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1,1,3,3-Tetramethyl-2-[2-(tritylsulfanyl)-ethyl]guanidine

Adam Neuba, Ulrich Flörke* and Gerald Henkel

Department Chemie, Fakultät für Naturwissenschaften, Universität Paderborn, Warburgerstrasse 100, D-33098 Paderborn, Germany
Correspondence e-mail: ulrich.floerke@upb.de

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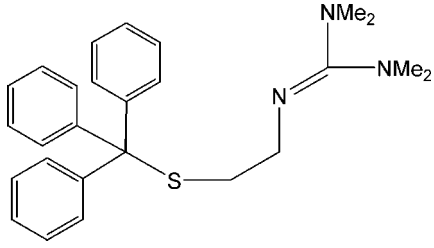
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.142; data-to-parameter ratio = 19.9.

The molecular structure of the title compound, $C_{26}H_{31}N_3S$, shows a guanidyl group bridged by an ethylene linker with a localized C=N bond to the tritylsulfanyl unit. The N—C—C—S group has a folded non-planar conformation, with a torsion angle of 66.04 (15)°. Intermolecular C—H···S hydrogen bonds link molecules into chains extended along [010].

Related literature

For related literature, see: Harmjanz (1997); Herres *et al.* (2005); Neuba, Flörke *et al.* (2007*a*,*b*); Neuba, Herres-Pawlis *et al.* (2007); Pohl *et al.* (2000); Schneider (2000); Waden (1999); Wenzhuo *et al.* (2003); Wittmann *et al.* (2001).



Experimental

Crystal data

$C_{26}H_{31}N_3S$
M_r = 417.60
Monoclinic, $P2_1/c$
a = 11.7059 (6) Å
b = 13.8102 (7) Å
c = 14.2886 (7) Å
β = 101.063 (1)°
V = 2267.0 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 120 (2) K
0.43 × 0.40 × 0.32 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.905, T_{max} = 0.951
19345 measured reflections
5380 independent reflections
4306 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.142
S = 1.04
5380 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C25—H25A···S1^{i}	0.95	2.95	3.7995 (18)	149

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2002); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2594).

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supplementary materials

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1,1,3,3-Tetramethyl-2-[2-(tritylsulfanyl)ethyl]guanidine

A. Neuba, U. Flörke and G. Henkel

Comment

The synthesis and characterization of molecules containing nitrogen and sulfur as donor functions is important for biomimetic coordination chemistry. The use of this molecules as ligands in the synthesis of copper-complexes as mimics for active centres like the CuA in cytochrome-c-oxidase and N_2O-reductase is currently of considerable interest in bioinorganic chemistry. In search of multifunctional ligands we have extended our studies to guanidyl-type systems with N-donor functions. The first derivative, the ligand bis(tetramethyl-guanidino)propylene (btmgp) and its complexes with Cu, Fe, Ni and Mn have recently been investigated (Harmjanz, 1997; Waden, 1999; Pohl *et al.*, 2000; Schneider, 2000; Wittmann *et al.*, 2001; Herres *et al.*, 2005; Neuba, Herres-Pawlis *et al.*, 2007). Recently, we reported about the molecular structure of *N*,*N*'-bis(1,3-dimethylimidazolidin-2-ylidene)-2,2'-dithiodianiline (II) and 2',2'-(2,2'-disulfanediylbis(2,1-phenylene))bis(1,1,3,3- tetramethylguanidine) (III) (Neuba, Flörke *et al.*, 2007*a*,b) with two guanidyl groups bridged by a diphenyldisulfanyl linker. Now the title compound is another member of the guanidine based ligand family incorporating a guanidine- and a sulfur donor function. I, II and III possess equal C═N bond lengths with 1.300 (2) in I, 1.297 (3) in II and 1.2812 (19) Å in III. Analogous to II and III the guanidyl double bond C═N in I is clearly localized. The N–C–C–S group has a folded nonplanar conformation with a torsion angle of 66.04 (15)°.

