planes.

Bond distances and angles within the dtc and mnt ligand of Au(dtc)(mnt) are essentially the same as those found in bis-(dtc) and bis-(mnt) complexes of gold.1,8’9,10 Some important dimensions of the 1.1-dithiolato cationic complex Au(dtc)2+, the 1.2-dithiolato anionic complex Au(mnt)2− and the neutral 1,1-dithiolato-1,2-dithiolato complex Au(dtc)(mnt), are tabulated in Table IV. In view of the discussions about metal-sulfur π-bonding in 1,1- and 1,2-dithiolato complexes of transition metals, we shall return to this topic in Section 3.1ii.

### TABLE I

Final atomic parameters (with e.s.d.) for Au(dtc)(mnt)

The estimated standard deviations are those obtained from the least squares refinement. The expression used for the anisotropic temperature factor is: $\exp \left( -\beta_{11} h^2 + \beta_{22} k^2 + \beta_{33} l^2 + 2\beta_{12} hl + 2\beta_{13} kl + 2\beta_{23} kl \right)$

<table>
<thead>
<tr>
<th>ATOM</th>
<th>X (Å)</th>
<th>Y (Å)</th>
<th>Z (Å)</th>
<th>$\beta_{11}$</th>
<th>$\beta_{22}$</th>
<th>$\beta_{33}$</th>
<th>$\beta_{12}$</th>
<th>$\beta_{13}$</th>
<th>$\beta_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>0.11650(4)</td>
<td>0.03400(2)</td>
<td>0.20826(6)</td>
<td>0.00502(3)</td>
<td>0.00074(1)</td>
<td>0.1097(8)</td>
<td>0.00011(2)</td>
<td>-0.00012(5)</td>
<td>-0.00028(3)</td>
</tr>
<tr>
<td>S(1)</td>
<td>0.2489(3)</td>
<td>0.0381(2)</td>
<td>0.1019(5)</td>
<td>0.0063(2)</td>
<td>0.0083(1)</td>
<td>0.0150(7)</td>
<td>-0.00001(1)</td>
<td>0.0014(4)</td>
<td>-0.0011(2)</td>
</tr>
<tr>
<td>S(2)</td>
<td>0.1575(3)</td>
<td>0.0643(1)</td>
<td>0.3637(5)</td>
<td>0.0070(3)</td>
<td>0.0009(1)</td>
<td>0.0132(7)</td>
<td>-0.00001(1)</td>
<td>0.0011(4)</td>
<td>-0.0003(2)</td>
</tr>
<tr>
<td>S(3)</td>
<td>0.0956(3)</td>
<td>-0.0494(1)</td>
<td>0.0284(5)</td>
<td>0.0060(3)</td>
<td>0.0012(1)</td>
<td>0.0144(7)</td>
<td>-0.00001(1)</td>
<td>0.0012(3)</td>
<td>-0.0011(2)</td>
</tr>
<tr>
<td>S(4)</td>
<td>-0.0159(3)</td>
<td>-0.0228(2)</td>
<td>0.3291(4)</td>
<td>0.0071(3)</td>
<td>0.0016(1)</td>
<td>0.0132(7)</td>
<td>-0.00007(1)</td>
<td>0.0013(3)</td>
<td>-0.0016(2)</td>
</tr>
<tr>
<td>N(1)</td>
<td>0.302(1)</td>
<td>0.114(1)</td>
<td>0.251(2)</td>
<td>0.005(1)</td>
<td>0.0001(1)</td>
<td>0.016(3)</td>
<td>0.00001(1)</td>
<td>-0.001(1)</td>
<td>0.001(1)</td>
</tr>
<tr>
<td>N(2)</td>
<td>-0.060(1)</td>
<td>-0.143(1)</td>
<td>-0.083(2)</td>
<td>0.001(1)</td>
<td>0.0001(1)</td>
<td>0.015(3)</td>
<td>-0.0001(1)</td>
<td>-0.001(1)</td>
<td>-0.0001(1)</td>
</tr>
<tr>
<td>C(1)</td>
<td>0.245(1)</td>
<td>0.077(1)</td>
<td>0.245(2)</td>
<td>0.006(1)</td>
<td>0.001(1)</td>
