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Dimethyl *N*-cyanodithioiminocarbonate

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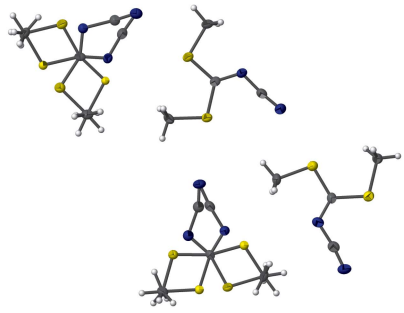
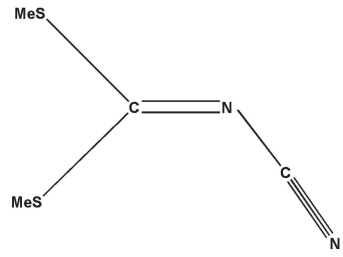
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_4H_6N_2S_2$, crystallizes with four independent molecules in the asymmetric unit. Two of the molecules are disordered about a pseudo twofold rotation axis. The mean values of the C—N bonds are 1.143 (5) Å for C≡N, 1.302 (5) Å for C=N and 1.341 (5) Å for the C—N single bond. In the crystal, molecules are linked *via* C—H···N hydrogen bonds, forming slabs parallel to the *bc* plane.

3D view



Chemical scheme



Structure description

Dimethyl cyaniminodithiocarbamate with its potential coordination power – two N and two S atoms – has been scarcely studied. To the best of our knowledge, only two crystalline structures incorporating this ligand are known, *viz. catena*-[bis(μ_2-chloro)bis[2,2-bis(methylthio)-*N*-cyanoazomethine]copper(I)] (Kojić-Prodić *et al.*, 1992) and dichloridobis(dimethyl *N*-cyanodithioiminocarbonate)cobalt (II) (Diop *et al.*, 2016). In our study of new compounds containing this ligand, we have undertaken reactions between the title compound, dimethyl cyanocarbonimidodithioate, and CrO_2Cl_2 expecting coordination to the Cr atom. However, only crystals of the title ligand were obtained and we report herein on its crystal structure.

The molecular structures of the four independent molecules (*A*, *B*, *C* and *D*) of the title compound are illustrated in Fig. 1. Two of the molecules, *B* and *D*, were found to have a small, but significant amount of disorder in the position of the sulfur atoms. The imido nitrogen and cyanide carbon are disordered in these two molecules, reflecting the orientation change of the methylthiol chains (Fig. 1). Bond lengths and angles in the major component and fully occupied molecules are in the expected ranges (Diop *et al.*, 2016) and show perfect planarity around the imido carbon atoms (average sum of angles is 359.99°).

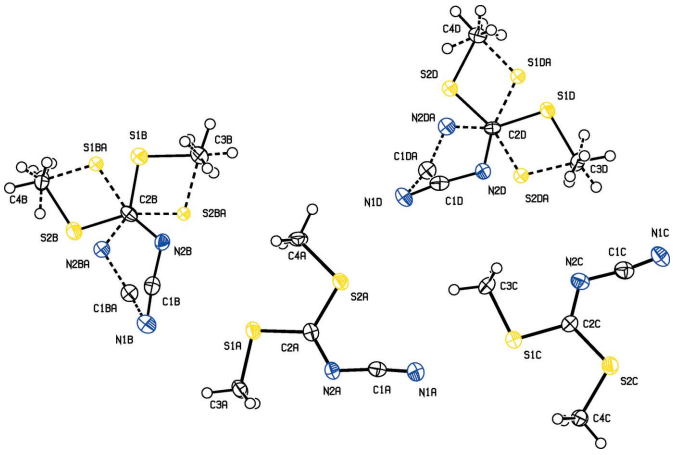


Figure 1
The molecular structure of the four independent molecules (*A*, *B*, *C* and *D*) of the title compound, with atom labelling. The minor components of the disordered molecules are shown with dashed bonds. Displacement ellipsoids are drawn at the 50% probability level.