Experimental

A solution of tetramethylchloroformamidinium chloride (5.13 g, 30 mmol) in dry MeCN was added dropwise to an ice-cooled solution of 2-(tritylthio)ethanamine (Wenzhuo *et al.*, 2003) (9.57 g, 30 mmol) and triethylamine (4.18 ml, 3.03 g, 30 mmol) in dry MeCN. After 3 h under reflux, a solution of NaOH (1.2 g, 30 mmol) in water was added. The solvents and NEt_3 were then evaporated under vacuum. In order to deprotonate the mono-hydrochloride, 50 wt% KOH (aqueous, 15 ml) was added and the free base was extracted into the THF phase (3 *x* 80 ml). The organic phase was dried with Na_2SO_4. After filtration, the solvent was evaporated under reduced pressure. The crude product was recrystallized in MeCN and the title compound was obtained as a white powder (yield 77.0%, 9 g). Colourless crystals suitable for X-ray diffraction were obtained by diffusion of Et_2O into a cold saturated MeCN solution. Spectroscopic analysis, ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.39 (d, 2H, CH_2), 2.62 (s, 12H, CH_3.), 3.10 (dd, 2H, CH_2), 7.17 (m, 3H, Try CH's.), 7.27 (m, 6H, Try CH's.), 7.43 (m, 6H, Try CH's.). ^{13}C NMR (125 MHz, $CDCl_3$): δ 35.1 (CH_2), 38.8 (CH_3), 39.5 (CH_3), 48.6 (CH_2), 66.2 (C_{quart}), 126.38 (CH_{arom}), 127.72 (CH_{arom}), 129.90 (CH_{arom}), 129.74 (CH_{arom}), 145.35 (C_{quart}), 160.65 (C_{gua}); IR (KBr, ν, cm^{-1}): 3045 (w), 2992 (w), 2950 (w), 3925 (*m*), 2871 (*m*), 2829 (*m*), 2792 (w), 1691 (*versus*, C═N), 1614 (*versus*, C═N), 1490 (*s*), 1446 (*s*), 1444 (*s*), 1363 (*s*), 1132 (*s*), 1024 (*m*), 744 (*s*), 698 (*versus*), 622 (*m*), 578 (w), 507 (w); EI—MS: m/*z* (%) 418 (2) [M^+], 243 (89), 215 (20), 174 (100), 128 (75), 85 (96), 71 (38); Elemental analysis (M = 418.23 g mol^{-1}): calcd. for $C_{36}H_{31}N_3S$: C 74.78, H: 7.48, N 10.06; found C: 73.1, H: 7.56, N: 10.11.

Refinement

Hydrogen atoms were refined at idealized positions riding on the carbon atoms with isotropic displacement parameters $U_{iso}(H) = 1.2U(C_{eq})$ or $1.5U(–CH_3)$. All CH_3 groups were allowed to rotate but not to tip.

Figures

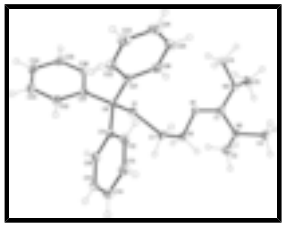

Fig. 1. Molecular structure of I. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. Crystal packing viewed along [100] with hydrogen bond indicated as dashed lines. H-atoms not involved are omitted.

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Crystal data

$C_{26}H_{31}N_3S$	$F_{000} = 896$
$M_r = 417.60$	$D_x = 1.224$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4979 reflections
$a = 11.7059$ (6) Å	$\theta = 2.5$–28.3º
$b = 13.8102$ (7) Å	$\mu = 0.16$ mm^{-1}
$c = 14.2886$ (7) Å	$T = 120$ (2) K
$\beta = 101.063$ (1)º	Block, colourless
$V = 2267.0$ (2) Å^3	0.43 × 0.40 × 0.32 mm
$Z = 4$	

Data collection

Bruker AXS SMART APEX diffractometer	5380 independent reflections
Radiation source: sealed tube	4306 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
$T = 120(2)$ K	$\theta_{max} = 27.9$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -15 \rightarrow 12$

T_{min} = 0.905, T_{max} = 0.951
19345 measured reflections

k = −18→18
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.142
S = 1.04
5380 reflections
271 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.0286P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.37632 (4)	0.13069 (3)	0.25946 (3)	0.01926 (13)
N1	0.56201 (12)	0.20942 (9)	0.43375 (9)	0.0192 (3)
N2	0.63255 (12)	0.22038 (9)	0.60122 (9)	0.0214 (3)
N3	0.70913 (12)	0.31770 (9)	0.49347 (9)	0.0219 (3)
C1	0.63107 (14)	0.24506 (10)	0.50601 (10)	0.0183 (3)
C2	0.65769 (17)	0.12119 (12)	0.63128 (13)	0.0285 (4)
H2A	0.6397	0.0782	0.5758	0.043*
H2B	0.6101	0.1031	0.6779	0.043*
H2C	0.7403	0.1152	0.6604	0.043*
C3	0.65892 (16)	0.29261 (12)	0.67636 (11)	0.0258 (4)
H3A	0.7421	0.2902	0.7045	0.039*
H3B	0.6133	0.2792	0.7257	0.039*
H3C	0.6391	0.3571	0.6495	0.039*
C4	0.69383 (18)	0.36216 (12)	0.39961 (12)	0.0302 (4)
H4A	0.7220	0.3179	0.3554	0.045*
H4B	0.7381	0.4228	0.4039	0.045*
H4C	0.6111	0.3758	0.3763	0.045*

