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A new orthorhombic polymorph of 1,1'-selenobis(*N,N*-diethylsulfanecarbothioamide)

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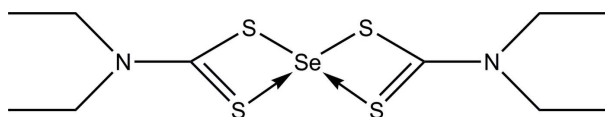
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 Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.038; wR factor = 0.076; data-to-parameter ratio = 18.7.

The title compound [systematic name: *N,N*-diethyl{[(diethylcarbamothioyl)sulfanyl]selenanyl}sulfanyl}carbothioamide], $\text{C}_{10}\text{H}_{20}\text{N}_2\text{S}_4\text{Se}$, crystallizes in a new form in the space group $Pca2_1$: the previously reported polymorph crystallizes in the space group $P2_12_12_1$. The new phase contains two independent molecules in the asymmetric unit. The Se atoms are tetracoordinated, with a distorted square-planar geometry. The ligands coordinate asymmetrically to the Se atoms, with one strong Se—S bond [range 2.2833 (13)–2.3041 (15) Å] and one weaker bond [range 2.7318 (14)–2.7873 (12) Å].

Related literature

For the characterization of the $P2_12_12_1$ polymorph, see: Conde *et al.* (1970); Husebye & Helland-Madsen (1970); Sugihara (1985). For the benzene solvate, see: Klapötke *et al.* (2008). For the synthesis of bis(*o*-formylphenyl)selenide acetal, see: Panda *et al.* (2001).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{20}\text{N}_2\text{S}_4\text{Se}$	$V = 3406.9 (7) \text{ \AA}^3$
$M_r = 375.52$	$Z = 8$
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 16.0338 (18) \text{ \AA}$	$\mu = 2.68 \text{ mm}^{-1}$
$b = 15.6376 (18) \text{ \AA}$	$T = 297 \text{ K}$
$c = 13.5880 (15) \text{ \AA}$	$0.27 \times 0.26 \times 0.19 \text{ mm}$

Data collection

Bruker SMART APEX diffractometer	17395 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	5896 independent reflections
$T_{\min} = 0.532$, $T_{\max} = 0.630$	4856 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	H-atom parameters constrained
$wR(F^2) = 0.076$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
$S = 0.94$	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
5896 reflections	Absolute structure: Flack (1983),
315 parameters	2755 Friedel pairs
1 restraint	Flack parameter: 0.007 (7)

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2326).

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supporting information

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A new orthorhombic polymorph of 1,1'-selenobis(*N,N*-diethylsulfanecarbothioamide)

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S1. Comment

In the crystal, the title compound contains two independent molecules in the asymmetric unit, with only slight differences in the bond distances and bond angles between the two molecules (Fig. 1). Both Se atoms are tetracoordinated with four S atoms arranged in a distorted square-planar geometry. The distortion of the coordination geometry is the result of the small bite and asymmetric coordination of the ligands. Each ligand coordinates strongly to the corresponding Se center through one S atom [range 2.2833 (13)–2.3041 (15) Å] and forms a weaker interaction through the second S atom [range 2.7318 (14)–2.7873 (12) Å].