In the crystal, C—H···N hydrogen bonds link the four molecules, forming slabs that lie parallel to (100); see Table 1 and Fig. 2.

Synthesis and crystallization

Dimethyl cyanocarbonimidodithioate was mixed in acetonitrile with CrO_2Cl_2 in a 1:1 ratio, giving a green solution. On slow evaporation of the solution at room temperature (303 K), a small number of colourless crystals of the title compound were obtained.

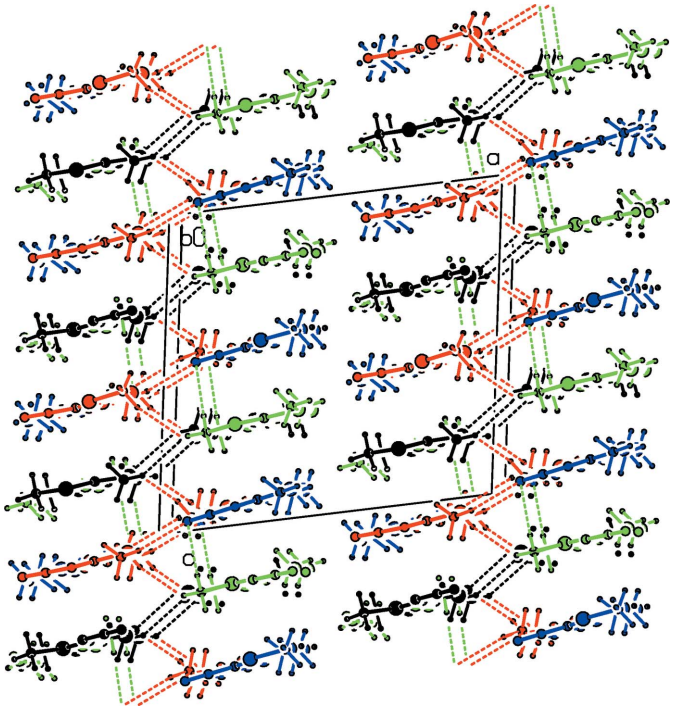


Figure 2
The crystal packing of the title compound, viewed approximately along the *b*-axis direction. The four independent molecules (*A* green, *B* black, *C* blue, *D* red) are linked *via* C—H···N hydrogen bonds (dashed lines; see Table 1).

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4*B*—H4*BB*···N1*B*^{i}	0.98	2.56	3.424 (5)	147
C3*D*—H3*DB*···N1*C*^{ii}	0.98	2.59	3.460 (5)	149
C4*D*—H4*DA*···N1*B*^{iii}	0.98	2.52	3.485 (6)	166

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+2, -y, -z+1$; (iii) $x+1, y, z$.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The disordered components of molecules B and D were refined with the occupancy of the disorder components summed to unity. The occupancy of each molecule was refined separately yielding a 0.92:0.08 and 0.90:0.10 ratio. Despite this small percentage, there was a significant improvement in the model upon inclusion of this disorder. The atomic displacement parameters of the inherent minor disordered component present in the cyanide nitrogen and carbon atoms were restrained to be similar to those of the associated major component.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_4H_6N_2S_2$
M_r	146.23
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	120
a, *b*, *c* (Å)	15.2211 (18), 12.2037 (15), 14.4716 (18)
β (°)	98.788 (5)
V (Å^3)	2656.6 (6)
Z	16
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.69
Crystal size (mm)	0.19 × 0.12 × 0.04
Data collection	
Diffractometer	Bruker Kappa X8 APEXIII
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.837, 0.983
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36932, 4868, 2986
R_{int}	0.105
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.106, 1.07
No. of reflections	4868
No. of parameters	331
No. of restraints	24
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.86, −0.37

Computer programs: *APEX3* (Bruker, 2015), *SAINT* (Bruker, 2015), *SHELXT* (Sheldrick, 2015*a*), *PLATON* (Spek, 2009), *SHELXL2014* (Sheldrick, 2015*b*) and *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