C5	0.83118 (15)	0.30039 (13)	0.53613 (14)	0.0304 (4)
H5A	0.8360	0.2663	0.5969	0.046*
H5B	0.8721	0.3625	0.5473	0.046*
H5C	0.8673	0.2608	0.4928	0.046*
C6	0.46551 (15)	0.14912 (11)	0.45075 (11)	0.0206 (3)
H6A	0.4501	0.1625	0.5153	0.025*
H6B	0.4870	0.0800	0.4481	0.025*
C7	0.35577 (15)	0.16880 (11)	0.37683 (11)	0.0210 (3)
H7A	0.3375	0.2388	0.3758	0.025*
H7B	0.2894	0.1332	0.3941	0.025*
C8	0.25120 (13)	0.18796 (10)	0.17909 (10)	0.0166 (3)
C11	0.14460 (14)	0.17146 (11)	0.22436 (10)	0.0180 (3)
C12	0.08681 (15)	0.24665 (12)	0.26000 (11)	0.0227 (4)
H12A	0.1092	0.3116	0.2511	0.027*
C13	−0.00305 (16)	0.22864 (13)	0.30841 (12)	0.0304 (4)
H13A	−0.0409	0.2813	0.3326	0.036*
C14	−0.03812 (17)	0.13497 (14)	0.32186 (13)	0.0314 (4)
H14A	−0.1005	0.1229	0.3541	0.038*
C15	0.01944 (16)	0.05859 (13)	0.28734 (12)	0.0282 (4)
H15A	−0.0031	−0.0062	0.2968	0.034*
C16	0.10907 (15)	0.07632 (11)	0.23935 (11)	0.0230 (4)
H16A	0.1474	0.0234	0.2161	0.028*
C21	0.27182 (14)	0.29662 (10)	0.16190 (11)	0.0185 (3)
C22	0.19375 (16)	0.34473 (11)	0.09053 (12)	0.0252 (4)
H22A	0.1304	0.3101	0.0540	0.030*
C23	0.20778 (18)	0.44233 (12)	0.07244 (13)	0.0321 (4)
H23A	0.1546	0.4738	0.0233	0.039*
C24	0.29889 (18)	0.49393 (12)	0.12566 (14)	0.0326 (4)
H24A	0.3076	0.5610	0.1140	0.039*
C25	0.37728 (17)	0.44727 (12)	0.19593 (13)	0.0293 (4)
H25A	0.4404	0.4824	0.2322	0.035*
C26	0.36434 (16)	0.34860 (11)	0.21394 (12)	0.0233 (4)
H26A	0.4191	0.3170	0.2620	0.028*
C31	0.24462 (15)	0.13587 (10)	0.08293 (11)	0.0177 (3)
C32	0.13857 (15)	0.10574 (11)	0.02863 (11)	0.0208 (3)
H32A	0.0688	0.1151	0.0521	0.025*
C33	0.13434 (16)	0.06201 (11)	−0.05986 (11)	0.0255 (4)
H33A	0.0615	0.0421	−0.0963	0.031*
C34	0.23468 (16)	0.04730 (11)	−0.09500 (11)	0.0262 (4)
H34A	0.2315	0.0166	−0.1550	0.031*
C35	0.34038 (16)	0.07776 (12)	−0.04186 (12)	0.0261 (4)
H35A	0.4100	0.0678	−0.0655	0.031*
C36	0.34505 (15)	0.12277 (11)	0.04577 (11)	0.0221 (4)
H36A	0.4177	0.1449	0.0807	0.027*

Atomic displacement parameters (Å^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