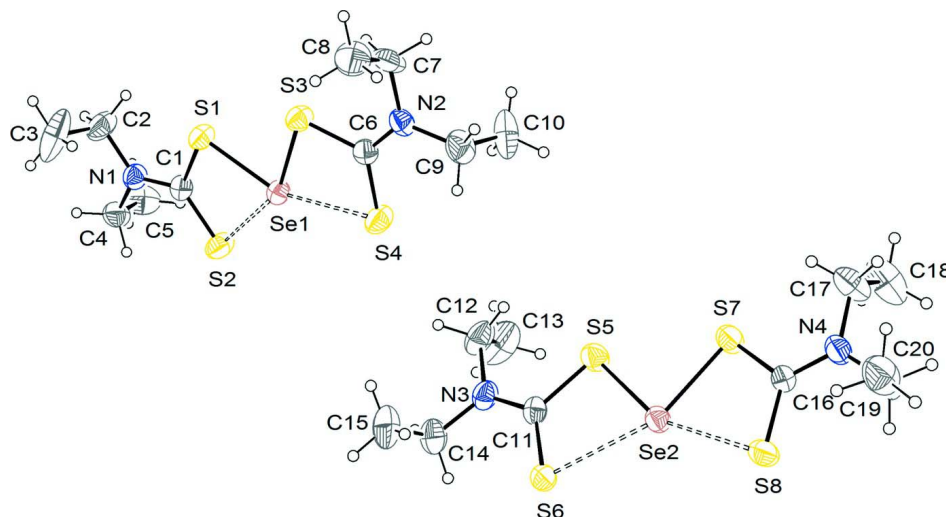
The molecular structure is similar to the ones published (Klapötke *et al.*, 2008; Sugihara, 1985; Husebye & Helland-Madsen, 1970; Conde *et al.*, 1970) in terms of structure parameters. Only one difference can be observed between the title compound and the benzene solvate (Klapötke *et al.*, 2008), the position of the Et groups from the ligands. While in the title compound the organic fragments from the same ligand are on the opposite sides of the coordination plane, in the benzene solvate they are on the same side.

S2. Experimental

The title compound was recovered as unreacted material after the reaction described for the synthesis of bis(*o*-formylphenyl)selenide acetal by Panda *et al.* (2001). Recrystallization from diethylether at -20°C over 72 h afforded suitable crystals.

S3. Refinement

All hydrogen atoms were placed in calculated positions using a riding model, with C—H = 0.96–0.97 Å and with $U_{\text{iso}} = 1.2$ or $1.5U_{\text{eq}}$ (C) for H. The methyl groups were allowed to rotate but not to tip.

**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

N,N-diethyl(((diethylcarbamothioyl)sulfanyl)selanyl)sulfanylcarbothioamide

Crystal data

$C_{10}H_{20}N_2S_4Se$

$M_r = 375.52$

Orthorhombic, $Pca2_1$

Hall symbol: $P\ 2c\ -2ac$

$a = 16.0338$ (18) Å

$b = 15.6376$ (18) Å

$c = 13.5880$ (15) Å

$V = 3406.9$ (7) Å³

$Z = 8$

$F(000) = 1536$

$D_x = 1.464$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 3414 reflections

$\theta = 2.4\text{--}21.5^\circ$

$\mu = 2.68$ mm⁻¹

$T = 297$ K

Block, orange

$0.27 \times 0.26 \times 0.19$ mm

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2001)

$T_{\min} = 0.532$, $T_{\max} = 0.630$

17395 measured reflections

5896 independent reflections

4856 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.046$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.4^\circ$

