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# 2-(2,2-Dimethyl-1,3,2-dithiagermetan-4-ylidene)-malononitrile

**Mehmet Akkurt,[a] Sema Öztürk,[a]* Tevfik Rıza Kök[b] and Frank W. Heinemann[c]**

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, and [c]Institut für Anorganische Chemie, Universität Erlangen-Nürnberg, Egerlandstrasse 1, D-91058 Erlangen, Germany

Correspondence e-mail: ozturk@erciyes.edu.tr

**Key indicators**

Single-crystal X-ray study
*T* = 294 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.046
*wR* factor = 0.073
Data-to-parameter ratio = 19.9

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

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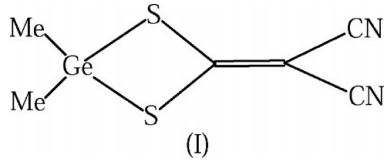
The title compound, $[Ge(CH_3)_2(C_4N_2S_2)]$, crystallizes in the space group *Pnma*, with two half-molecules in the asymmetric unit. The C atoms of the two methyl groups lie on the same mirror plane as the Ge atom and the –C═C– group. The S atoms and nitrile groups are each symmetry-related across the mirror plane. The structure is stabilized by intermolecular C—H···N hydrogen interactions.

## Comment

The title compound, (I), is another example of our newly synthesized Ge complexes (Akkurt *et al.*, 2003; Öztürk *et al.*, 2003). A view of (I) showing the atom-labelling scheme is shown in Fig. 1 and selected geometric parameters are given in Table 1.




(I)

The central Ge atom in the structure of (I) is coordinated by two S and two C atoms, with the Ge—S and Ge—C distances in agreement with the literature values (Akkurt *et al.*, 2003; Öztürk *et al.*, 2003).

There are two independent molecules, *A* and *B*, of similar conformation; half of each molecule is in the asymmetric unit of (I). The two methyl groups are not related by mirror symmetry, but the C atoms lie on the same mirror plane as the Ge atom and the –C═C– group. The S atoms and nitrile groups are each symmetry-related across the mirror plane.

The dithiagermetane rings are nearly planar, with maximum deviations of 0.156 (4) and 0.140 (4) Å for atom C3 in molecules *A* and *B*, respectively (*PARST*; Nardelli, 1995). The dihedral angle between the weighted least-squares planes of

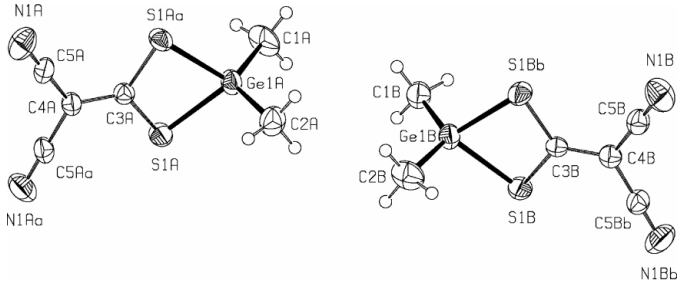



**Figure 1**
A view of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

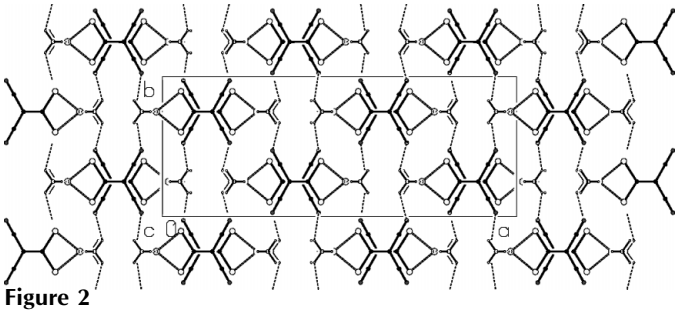



**Figure 2**
A view, along the *c* axis, of the packing and hydrogen bonding (dashed lines) in (I).

the dithiagermetane rings of molecules *A* and *B* is 13.19 (3)°.

The C—Ge—C and S—Ge—S angles are 123.1 (3) and 78.82 (3)°, respectively, in molecule *A*, and 124.3 (3) and 78.75 (3)°, respectively, in molecule *B*. The C—Ge—S angles are in the range 109.26 (12)–113.90 (16)° in molecule *A* and 109.96 (16)–112.39 (11)° in molecule *B*.

