metal-organic papers

2,2-Dimethoxy-1,3,2-dithiagermole-4,5-dicarbonitrile

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The title molecule, $[Ge(CH_3O)_2(C_4N_2S_2)]$, exhibits a non-planar geometry and the Ge atom is coordinated by two S and the O atoms of two methoxy groups. The five-membered ring adopts an envelope conformation. A mirror plane passes through the Ge atom, the methoxy groups and the mid-point of the C=C bond.

Comment

The title compound, (I), is another example of our newly synthesized germanium complexes (Akkurt *et al.*, 2003).

A mirror plane passes through the Ge atom, the methoxy groups and the mid-point of the C=C bond. The Ge—S distance is 2.2662 (8) Å, and the Ge—O distances are 1.945 (5) and 1.936 (4) Å. The O—Ge—O and S—Ge—S angles are in the range 108.95 (9)–110.95 (9)°. The average C—C bond length is 1.3945 (4) Å and the C≡N bond length is 1.143 (4) Å, in agreement with the literature values (Allen *et al.*, 1987; Liu *et al.*, 2002)

The five-membered ring is in an envelope conformation; the puckering parameters (Cremer & Pople, 1975) are Q_2 = 0.156 (2) Å and φ = 360.0 (9)°. The torsion angle S1—Ge1—O2—C4 is −51.07 (4)°, while S1—Ge1—O1—C3 is 51.98 (6)°.
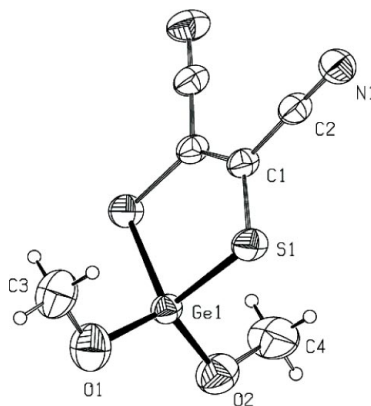

Figure 1
View of the title compound, (I), with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

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Experimental

The title compound was prepared according to the method of Akkurt *et al.* (2003).

Crystal data

[Ge(CH$_3$O)$_2$(C$_4$N$_2$S$_2$)]
$M_r = 272.86$
Orthorhombic, $Pnnm$
$a = 12.2960\,(8)$ Å
$b = 9.7463\,(7)$ Å
$c = 9.9583\,(7)$ Å
$V = 1193.41\,(14)$ Å^3
$Z = 4$
$D_x = 1.519$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 3800
  reflections
$\theta = 5.3$–$56.1°$
$\mu = 2.89$ mm^{-1}
$T = 293$ K
Block, colourless
$0.40 \times 0.36 \times 0.28$ mm

Data collection

Siemens SMART CCD area-
  detector diffractometer
ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
  $T_{min} = 0.350$, $T_{max} = 0.445$
6631 measured reflections

1469 independent reflections
1230 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 28.3°$
$h = -16 \rightarrow 11$
$k = -10 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.101$
$S = 1.03$
1469 reflections
67 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.053P)^2$
  $+ 0.6463P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.51$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

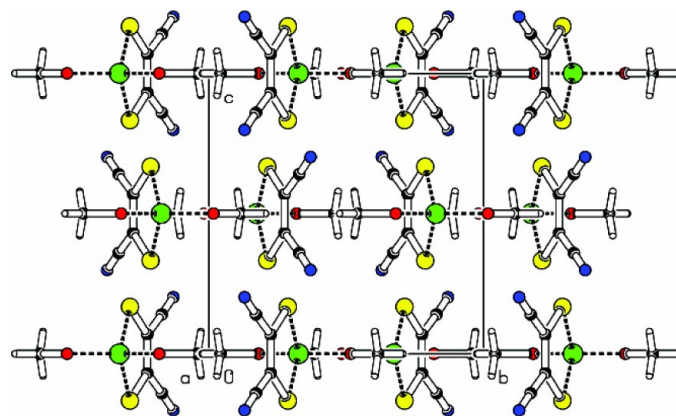|			
Ge1—S1	2.2662 (8)	O2—C4	1.467 (8)
Ge1—O1	1.945 (5)	N1—C2	1.143 (4)
Ge1—O2	1.936 (4)	C1—C2	1.425 (4)
S1—C1	1.743 (3)	C1—C1^i	1.364 (4)
O1—C3	1.437 (10)		
S1—Ge1—O1	110.95 (11)	Ge1—O2—C4	114.0 (4)
S1—Ge1—O2	108.95 (9)	S1—C1—C2	115.4 (2)
S1—Ge1—S1^i	94.74 (3)	S1—C1—C1^i	124.4 (2)
O1—Ge1—O2	119.5 (2)	C2—C1—C1^i	120.2 (2)
Ge1—S1—C1	97.60 (10)	N1—C2—C1	177.9 (3)
Ge1—O1—C3	114.6 (5)		
O1—Ge1—S1—C1	−123.77 (18)	O2—Ge1—O1—C3	180.00
O2—Ge1—S1—C1	102.70 (15)	S1—Ge1—O2—C4	−51.07 (4)
S1—Ge1—O1—C3	51.98 (6)	O1—Ge1—O2—C4	180.00

Symmetry code: (i) $x, y, -z$.

Figure 2
The packing of (I), viewed along the *a* axis.

The methyl H atoms were constrained to an ideal geometry (C—H = 0.96 Å), with $U_{iso}(H) = 1.5U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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