$h = -18 \rightarrow 19$

$k = -18 \rightarrow 17$

$l = -16 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.076$

$S = 0.94$

5896 reflections

315 parameters

1 restraint

0 constraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2)]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack (1983), 2755 Friedel
 pairs
 Absolute structure parameter: 0.007 (7)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.2875 (3)	0.5449 (3)	0.9917 (3)	0.0528 (11)
C2	0.2975 (4)	0.4729 (4)	1.1515 (5)	0.0899 (18)
H2A	0.2578	0.4655	1.2046	0.108*
H2B	0.3357	0.5184	1.1697	0.108*
C3	0.3460 (5)	0.3900 (6)	1.1355 (9)	0.172 (4)
H3A	0.3078	0.3448	1.1194	0.258*
H3B	0.3757	0.3756	1.1946	0.258*
H3C	0.3849	0.3976	1.0825	0.258*
C4	0.1673 (3)	0.4642 (4)	1.0520 (4)	0.0766 (16)
H4A	0.1626	0.4094	1.0849	0.092*
H4B	0.1542	0.4558	0.9830	0.092*
C5	0.1059 (3)	0.5257 (5)	1.0961 (5)	0.106 (2)
H5A	0.1192	0.5346	1.1642	0.159*
H5B	0.0506	0.5025	1.0907	0.159*
H5C	0.1086	0.5792	1.0616	0.159*
C6	0.5408 (3)	0.7480 (3)	0.7986 (4)	0.0540 (12)
C7	0.6744 (3)	0.7964 (4)	0.8659 (5)	0.0879 (18)
H7A	0.6486	0.7904	0.9301	0.105*
H7B	0.7018	0.8517	0.8639	0.105*
C8	0.7384 (4)	0.7283 (4)	0.8539 (6)	0.104 (2)
H8A	0.7117	0.6734	0.8543	0.156*
H8B	0.7777	0.7314	0.9071	0.156*
H8C	0.7671	0.7362	0.7925	0.156*
C9	0.6213 (4)	0.8503 (4)	0.7051 (5)	0.0860 (18)
H9A	0.5988	0.8232	0.6466	0.103*
H9B	0.6806	0.8588	0.6949	0.103*
C10	0.5794 (4)	0.9369 (4)	0.7195 (7)	0.130 (3)
H10A	0.5209	0.9287	0.7309	0.195*
H10B	0.5872	0.9711	0.6616	0.195*
H10C	0.6038	0.9653	0.7751	0.195*
C11	0.5475 (2)	0.7900 (3)	0.2665 (4)	0.0511 (11)
C12	0.4976 (4)	0.7850 (4)	0.4376 (4)	0.0868 (18)
H12A	0.5448	0.8218	0.4516	0.104*
H12B	0.4982	0.7387	0.4850	0.104*
C13	0.4186 (5)	0.8354 (5)	0.4500 (6)	0.136 (3)
H13A	0.4187	0.8829	0.4053	0.205*
H13B	0.4150	0.8561	0.5164	0.205*
H13C	0.3715	0.7993	0.4364	0.205*
C14	0.4681 (3)	0.6663 (3)	0.3214 (5)	0.0836 (18)
H14A	0.4498	0.6628	0.2535	0.100*
H14B	0.4193	0.6611	0.3632	0.100*