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Crystal data

$C_4H_6N_2S_2$
M_r = 146.23
Monoclinic, $P2_1/c$
a = 15.2211 (18) Å
b = 12.2037 (15) Å
c = 14.4716 (18) Å
β = 98.788 (5)°
V = 2656.6 (6) Å^3
Z = 16
$F(000)$ = 1216
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2731 reflections
θ = 2.5–24.0°
μ = 0.69 mm^{-1}
T = 120 K
Plate, colourless
0.19 × 0.12 × 0.04 mm

Data collection

Bruker Kappa X8 APEXIII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.33 pixels mm^{-1}
ω and φ–scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.837, T_{max} = 0.983
36932 measured reflections
4868 independent reflections
2986 reflections with $I > 2\sigma(I)$
R_{int} = 0.105
θ_{max} = 25.4°, θ_{min} = 1.4°
h = −18→18
k = −10→14
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.106
S = 1.07
4868 reflections
331 parameters
24 restraints
Primary atom site location: real-space vector search
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 2.1088P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
S1A	0.23225 (6)	0.34721 (9)	0.68456 (7)	0.0256 (3)	
S2A	0.42019 (6)	0.30624 (9)	0.66254 (7)	0.0247 (3)	
N1A	0.4260 (2)	0.0211 (3)	0.6710 (3)	0.0346 (9)	
N2A	0.3025 (2)	0.1506 (3)	0.6812 (2)	0.0240 (8)	
C1A	0.3717 (3)	0.0847 (4)	0.6751 (3)	0.0278 (10)	
C2A	0.3160 (2)	0.2562 (3)	0.6760 (3)	0.0212 (9)	
C3A	0.1432 (2)	0.2571 (3)	0.6995 (3)	0.0290 (10)	
H3AA	0.1318	0.2071	0.6461	0.044*	
H3AB	0.0895	0.3000	0.7037	0.044*	
H3AC	0.1593	0.2146	0.7571	0.044*	
C4A	0.4042 (3)	0.4514 (3)	0.6502 (3)	0.0282 (10)	
H4AA	0.3580	0.4664	0.5968	0.042*	
H4AB	0.4600	0.4860	0.6397	0.042*	
H4AC	0.3860	0.4812	0.7072	0.042*	
S1B	0.27136 (7)	0.84989 (10)	0.67592 (8)	0.0282 (3)	0.912 (2)
S2B	0.08290 (7)	0.80878 (10)	0.69178 (8)	0.0272 (3)	0.912 (2)
N2B	0.2056 (2)	0.6533 (3)	0.6944 (2)	0.0229 (8)	0.912 (2)
C1B	0.1383 (3)	0.5860 (4)	0.7034 (3)	0.0272 (12)	0.912 (2)
S1BA	0.1982 (7)	0.9020 (9)	0.6848 (7)	0.018 (3)*	0.088 (2)
S2BA	0.2706 (7)	0.6740 (8)	0.6838 (7)	0.015 (3)*	0.088 (2)
N2BA	0.106 (2)	0.732 (3)	0.702 (3)	0.023 (3)*	0.088 (2)
C1BA	0.095 (4)	0.607 (5)	0.705 (4)	0.026 (3)*	0.088 (2)
N1B	0.0844 (2)	0.5224 (3)	0.7107 (2)	0.0334 (9)	
C2B	0.1882 (2)	0.7574 (3)	0.6888 (3)	0.0223 (9)	
C3B	0.3641 (3)	0.7605 (3)	0.6732 (3)	0.0319 (11)	
H3BA	0.3789	0.7239	0.7338	0.048*	0.912 (2)
H3BB	0.4153	0.8033	0.6602	0.048*	0.912 (2)
H3BC	0.3488	0.7055	0.6240	0.048*	0.912 (2)
H3BD	0.3507	0.8053	0.6165	0.048*	0.088 (2)
H3BE	0.4164	0.7150	0.6692	0.048*	0.088 (2)
H3BF	0.3760	0.8085	0.7280	0.048*	0.088 (2)
C4B	0.0934 (3)	0.9533 (3)	0.6822 (3)	0.0319 (11)	
H4BA	0.1391	0.9799	0.7323	0.048*	0.912 (2)
H4BB	0.0365	0.9882	0.6875	0.048*	0.912 (2)
H4BC	0.1106	0.9714	0.6214	0.048*	0.912 (2)
H4BD	0.0941	1.0097	0.7305	0.048*	0.088 (2)
H4BE	0.0531	0.8940	0.6939	0.048*	0.088 (2)
H4BF	0.0730	0.9855	0.6206	0.048*	0.088 (2)
S1C	0.59095 (7)	−0.06797 (9)	0.58903 (7)	0.0273 (3)	
S2C	0.70112 (7)	−0.26439 (9)	0.57075 (8)	0.0274 (3)	
N1C	0.9006 (2)	−0.1351 (3)	0.5268 (2)	0.0347 (9)	
N2C	0.7551 (2)	−0.0593 (3)	0.5548 (2)	0.0280 (8)	
C1C	0.8319 (3)	−0.1058 (3)	0.5399 (3)	0.0286 (10)	
C2C	0.6907 (3)	−0.1234 (3)	0.5689 (3)	0.0205 (9)	
C3C	0.6149 (3)	0.0749 (3)	0.5822 (3)	0.0312 (10)	