<td>0.013(3)</td>
<td>0.00001(1)</td>
<td>-0.003(1)</td>
<td>-0.0000(1)</td>
</tr>
<tr>
<td>C(2)</td>
<td>0.360(1)</td>
<td>0.120(1)</td>
<td>0.142(2)</td>
<td>0.006(1)</td>
<td>0.001(2)</td>
<td>0.019(3)</td>
<td>-0.0000(1)</td>
<td>0.002(2)</td>
<td>0.001(1)</td>
</tr>
<tr>
<td>C(3)</td>
<td>0.355(1)</td>
<td>0.155(1)</td>
<td>0.024(2)</td>
<td>0.010(2)</td>
<td>0.001(2)</td>
<td>0.015(3)</td>
<td>0.00000(1)</td>
<td>0.002(2)</td>
<td>0.001(1)</td>
</tr>
<tr>
<td>C(4)</td>
<td>0.430(1)</td>
<td>0.157(1)</td>
<td>-0.068(3)</td>
<td>0.011(2)</td>
<td>0.002(1)</td>
<td>0.026(5)</td>
<td>-0.0001(1)</td>
<td>0.008(2)</td>
<td>0.000(1)</td>
</tr>
<tr>
<td>C(5)</td>
<td>0.412(2)</td>
<td>0.191(1)</td>
<td>-0.205(3)</td>
<td>0.014(2)</td>
<td>0.005(1)</td>
<td>0.025(4)</td>
<td>-0.0001(1)</td>
<td>0.009(3)</td>
<td>0.003(2)</td>
</tr>
<tr>
<td>C(6)</td>
<td>0.292(1)</td>
<td>0.147(1)</td>
<td>0.373(2)</td>
<td>0.007(1)</td>
<td>0.0001(1)</td>
<td>0.010(2)</td>
<td>0.00001(1)</td>
<td>-0.001(1)</td>
<td>-0.0001(1)</td>
</tr>
<tr>
<td>C(7)</td>
<td>0.221(1)</td>
<td>0.185(1)</td>
<td>0.334(2)</td>
<td>0.008(1)</td>
<td>0.001(1)</td>
<td>0.015(3)</td>
<td>0.0001(1)</td>
<td>-0.003(2)</td>
<td>-0.001(1)</td>
</tr>
<tr>
<td>C(8)</td>
<td>0.204(2)</td>
<td>0.217(1)</td>
<td>0.465(2)</td>
<td>0.013(2)</td>
<td>0.002(2)</td>
<td>0.019(4)</td>
<td>0.0001(1)</td>
<td>-0.003(2)</td>
<td>-0.002(1)</td>
</tr>
<tr>
<td>C(9)</td>
<td>0.134(2)</td>
<td>0.253(1)</td>
<td>0.426(3)</td>
<td>0.017(3)</td>
<td>0.002(2)</td>
<td>0.032(6)</td>
<td>0.0003(1)</td>
<td>-0.003(3)</td>
<td>-0.004(1)</td>
</tr>
<tr>
<td>C(10)</td>
<td>-0.007(1)</td>
<td>-0.075(1)</td>
<td>0.086(2)</td>
<td>0.006(1)</td>
<td>0.001(1)</td>
<td>0.009(2)</td>
<td>-0.00001(1)</td>
<td>0.000(1)</td>
<td>0.000(1)</td>
</tr>
<tr>
<td>C(11)</td>
<td>-0.055(1)</td>
<td>-0.064(1)</td>
<td>0.210(2)</td>
<td>0.006(1)</td>
<td>0.001(1)</td>
<td>0.012(2)</td>
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<td>0.000(2)</td>
<td>-0.000(1)</td>
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<td>C(12)</td>
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<td>-0.114(1)</td>
<td>-0.004(2)</td>
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<td>0.001(1)</td>
<td>0.010(3)</td>
<td>-0.0001(1)</td>
<td>0.002(2)</td>
<td>0.000(1)</td>
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<tr>
<td>C(13)</td>
<td>-0.138(1)</td>
<td>-0.089(1)</td>
<td>0.248(2)</td>
<td>0.008(1)</td>
<td>0.002(1)</td>
<td>0.012(3)</td>
<td>-0.0001(1)</td>
<td>0.002(1)</td>
<td>-0.001(1)</td>
</tr>
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</table>
TABLE II