C15	0.5265 (5)	0.5937 (4)	0.3426 (7)	0.127 (3)
H15A	0.5748	0.5984	0.3011	0.190*
H15B	0.4987	0.5405	0.3297	0.190*
H15C	0.5433	0.5958	0.4103	0.190*
C16	0.7525 (3)	1.0497 (3)	0.0838 (3)	0.0551 (12)
C17	0.8189 (3)	1.1743 (4)	0.1579 (5)	0.093 (2)
H17A	0.8760	1.1945	0.1537	0.112*
H17B	0.8135	1.1422	0.2186	0.112*
C18	0.7628 (4)	1.2492 (4)	0.1626 (7)	0.127 (3)
H18A	0.7674	1.2815	0.1028	0.191*
H18B	0.7782	1.2846	0.2174	0.191*
H18C	0.7063	1.2302	0.1707	0.191*
C19	0.8443 (4)	1.1369 (4)	-0.0176 (5)	0.0847 (18)
H19A	0.8535	1.1982	-0.0209	0.102*
H19B	0.8079	1.1213	-0.0717	0.102*
C20	0.9255 (4)	1.0925 (4)	-0.0301 (5)	0.105 (2)
H20A	0.9640	1.1124	0.0188	0.158*
H20B	0.9473	1.1043	-0.0945	0.158*
H20C	0.9175	1.0320	-0.0228	0.158*
N1	0.2536 (3)	0.4961 (2)	1.0614 (3)	0.0615 (11)
N2	0.6087 (2)	0.7942 (2)	0.7896 (3)	0.0598 (10)
N3	0.5070 (3)	0.7493 (3)	0.3382 (3)	0.0637 (11)
N4	0.8028 (2)	1.1167 (3)	0.0749 (3)	0.0633 (11)
S1	0.38904 (8)	0.58095 (9)	1.01289 (10)	0.0616 (3)
S2	0.24068 (9)	0.57133 (9)	0.88656 (11)	0.0775 (4)
S3	0.52830 (8)	0.68637 (9)	0.90454 (10)	0.0632 (3)
S4	0.46334 (8)	0.74428 (10)	0.71483 (10)	0.0758 (4)
S5	0.58959 (8)	0.88991 (8)	0.29503 (10)	0.0669 (4)
S6	0.56063 (7)	0.75098 (8)	0.15308 (10)	0.0597 (3)
S7	0.70132 (9)	1.03237 (8)	0.19479 (10)	0.0675 (4)
S8	0.73695 (10)	0.97916 (9)	-0.00757 (10)	0.0794 (4)
Se1	0.39627 (3)	0.64649 (3)	0.86143 (4)	0.05358 (13)
Se2	0.64458 (3)	0.90662 (3)	0.13955 (4)	0.05516 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.053 (3)	0.051 (3)	0.055 (3)	0.006 (2)	0.009 (2)	0.002 (2)
C2	0.091 (4)	0.120 (5)	0.058 (4)	-0.010 (4)	-0.002 (4)	0.030 (4)
C3	0.183 (8)	0.161 (8)	0.171 (9)	0.073 (7)	0.025 (8)	0.103 (8)
C4	0.082 (4)	0.083 (4)	0.065 (4)	-0.028 (3)	0.004 (3)	0.002 (3)
C5	0.062 (4)	0.154 (7)	0.101 (5)	-0.020 (4)	0.015 (4)	-0.019 (5)
C6	0.061 (3)	0.052 (3)	0.049 (3)	0.004 (2)	0.010 (2)	-0.007 (2)
C7	0.094 (4)	0.098 (5)	0.071 (4)	-0.043 (4)	-0.007 (4)	-0.022 (4)
C8	0.068 (4)	0.120 (5)	0.123 (6)	-0.009 (4)	-0.018 (4)	0.013 (5)
C9	0.077 (4)	0.089 (5)	0.093 (5)	-0.022 (3)	0.020 (3)	0.005 (4)
C10	0.126 (6)	0.075 (5)	0.188 (9)	-0.001 (4)	0.034 (6)	0.053 (5)
C11	0.043 (2)	0.050 (3)	0.061 (3)	0.004 (2)	0.002 (2)	0.009 (2)