H3CA	0.6665	0.0932	0.6289	0.047*	
H3CB	0.5633	0.1176	0.5944	0.047*	
H3CC	0.6280	0.0922	0.5196	0.047*	
C4C	0.5942 (2)	−0.3166 (3)	0.5872 (3)	0.0248 (10)	
H4CA	0.5770	−0.2846	0.6439	0.037*	
H4CB	0.5974	−0.3965	0.5936	0.037*	
H4CC	0.5500	−0.2973	0.5331	0.037*	
S1D	0.91532 (7)	0.31363 (9)	0.54631 (8)	0.0239 (3)	0.906 (2)
S2D	0.79660 (7)	0.50375 (9)	0.55930 (8)	0.0264 (3)	0.906 (2)
N2D	0.7486 (2)	0.2970 (3)	0.5728 (2)	0.0243 (9)	0.906 (2)
C1D	0.6687 (4)	0.3409 (4)	0.5792 (4)	0.0274 (13)	0.906 (2)
S1DA	0.9169 (6)	0.4230 (9)	0.5617 (7)	0.019 (3)*	0.094 (2)
S2DA	0.7999 (7)	0.2306 (9)	0.5670 (7)	0.019 (3)*	0.094 (2)
N2DA	0.748 (2)	0.437 (3)	0.571 (2)	0.026 (3)*	0.094 (2)
C1DA	0.663 (5)	0.384 (5)	0.569 (4)	0.028 (3)*	0.094 (2)
N1D	0.5982 (2)	0.3688 (3)	0.5835 (3)	0.0347 (9)	
C2D	0.8131 (2)	0.3638 (3)	0.5613 (3)	0.0190 (9)	
C3D	0.9013 (3)	0.1702 (3)	0.5593 (3)	0.0259 (10)	
H3DA	0.8916	0.1542	0.6233	0.039*	0.906 (2)
H3DB	0.9548	0.1319	0.5465	0.039*	0.906 (2)
H3DC	0.8499	0.1453	0.5152	0.039*	0.906 (2)
H3DD	0.9385	0.1711	0.6208	0.039*	0.094 (2)
H3DE	0.9311	0.2109	0.5146	0.039*	0.094 (2)
H3DF	0.8918	0.0942	0.5380	0.039*	0.094 (2)
C4D	0.8994 (2)	0.5620 (3)	0.5400 (3)	0.0306 (10)	
H4DA	0.9441	0.5511	0.5956	0.046*	0.906 (2)
H4DB	0.8914	0.6407	0.5277	0.046*	0.906 (2)
H4DC	0.9192	0.5265	0.4861	0.046*	0.906 (2)
H4DD	0.9463	0.6043	0.5780	0.046*	0.094 (2)
H4DE	0.8414	0.5832	0.5561	0.046*	0.094 (2)
H4DF	0.9004	0.5769	0.4736	0.046*	0.094 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1A	0.0203 (5)	0.0274 (6)	0.0291 (6)	0.0038 (5)	0.0044 (4)	0.0013 (5)
S2A	0.0189 (5)	0.0278 (6)	0.0274 (6)	0.0009 (5)	0.0036 (4)	0.0017 (5)
N1A	0.031 (2)	0.031 (2)	0.046 (2)	0.0022 (19)	0.0149 (18)	0.0002 (18)
N2A	0.0201 (18)	0.027 (2)	0.026 (2)	0.0028 (16)	0.0042 (14)	0.0004 (16)
C1A	0.026 (2)	0.026 (3)	0.032 (3)	−0.005 (2)	0.0073 (19)	0.001 (2)
C2A	0.020 (2)	0.028 (3)	0.014 (2)	0.0026 (18)	−0.0016 (16)	0.0002 (17)
C3A	0.019 (2)	0.034 (3)	0.034 (3)	0.0008 (19)	0.0062 (19)	−0.003 (2)
C4A	0.028 (2)	0.024 (2)	0.033 (3)	−0.0053 (19)	0.0051 (19)	0.008 (2)
S1B	0.0238 (6)	0.0277 (7)	0.0331 (7)	−0.0003 (5)	0.0045 (5)	0.0012 (6)
S2B	0.0227 (6)	0.0288 (8)	0.0311 (7)	0.0032 (5)	0.0070 (5)	0.0027 (6)
N2B	0.021 (2)	0.0211 (19)	0.026 (2)	0.0025 (17)	0.0009 (15)	0.0005 (16)
C1B	0.027 (3)	0.026 (3)	0.028 (2)	0.004 (2)	0.003 (2)	−0.002 (2)
N1B	0.027 (2)	0.036 (2)	0.038 (2)	−0.0022 (19)	0.0065 (17)	0.0002 (19)