Hydrogen parameters

Unrefined results (see text). The first index of the numbering identifies the parent carbon atom. The isotropic temperature factors are the same as those of the parent carbon atom.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>B (Å²)</th>
</tr>
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<tbody>
<tr>
<td>H(21)</td>
<td>0.39</td>
<td>0.08</td>
<td>0.09</td>
<td>5.5</td>
</tr>
<tr>
<td>H(22)</td>
<td>0.45</td>
<td>0.13</td>
<td>0.19</td>
<td>5.5</td>
</tr>
<tr>
<td>H(31)</td>
<td>0.35</td>
<td>0.19</td>
<td>0.06</td>
<td>5.8</td>
</tr>
<tr>
<td>H(32)</td>
<td>0.29</td>
<td>0.15</td>
<td>-0.03</td>
<td>5.0</td>
</tr>
<tr>
<td>H(41)</td>
<td>0.50</td>
<td>0.17</td>
<td>-0.04</td>
<td>6.0</td>
</tr>
<tr>
<td>H(42)</td>
<td>0.44</td>
<td>0.12</td>
<td>-0.14</td>
<td>8.0</td>
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<tr>
<td>H(51)</td>
<td>0.46</td>
<td>0.19</td>
<td>-0.29</td>
<td>10.0</td>
</tr>
<tr>
<td>H(52)</td>
<td>0.41</td>
<td>0.23</td>
<td>-0.16</td>
<td>10.0</td>
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<tr>
<td>H(53)</td>
<td>0.34</td>
<td>0.19</td>
<td>-0.25</td>
<td>10.0</td>
</tr>
<tr>
<td>H(61)</td>
<td>0.36</td>
<td>0.61</td>
<td>0.40</td>
<td>4.5</td>
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<td>H(62)</td>
<td>0.27</td>
<td>0.13</td>
<td>0.47</td>
<td>4.5</td>
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<tr>
<td>H(71)</td>
<td>0.25</td>
<td>0.21</td>
<td>0.24</td>
<td>5.9</td>
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<tr>
<td>H(72)</td>
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<td>0.17</td>
<td>0.29</td>
<td>5.9</td>
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<tr>
<td>H(81)</td>
<td>0.27</td>
<td>0.23</td>
<td>0.50</td>
<td>7.0</td>
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<td>H(82)</td>
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<td>0.19</td>
<td>0.56</td>
<td>7.0</td>
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<tr>
<td>H(91)</td>
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<td>0.28</td>
<td>0.50</td>
<td>10.0</td>
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<tr>
<td>H(92)</td>
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<td>0.27</td>
<td>0.32</td>
<td>10.0</td>
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<td>H(93)</td>
<td>0.06</td>
<td>0.23</td>
<td>0.41</td>
<td>10.0</td>
</tr>
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</table>

TABLE III

Intermolecular sulfur-sulfur contacts in Au(dtc)(mnt)

<table>
<thead>
<tr>
<th>Contact</th>
<th>Distance (Å)</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.438(6)</td>
<td>distances between members of one pair (see text)</td>
</tr>
<tr>
<td>2</td>
<td>3.658(6)</td>
<td>distances between members of different pairs (see text)</td>
</tr>
<tr>
<td>3</td>
<td>3.804(6)</td>
<td>van der Waals contact</td>
</tr>
<tr>
<td>4</td>
<td>3.814(6)</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>3.915(6)</td>
<td></td>
</tr>
</tbody>
</table>

As mentioned above, the interligand S–Au–S angles differ by 4.1°. To investigate whether this irregular coordination of the gold atom by the dtc and mnt
ligand in Au(dtc)(mnt) is caused by intermolecular forces peculiar to the crystalline state, or whether it also exists in solution. $^1$H NMR spectra of the complex were recorded at various temperatures. No splitting of the N-alkyl proton resonances could be observed at temperatures as low as $-60^\circ$C. From this result no definitive conclusion is possible, however, since the absence of splitting might also be due to an undetectably small difference in the magnetic environments of the N-alkyl groups.$^{14}$