C12	0.108 (4)	0.098 (5)	0.055 (4)	0.016 (4)	0.023 (3)	0.017 (3)
C13	0.151 (6)	0.162 (8)	0.096 (6)	0.070 (6)	0.046 (5)	0.010 (5)
C14	0.083 (4)	0.076 (4)	0.092 (5)	-0.015 (3)	0.017 (3)	0.017 (3)
C15	0.170 (7)	0.070 (4)	0.141 (7)	0.010 (4)	-0.009 (6)	0.035 (5)
C16	0.063 (3)	0.045 (3)	0.057 (3)	-0.005 (2)	-0.004 (3)	0.002 (2)
C17	0.080 (4)	0.084 (4)	0.115 (6)	-0.024 (3)	0.012 (4)	-0.033 (4)
C18	0.088 (4)	0.090 (5)	0.204 (9)	-0.012 (4)	0.050 (5)	-0.042 (5)
C19	0.105 (5)	0.069 (4)	0.080 (4)	-0.035 (3)	0.016 (4)	0.006 (3)
C20	0.110 (5)	0.104 (5)	0.101 (5)	-0.028 (4)	0.036 (5)	-0.018 (4)
N1	0.063 (3)	0.064 (3)	0.058 (3)	-0.004 (2)	0.004 (2)	0.007 (2)
N2	0.062 (2)	0.054 (2)	0.064 (3)	-0.0117 (19)	0.010 (2)	-0.005 (2)
N3	0.072 (3)	0.066 (3)	0.053 (3)	0.001 (2)	0.013 (2)	0.009 (2)
N4	0.068 (3)	0.053 (2)	0.070 (3)	-0.014 (2)	0.003 (2)	-0.002 (2)
S1	0.0544 (7)	0.0774 (9)	0.0529 (8)	-0.0004 (6)	-0.0011 (6)	0.0125 (6)
S2	0.0656 (8)	0.1032 (10)	0.0637 (9)	-0.0092 (8)	-0.0120 (7)	0.0199 (8)
S3	0.0588 (7)	0.0774 (9)	0.0534 (8)	-0.0031 (6)	0.0000 (6)	0.0056 (7)
S4	0.0649 (8)	0.0990 (11)	0.0635 (10)	-0.0127 (7)	-0.0047 (7)	0.0243 (8)
S5	0.0789 (9)	0.0604 (8)	0.0614 (8)	-0.0046 (6)	0.0107 (7)	-0.0104 (7)
S6	0.0708 (7)	0.0561 (7)	0.0522 (7)	-0.0081 (6)	0.0056 (7)	-0.0016 (6)
S7	0.0809 (9)	0.0592 (8)	0.0624 (8)	-0.0170 (7)	0.0135 (7)	-0.0101 (7)
S8	0.1033 (10)	0.0782 (10)	0.0565 (9)	-0.0355 (8)	0.0075 (8)	-0.0147 (7)
Se1	0.0552 (3)	0.0547 (3)	0.0509 (3)	0.0034 (2)	0.0032 (3)	0.0038 (2)
Se2	0.0558 (3)	0.0524 (3)	0.0572 (3)	-0.0074 (2)	0.0025 (3)	-0.0011 (3)

Geometric parameters (Å, °)

C1—N1	1.332 (6)	C12—C13	1.501 (8)
C1—S2	1.666 (5)	C12—H12A	0.9700
C1—S1	1.747 (5)	C12—H12B	0.9700
C2—N1	1.458 (7)	C13—H13A	0.9600
C2—C3	1.527 (10)	C13—H13B	0.9600
C2—H2A	0.9700	C13—H13C	0.9600
C2—H2B	0.9700	C14—N3	1.457 (7)
C3—H3A	0.9600	C14—C15	1.499 (8)
C3—H3B	0.9600	C14—H14A	0.9700
C3—H3C	0.9600	C14—H14B	0.9700
C4—N1	1.476 (6)	C15—H15A	0.9600
C4—C5	1.501 (8)	C15—H15B	0.9600
C4—H4A	0.9700	C15—H15C	0.9600
C4—H4B	0.9700	C16—N4	1.327 (6)
C5—H5A	0.9600	C16—S8	1.680 (5)
C5—H5B	0.9600	C16—S7	1.738 (5)
C5—H5C	0.9600	C17—N4	1.467 (7)
C6—N2	1.312 (5)	C17—C18	1.478 (8)
C6—S4	1.685 (5)	C17—H17A	0.9700
C6—S3	1.744 (5)	C17—H17B	0.9700
C7—N2	1.479 (7)	C18—H18A	0.9600
C7—C8	1.488 (8)	C18—H18B	0.9600