C2B	0.016 (2)	0.030 (3)	0.020 (2)	−0.0035 (19)	0.0013 (17)	−0.0009 (19)
C3B	0.021 (2)	0.034 (3)	0.041 (3)	−0.002 (2)	0.0040 (19)	−0.001 (2)
C4B	0.030 (2)	0.027 (3)	0.039 (3)	0.009 (2)	0.009 (2)	0.001 (2)
S1C	0.0234 (6)	0.0266 (6)	0.0325 (6)	0.0013 (5)	0.0065 (5)	−0.0002 (5)
S2C	0.0254 (6)	0.0278 (6)	0.0294 (6)	0.0012 (5)	0.0054 (5)	−0.0028 (5)
N1C	0.023 (2)	0.044 (3)	0.038 (2)	0.0007 (18)	0.0068 (17)	0.0020 (19)
N2C	0.0251 (18)	0.031 (2)	0.029 (2)	−0.0032 (18)	0.0058 (15)	0.0031 (17)
C1C	0.025 (3)	0.032 (3)	0.027 (3)	−0.003 (2)	−0.003 (2)	0.003 (2)
C2C	0.025 (2)	0.021 (2)	0.013 (2)	0.0006 (18)	−0.0015 (17)	0.0003 (17)
C3C	0.033 (3)	0.018 (2)	0.043 (3)	0.003 (2)	0.008 (2)	0.003 (2)
C4C	0.026 (2)	0.025 (2)	0.025 (2)	−0.0024 (19)	0.0062 (18)	−0.0044 (19)
S1D	0.0183 (6)	0.0252 (7)	0.0289 (7)	0.0019 (5)	0.0057 (5)	0.0028 (5)
S2D	0.0203 (6)	0.0226 (7)	0.0369 (7)	0.0004 (5)	0.0063 (5)	0.0020 (6)
N2D	0.0216 (19)	0.023 (2)	0.029 (2)	0.0009 (17)	0.0066 (16)	0.0011 (17)
C1D	0.029 (3)	0.024 (3)	0.030 (3)	−0.006 (3)	0.006 (2)	0.003 (2)
N1D	0.019 (2)	0.038 (2)	0.047 (2)	0.0007 (18)	0.0083 (17)	0.0005 (19)
C2D	0.022 (2)	0.018 (2)	0.017 (2)	−0.0032 (18)	0.0034 (16)	0.0033 (17)
C3D	0.030 (2)	0.021 (2)	0.028 (2)	0.0073 (19)	0.0076 (18)	0.0015 (19)
C4D	0.024 (2)	0.027 (3)	0.041 (3)	−0.004 (2)	0.007 (2)	0.003 (2)