The structure of (I) is stabilized by two intermolecular C—H···N interactions, as detailed in Table 2 (Fig. 2).

## Experimental

The title compound was prepared according to the method described by Akkurt *et al.* (2003). Analysis calculated for $C_6H_6GeN_2S_2$: C 29.67, H 2.49, N 11.53, S 26.40%; found: C 29.71, H 2.51, N, 11.60, S 26.57%; m.p.: 553 K; IR ($\nu$, cm$^{-1}$): 2210 (C—N), 640 (C—S), 405 (Ge—S); $^1$H NMR ($\delta$, p.p.m.): 2.48; $^{13}$C NMR ($\delta$, p.p.m.): 13.46 ($CH_3$), 182.4 (C═C), 114.42 (CN).

*Crystal data*

$[Ge(CH_3)_2(C_4N_2S_2)]$
$M_r$ = 242.88
Orthorhombic, *Pnma*
$a$ = 25.1259 (19) Å
$b$ = 9.9284 (8) Å
$c$ = 7.5207 (4) Å
$V$ = 1876.1 (2) Å$^3$
$Z$ = 8
$D_x$ = 1.720 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 116 reflections
$\theta$ = 6.0–20.0°
$\mu$ = 3.65 mm$^{-1}$
$T$ = 294 (2) K
Block, colourless
0.18 × 0.08 × 0.07 mm

*Data collection*

Nonius KappaCCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min}$ = 0.560, $T_{max}$ = 0.784
25 208 measured reflections
2452 independent reflections
1413 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.074
$\theta_{max}$ = 28.5°
$h = -33 \rightarrow 33$
$k = -13 \rightarrow 13$
$l = -9 \rightarrow 9$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.073
$S$ = 1.05
2452 reflections
123 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 0.922P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.74 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ge1*A*—S1*A* | 2.2871 (9) | Ge1*B*—C2*B* | 1.933 (6) |
| Ge1*A*—C1*A* | 1.934 (6) | S1*A*—C3*A* | 1.736 (2) |
| Ge1*A*—C2*A* | 1.929 (5) | S1*B*—C3*B* | 1.731 (2) |
| Ge1*B*—S1*B* | 2.2846 (9) | N1*A*—C5*A* | 1.144 (5) |
| Ge1*B*—C1*B* | 1.905 (5) | N1*B*—C5*B* | 1.139 (5) |
| | | | |
| S1*A*—Ge1*A*—C1*A* | 113.90 (16) | Ge1*A*—S1*A*—C3*A* | 83.44 (12) |
| S1*A*—Ge1*A*—C2*A* | 109.26 (12) | Ge1*B*—S1*B*—C3*B* | 83.45 (12) |
| C1*A*—Ge1*A*—C2*A* | 123.1 (3) | S1*A*—C3*A*—C4*A* | 123.20 (12) |
| C1*B*—Ge1*B*—C2*B* | 124.3 (3) | N1*A*—C5*A*—C4*A* | 179.3 (4) |
| S1*B*—Ge1*B*—C1*B* | 112.39 (11) | S1*B*—C3*B*—C4*B* | 123.11 (12) |
| S1*B*—Ge1*B*—C2*B* | 109.96 (16) | N1*B*—C5*B*—C4*B* | 178.8 (4) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1*A*—H2···N1*B*$^{i}$ | 0.96 | 2.61 | 3.182 (5) | 119 |
| C2*B*—H11···N1*A*$^{ii}$ | 0.96 | 2.62 | 3.194 (5) | 119 |

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

All H atoms were positioned geometrically in their ideal positions (C—H = 0.96 Å) and refined using a riding model, with fixed individual displacement parameters [$U_{iso}$(H) = 1.5$U_{eq}$(C)].

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *EVALCCD* (Duisenberg *et al.*, 2003); data reduction: *EVALCCD*; 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).

## References

Akkurt, M., Öztürk, S., Kök, T. R. & Fun, H.-K. (2003). *Acta Cryst.* E**59**, m664–m665.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Öztürk, S., Akkurt, M., Kök, T. R. & Fun, H.-K. (2003). *Acta Cryst.* E**59**, m1018–m1019.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (2002). *SADABS*. Version 2.03. University of Göttingen, Germany.