C7—H7A	0.9700	C18—H18C	0.9600
C7—H7B	0.9700	C19—N4	1.457 (7)
C8—H8A	0.9600	C19—C20	1.485 (8)
C8—H8B	0.9600	C19—H19A	0.9700
C8—H8C	0.9600	C19—H19B	0.9700
C9—N2	1.460 (7)	C20—H20A	0.9600
C9—C10	1.523 (8)	C20—H20B	0.9600
C9—H9A	0.9700	C20—H20C	0.9600
C9—H9B	0.9700	S1—Se1	2.3020 (14)
C10—H10A	0.9600	S3—Se1	2.2833 (13)
C10—H10B	0.9600	S5—Se2	2.3041 (15)
C10—H10C	0.9600	S7—Se2	2.2930 (13)
C11—N3	1.332 (6)	S8—Se2	2.7343 (15)
C11—S6	1.671 (5)	S6—Se2	2.7873 (12)
C11—S5	1.746 (5)	S2—Se1	2.7788 (15)
C12—N3	1.470 (7)	S4—Se1	2.7318 (14)
N1—C1—S2	124.6 (3)	C12—C13—H13A	109.5
N1—C1—S1	116.6 (3)	C12—C13—H13B	109.5
S2—C1—S1	118.7 (3)	H13A—C13—H13B	109.5
N1—C2—C3	109.7 (6)	C12—C13—H13C	109.5
N1—C2—H2A	109.7	H13A—C13—H13C	109.5
C3—C2—H2A	109.7	H13B—C13—H13C	109.5
N1—C2—H2B	109.7	N3—C14—C15	112.2 (5)
C3—C2—H2B	109.7	N3—C14—H14A	109.2
H2A—C2—H2B	108.2	C15—C14—H14A	109.2
C2—C3—H3A	109.5	N3—C14—H14B	109.2
C2—C3—H3B	109.5	C15—C14—H14B	109.2
H3A—C3—H3B	109.5	H14A—C14—H14B	107.9
C2—C3—H3C	109.5	C14—C15—H15A	109.5
H3A—C3—H3C	109.5	C14—C15—H15B	109.5
H3B—C3—H3C	109.5	H15A—C15—H15B	109.5
N1—C4—C5	111.3 (5)	C14—C15—H15C	109.5
N1—C4—H4A	109.4	H15A—C15—H15C	109.5
C5—C4—H4A	109.4	H15B—C15—H15C	109.5
N1—C4—H4B	109.4	N4—C16—S8	122.7 (4)
C5—C4—H4B	109.4	N4—C16—S7	119.3 (4)
H4A—C4—H4B	108.0	S8—C16—S7	118.0 (3)
C4—C5—H5A	109.5	N4—C17—C18	114.4 (6)
C4—C5—H5B	109.5	N4—C17—H17A	108.7
H5A—C5—H5B	109.5	C18—C17—H17A	108.7
C4—C5—H5C	109.5	N4—C17—H17B	108.7
H5A—C5—H5C	109.5	C18—C17—H17B	108.7
H5B—C5—H5C	109.5	H17A—C17—H17B	107.6
N2—C6—S4	124.6 (4)	C17—C18—H18A	109.5
N2—C6—S3	118.4 (4)	C17—C18—H18B	109.5
S4—C6—S3	117.0 (3)	H18A—C18—H18B	109.5
N2—C7—C8	113.4 (5)	C17—C18—H18C	109.5