Geometric parameters (Å, º)

S1A—C2A	1.709 (4)	S1C—C2C	1.726 (4)
S1A—C3A	1.785 (4)	S1C—C3C	1.787 (4)
S2A—C2A	1.738 (4)	S2C—C2C	1.727 (4)
S2A—C4A	1.794 (4)	S2C—C4C	1.797 (4)
N1A—C1A	1.143 (5)	N1C—C1C	1.147 (5)
N2A—C2A	1.309 (5)	N2C—C2C	1.295 (5)
N2A—C1A	1.339 (5)	N2C—C1C	1.347 (5)
C3A—H3AA	0.9800	C3C—H3CA	0.9800
C3A—H3AB	0.9800	C3C—H3CB	0.9800
C3A—H3AC	0.9800	C3C—H3CC	0.9800
C4A—H4AA	0.9800	C4C—H4CA	0.9800
C4A—H4AB	0.9800	C4C—H4CB	0.9800
C4A—H4AC	0.9800	C4C—H4CC	0.9800
S1B—C2B	1.727 (4)	S1D—C2D	1.717 (4)
S1B—C3B	1.788 (4)	S1D—C3D	1.777 (4)
S2B—C2B	1.728 (4)	S2D—C2D	1.725 (4)
S2B—C4B	1.778 (4)	S2D—C4D	1.779 (4)
N2B—C2B	1.297 (5)	N2D—C2D	1.306 (5)
N2B—C1B	1.336 (6)	N2D—C1D	1.344 (7)
C1B—N1B	1.145 (6)	C1D—N1D	1.136 (6)
S1BA—C4B	1.707 (11)	S1DA—C2D	1.736 (10)
S1BA—C2B	1.773 (12)	S1DA—C4D	1.740 (11)
S2BA—C2B	1.625 (11)	S2DA—C2D	1.642 (11)
S2BA—C3B	1.797 (12)	S2DA—C3D	1.730 (11)
N2BA—C2B	1.32 (4)	N2DA—C2D	1.36 (3)
N2BA—C1BA	1.55 (7)	N2DA—C1DA	1.43 (7)