The ultraviolet spectrum of Au(dtc)(mnt) is clearly different from that of the isomeric complex Au(dtc)$_2^+$Au(mnt)$_2^-$ (Table V). The structure of the last compound in the solid state was proved to consist of two gold(III)-containing complex ions, Au(dtc)$_2^+$ and Au(mnt)$_2^-$. The spectral data show that the spectrum of this compound is best described as the sum-spectrum of the spectra of the compounds Au(dtc)$_2$Br and (C$_4$H$_9$)$_4$N Au(mnt)$_2$. This demonstrates that in solution the Au(dtc)$_2^+$Au(mnt)$_2^-$-complex is still ionic and shows no rearrangement reaction to Au(dtc)(mnt). Such a rearrangement reaction is shown by the Au(dtc)$_2^+$AuBr$_4^-$ complex, that in solution rearranges to Br$_2$Au(dtc).$^9$ Thus, the different stereochemical patterns found in the solid state for both the isomers with stoichiometric formula Au(dtc)(mnt), are retained in solution.

![Figure 1](https://example.com/figure1.png)

**Figure 1** Dimensions of Au(dtc)(mnt), with estimated standard deviations
FIGURE 2 Projection of the structure of Au(dtc)(mnt) along the \(b\)-axis. Butyl chains and CN groups are omitted.

TABLE IV
Bond distances and angles in Au(dtc)\(^{2+}\), Au(mnt)\(^{2-}\) and Au(dtc)(mnt)

<table>
<thead>
<tr>
<th>Complex</th>
<th>Bond Distances (Å)</th>
<th>Angles (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Au–S</td>
<td>S–C</td>
</tr>
<tr>
<td>Au(dtc)(^{2+})</td>
<td>2.333(7)</td>
<td>1.76(3)</td>
</tr>
<tr>
<td>Au(mnt)(^{2-})</td>
<td>2.309(4)</td>
<td>1.75(2)</td>
</tr>
<tr>
<td></td>
<td>(\mathrm{dtc-lig.})</td>
<td>2.327(5)</td>
</tr>
<tr>
<td></td>
<td>(\mathrm{mnt-lig.})</td>
<td>2.294(5)</td>
</tr>
</tbody>
</table>

All values are averages of symmetry-independent values.

\(^{a}\) Average values from references 1, 8, 9 and 10.

\(^{b}\) C–N distance and S–C–S angle in dtc, and C–C distance and S–C–C angle in mnt.

TABLE V
Electronic Spectra of Goldthiolato complexes in \(\text{CH}_2\text{Cl}_2\) solutions

<table>
<thead>
<tr>
<th>Complex</th>
<th>Band maxima (kK)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au(dtc)(_2)Br</td>
<td></td>
</tr>
<tr>
<td></td>
<td>36.1(38,700)</td>
</tr>
<tr>
<td>((\text{C}_2\text{H}_5)_2\text{NAu(mnt)})_2</td>
<td>38.4(46,600)</td>
</tr>
<tr>
<td>Au(dtc)(_2)Au(mnt)(_2)</td>
<td>37.6(81,400)</td>
</tr>
<tr>
<td>Au(dtc)(mnt)</td>
<td>38.7(23,700)</td>
</tr>
</tbody>
</table>

Band maxima in kK: parentheses indicate \(\epsilon\)(mole\(^{-1}\)cm\(^{-1}\)).
ACKNOWLEDGEMENTS

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REFERENCES AND NOTES

4. Recently the crystal structure determination of a mixed-ligand tris-complex, Fe(S₂CNet₂)₂(S₂C₂(CF₃)₂) has been reported. D. L. Johnstone, W. L. Rohrbough and W. Dew. Horrocks, Inorg. Chem. 10, 1474 (1971).
7. The weights used in the least-squares calculation of mean planes through groups of atoms are based upon the accuracy of the positional parameters.