N2—C7—H7A	108.9	H18A—C18—H18C	109.5
C8—C7—H7A	108.9	H18B—C18—H18C	109.5
N2—C7—H7B	108.9	N4—C19—C20	113.4 (6)
C8—C7—H7B	108.9	N4—C19—H19A	108.9
H7A—C7—H7B	107.7	C20—C19—H19A	108.9
C7—C8—H8A	109.5	N4—C19—H19B	108.9
C7—C8—H8B	109.5	C20—C19—H19B	108.9
H8A—C8—H8B	109.5	H19A—C19—H19B	107.7
C7—C8—H8C	109.5	C19—C20—H20A	109.5
H8A—C8—H8C	109.5	C19—C20—H20B	109.5
H8B—C8—H8C	109.5	H20A—C20—H20B	109.5
N2—C9—C10	111.8 (5)	C19—C20—H20C	109.5
N2—C9—H9A	109.2	H20A—C20—H20C	109.5
C10—C9—H9A	109.2	H20B—C20—H20C	109.5
N2—C9—H9B	109.2	C1—N1—C2	122.8 (4)
C10—C9—H9B	109.2	C1—N1—C4	121.0 (4)
H9A—C9—H9B	107.9	C2—N1—C4	116.2 (4)
C9—C10—H10A	109.5	C6—N2—C9	121.3 (5)
C9—C10—H10B	109.5	C6—N2—C7	122.6 (4)
H10A—C10—H10B	109.5	C9—N2—C7	116.0 (4)
C9—C10—H10C	109.5	C11—N3—C14	121.3 (4)
H10A—C10—H10C	109.5	C11—N3—C12	122.7 (4)
H10B—C10—H10C	109.5	C14—N3—C12	116.0 (5)
N3—C11—S6	124.1 (4)	C16—N4—C19	121.9 (4)
N3—C11—S5	117.0 (4)	C16—N4—C17	121.4 (5)
S6—C11—S5	118.9 (3)	C19—N4—C17	116.7 (4)
N3—C12—C13	112.9 (6)	C1—S1—Se1	92.48 (16)
N3—C12—H12A	109.0	C6—S3—Se1	92.62 (16)
C13—C12—H12A	109.0	C11—S5—Se2	92.63 (16)
N3—C12—H12B	109.0	C16—S7—Se2	92.13 (16)
C13—C12—H12B	109.0	S3—Se1—S1	86.50 (5)
H12A—C12—H12B	107.8	S7—Se2—S5	87.07 (5)
S2—C1—N1—C2	178.6 (4)	C13—C12—N3—C11	92.4 (7)
S1—C1—N1—C2	-0.1 (6)	C13—C12—N3—C14	-86.8 (7)
S2—C1—N1—C4	-3.0 (7)	S8—C16—N4—C19	4.1 (7)
S1—C1—N1—C4	178.4 (4)	S7—C16—N4—C19	-177.0 (4)
C3—C2—N1—C1	-89.6 (7)	S8—C16—N4—C17	-176.3 (4)
C3—C2—N1—C4	91.9 (6)	S7—C16—N4—C17	2.5 (7)
C5—C4—N1—C1	-89.9 (6)	C20—C19—N4—C16	-87.4 (6)
C5—C4—N1—C2	88.7 (6)	C20—C19—N4—C17	93.0 (6)
S4—C6—N2—C9	2.5 (7)	C18—C17—N4—C16	-92.6 (7)
S3—C6—N2—C9	-177.1 (4)	C18—C17—N4—C19	87.0 (7)
S4—C6—N2—C7	179.0 (4)	N1—C1—S1—Se1	176.8 (3)
S3—C6—N2—C7	-0.5 (6)	S2—C1—S1—Se1	-2.0 (3)
C10—C9—N2—C6	84.1 (7)	N2—C6—S3—Se1	174.3 (3)
C10—C9—N2—C7	-92.7 (6)	S4—C6—S3—Se1	-5.3 (3)
C8—C7—N2—C6	88.1 (6)	N3—C11—S5—Se2	179.0 (3)

C8—C7—N2—C9	-95.2 (6)	S6—C11—S5—Se2	-0.6 (3)
S6—C11—N3—C14	-1.7 (7)	N4—C16—S7—Se2	-176.1 (4)
S5—C11—N3—C14	178.8 (4)	S8—C16—S7—Se2	2.8 (3)
S6—C11—N3—C12	179.2 (4)	C6—S3—Se1—S1	-174.55 (15)
S5—C11—N3—C12	-0.4 (6)	C1—S1—Se1—S3	-179.80 (16)
C15—C14—N3—C11	90.1 (7)	C16—S7—Se2—S5	176.19 (17)
C15—C14—N3—C12	-90.7 (6)	C11—S5—Se2—S7	-176.75 (15)