C1BA—N1B	1.05 (6)	C1DA—N1D	1.06 (7)
C3B—H3BA	0.9800	C3D—H3DA	0.9800
C3B—H3BB	0.9800	C3D—H3DB	0.9800
C3B—H3BC	0.9800	C3D—H3DC	0.9800
C3B—H3BD	0.9800	C3D—H3DD	0.9800
C3B—H3BE	0.9800	C3D—H3DE	0.9800
C3B—H3BF	0.9800	C3D—H3DF	0.9800
C4B—H4BA	0.9800	C4D—H4DA	0.9800
C4B—H4BB	0.9800	C4D—H4DB	0.9800
C4B—H4BC	0.9800	C4D—H4DC	0.9800
C4B—H4BD	0.9800	C4D—H4DD	0.9800
C4B—H4BE	0.9800	C4D—H4DE	0.9800
C4B—H4BF	0.9800	C4D—H4DF	0.9800
C2A—S1A—C3A	101.4 (2)	C2C—S1C—C3C	100.45 (19)
C2A—S2A—C4A	104.26 (19)	C2C—S2C—C4C	105.78 (19)
C2A—N2A—C1A	117.1 (3)	C2C—N2C—C1C	117.9 (4)
N1A—C1A—N2A	174.1 (4)	N1C—C1C—N2C	173.3 (5)
N2A—C2A—S1A	120.7 (3)	N2C—C2C—S1C	119.7 (3)
N2A—C2A—S2A	120.4 (3)	N2C—C2C—S2C	122.3 (3)
S1A—C2A—S2A	118.9 (2)	S1C—C2C—S2C	118.0 (2)
S1A—C3A—H3AA	109.5	S1C—C3C—H3CA	109.5
S1A—C3A—H3AB	109.5	S1C—C3C—H3CB	109.5
H3AA—C3A—H3AB	109.5	H3CA—C3C—H3CB	109.5
S1A—C3A—H3AC	109.5	S1C—C3C—H3CC	109.5
H3AA—C3A—H3AC	109.5	H3CA—C3C—H3CC	109.5
H3AB—C3A—H3AC	109.5	H3CB—C3C—H3CC	109.5
S2A—C4A—H4AA	109.5	S2C—C4C—H4CA	109.5
S2A—C4A—H4AB	109.5	S2C—C4C—H4CB	109.5
H4AA—C4A—H4AB	109.5	H4CA—C4C—H4CB	109.5
S2A—C4A—H4AC	109.5	S2C—C4C—H4CC	109.5
H4AA—C4A—H4AC	109.5	H4CA—C4C—H4CC	109.5
H4AB—C4A—H4AC	109.5	H4CB—C4C—H4CC	109.5
C2B—S1B—C3B	101.4 (2)	C2D—S1D—C3D	102.28 (18)
C2B—S2B—C4B	105.2 (2)	C2D—S2D—C4D	105.62 (19)
C2B—N2B—C1B	117.1 (4)	C2D—N2D—C1D	117.7 (4)
N1B—C1B—N2B	175.4 (5)	N1D—C1D—N2D	173.9 (5)
C4B—S1BA—C2B	106.3 (6)	C2D—S1DA—C4D	106.9 (6)
C2B—S2BA—C3B	105.2 (6)	C2D—S2DA—C3D	107.6 (6)
C2B—N2BA—C1BA	110 (4)	C2D—N2DA—C1DA	111 (4)
N1B—C1BA—N2BA	177 (5)	N1D—C1DA—N2DA	159 (6)
N2BA—C2B—S2BA	127.7 (19)	N2DA—C2D—S2DA	123.3 (16)
N2B—C2B—S1B	120.0 (3)	N2D—C2D—S1D	120.5 (3)
N2B—C2B—S2B	122.4 (3)	N2D—C2D—S2D	120.6 (3)
S1B—C2B—S2B	117.6 (2)	S1D—C2D—S2D	118.9 (2)
N2BA—C2B—S1BA	108.7 (19)	N2DA—C2D—S1DA	114.0 (16)
S2BA—C2B—S1BA	123.4 (6)	S2DA—C2D—S1DA	122.0 (5)
S1B—C3B—H3BA	109.5	S1D—C3D—H3DA	109.5

S1B—C3B—H3BB	109.5	S1D—C3D—H3DB	109.5
H3BA—C3B—H3BB	109.5	H3DA—C3D—H3DB	109.5
S1B—C3B—H3BC	109.5	S1D—C3D—H3DC	109.5
H3BA—C3B—H3BC	109.5	H3DA—C3D—H3DC	109.5
H3BB—C3B—H3BC	109.5	H3DB—C3D—H3DC	109.5
S2BA—C3B—H3BD	109.5	S2DA—C3D—H3DD	109.5
S2BA—C3B—H3BE	109.5	S2DA—C3D—H3DE	109.5
H3BD—C3B—H3BE	109.5	H3DD—C3D—H3DE	109.5
S2BA—C3B—H3BF	109.5	S2DA—C3D—H3DF	109.5
H3BD—C3B—H3BF	109.5	H3DD—C3D—H3DF	109.5
H3BE—C3B—H3BF	109.5	H3DE—C3D—H3DF	109.5
S2B—C4B—H4BA	109.5	S2D—C4D—H4DA	109.5
S2B—C4B—H4BB	109.5	S2D—C4D—H4DB	109.5
H4BA—C4B—H4BB	109.5	H4DA—C4D—H4DB	109.5
S2B—C4B—H4BC	109.5	S2D—C4D—H4DC	109.5
H4BA—C4B—H4BC	109.5	H4DA—C4D—H4DC	109.5
H4BB—C4B—H4BC	109.5	H4DB—C4D—H4DC	109.5
S1BA—C4B—H4BD	109.5	S1DA—C4D—H4DD	109.5
S1BA—C4B—H4BE	109.5	S1DA—C4D—H4DE	109.5
H4BD—C4B—H4BE	109.5	H4DD—C4D—H4DE	109.5
S1BA—C4B—H4BF	109.5	S1DA—C4D—H4DF	109.5
H4BD—C4B—H4BF	109.5	H4DD—C4D—H4DF	109.5
H4BE—C4B—H4BF	109.5	H4DE—C4D—H4DF	109.5

C1A—N2A—C2A—S1A	−179.2 (3)	C1C—N2C—C2C—S2C	0.9 (5)
C1A—N2A—C2A—S2A	−0.4 (5)	C3C—S1C—C2C—N2C	0.1 (4)
C3A—S1A—C2A—N2A	0.0 (4)	C3C—S1C—C2C—S2C	178.9 (2)
C3A—S1A—C2A—S2A	−178.8 (2)	C4C—S2C—C2C—N2C	−177.5 (3)
C4A—S2A—C2A—N2A	175.8 (3)	C4C—S2C—C2C—S1C	3.8 (3)
C4A—S2A—C2A—S1A	−5.4 (3)	C2D—N2DA—C1DA—N1D	149 (15)
C1B—N2B—C2B—S1B	−179.4 (3)	C1D—N2D—C2D—S1D	−176.5 (4)
C1B—N2B—C2B—S2B	−0.5 (5)	C1D—N2D—C2D—S2D	2.6 (5)
C1BA—N2BA—C2B—S2BA	−5 (4)	C1DA—N2DA—C2D—S2DA	−11 (4)
C1BA—N2BA—C2B—S1BA	180 (3)	C1DA—N2DA—C2D—S1DA	179 (3)
C3B—S2BA—C2B—N2BA	−176 (2)	C3D—S2DA—C2D—N2DA	−176.0 (17)
C3B—S2BA—C2B—S1BA	−0.5 (9)	C3D—S2DA—C2D—S1DA	−6.8 (8)
C3B—S1B—C2B—N2B	0.6 (4)	C3D—S1D—C2D—N2D	−3.6 (4)
C3B—S1B—C2B—S2B	−178.4 (2)	C3D—S1D—C2D—S2D	177.4 (2)
C4B—S2B—C2B—N2B	179.9 (3)	C4D—S2D—C2D—N2D	−178.8 (3)
C4B—S2B—C2B—S1B	−1.2 (3)	C4D—S2D—C2D—S1D	0.2 (3)
C4B—S1BA—C2B—N2BA	−9.0 (18)	C4D—S1DA—C2D—N2DA	−17.2 (17)
C4B—S1BA—C2B—S2BA	175.0 (5)	C4D—S1DA—C2D—S2DA	172.6 (6)
C1C—N2C—C2C—S1C	179.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4*B*—H4*BB*···N1*B*^{i}	0.98	2.56	3.424 (5)	147

C3*D*—H3*DB*···N1*C*^{ii}	0.98	2.59	3.460 (5)	149
C4*D*—H4*DA*···N1*B*^{iii}	0.98	2.52	3.485 (6)	166

Symmetry codes: (i) $-x$, $y+1/2$, $-z+3/2$; (ii) $-x+2$, $-y$, $-z+1$; (iii) $x+1$, y, z.