S1	0.0185 (2)	0.0212 (2)	0.0170 (2)	0.00201 (14)	0.00065 (16)	−0.00119 (14)
N1	0.0197 (7)	0.0192 (6)	0.0183 (6)	−0.0034 (5)	0.0029 (5)	−0.0001 (5)
N2	0.0240 (8)	0.0220 (6)	0.0164 (6)	−0.0020 (5)	−0.0004 (5)	0.0007 (5)
N3	0.0217 (8)	0.0252 (6)	0.0190 (7)	−0.0079 (5)	0.0043 (6)	−0.0014 (5)
C1	0.0193 (9)	0.0185 (7)	0.0173 (7)	0.0015 (6)	0.0038 (6)	0.0004 (5)
C2	0.0311 (11)	0.0262 (8)	0.0259 (9)	0.0004 (7)	−0.0007 (7)	0.0066 (7)
C3	0.0252 (10)	0.0322 (8)	0.0192 (8)	−0.0032 (7)	0.0025 (7)	−0.0046 (6)
C4	0.0392 (12)	0.0290 (9)	0.0244 (9)	−0.0121 (7)	0.0107 (8)	0.0002 (7)
C5	0.0216 (10)	0.0335 (9)	0.0374 (10)	−0.0061 (7)	0.0085 (8)	−0.0082 (8)
C6	0.0223 (9)	0.0213 (7)	0.0167 (8)	−0.0047 (6)	0.0001 (6)	0.0010 (6)
C7	0.0208 (9)	0.0260 (8)	0.0156 (7)	−0.0026 (6)	0.0018 (6)	−0.0013 (6)
C8	0.0162 (8)	0.0161 (6)	0.0166 (7)	0.0005 (5)	0.0008 (6)	−0.0004 (5)
C11	0.0151 (8)	0.0225 (7)	0.0149 (7)	−0.0023 (6)	−0.0008 (6)	−0.0002 (5)
C12	0.0201 (9)	0.0254 (7)	0.0229 (8)	−0.0034 (6)	0.0046 (7)	−0.0029 (6)
C13	0.0268 (11)	0.0368 (9)	0.0290 (9)	−0.0013 (7)	0.0090 (8)	−0.0070 (7)
C14	0.0233 (10)	0.0470 (11)	0.0254 (9)	−0.0090 (8)	0.0087 (7)	0.0000 (8)
C15	0.0274 (10)	0.0313 (9)	0.0255 (9)	−0.0117 (7)	0.0038 (7)	0.0023 (7)
C16	0.0229 (9)	0.0226 (7)	0.0220 (8)	−0.0044 (6)	0.0007 (7)	−0.0005 (6)
C21	0.0207 (9)	0.0166 (7)	0.0202 (8)	−0.0004 (6)	0.0089 (6)	−0.0016 (6)
C22	0.0281 (10)	0.0218 (7)	0.0260 (9)	0.0025 (7)	0.0062 (7)	0.0003 (6)
C23	0.0417 (12)	0.0242 (8)	0.0331 (10)	0.0086 (8)	0.0135 (8)	0.0058 (7)
C24	0.0430 (12)	0.0180 (7)	0.0443 (11)	−0.0001 (7)	0.0267 (9)	0.0007 (7)
C25	0.0319 (11)	0.0230 (8)	0.0375 (10)	−0.0081 (7)	0.0181 (8)	−0.0071 (7)
C26	0.0245 (9)	0.0226 (7)	0.0244 (8)	−0.0040 (6)	0.0086 (7)	−0.0024 (6)
C31	0.0215 (9)	0.0144 (6)	0.0162 (7)	0.0001 (5)	0.0012 (6)	0.0012 (5)
C32	0.0184 (9)	0.0222 (7)	0.0213 (8)	0.0014 (6)	0.0025 (6)	−0.0002 (6)
C33	0.0312 (10)	0.0220 (7)	0.0204 (8)	−0.0008 (6)	−0.0027 (7)	−0.0009 (6)
C34	0.0395 (11)	0.0209 (7)	0.0181 (8)	0.0009 (7)	0.0058 (7)	−0.0018 (6)
C35	0.0314 (11)	0.0278 (8)	0.0218 (8)	0.0024 (7)	0.0119 (7)	0.0005 (6)
C36	0.0230 (10)	0.0231 (7)	0.0202 (8)	−0.0019 (6)	0.0039 (7)	0.0005 (6)

Geometric parameters (Å, °)

S1—C7	1.8172 (16)	C12—C13	1.388 (3)
S1—C8	1.8559 (15)	C12—H12A	0.9500
N1—C1	1.2812 (19)	C13—C14	1.382 (3)
N1—C6	1.461 (2)	C13—H13A	0.9500
N2—C1	1.3993 (19)	C14—C15	1.392 (3)
N2—C2	1.449 (2)	C14—H14A	0.9500
N2—C3	1.455 (2)	C15—C16	1.381 (2)
N3—C1	1.392 (2)	C15—H15A	0.9500
N3—C4	1.454 (2)	C16—H16A	0.9500
N3—C5	1.461 (2)	C21—C26	1.390 (2)
C2—H2A	0.9800	C21—C22	1.400 (2)
C2—H2B	0.9800	C22—C23	1.388 (2)
C2—H2C	0.9800	C22—H22A	0.9500
C3—H3A	0.9800	C23—C24	1.383 (3)
C3—H3B	0.9800	C23—H23A	0.9500
C3—H3C	0.9800	C24—C25	1.383 (3)

C4—H4A	0.9800	C24—H24A	0.9500
C4—H4B	0.9800	C25—C26	1.400 (2)
C4—H4C	0.9800	C25—H25A	0.9500
C5—H5A	0.9800	C26—H26A	0.9500
C5—H5B	0.9800	C31—C36	1.391 (2)
C5—H5C	0.9800	C31—C32	1.395 (2)
C6—C7	1.523 (2)	C32—C33	1.394 (2)
C6—H6A	0.9900	C32—H32A	0.9500
C6—H6B	0.9900	C33—C34	1.378 (3)
C7—H7A	0.9900	C33—H33A	0.9500
C7—H7B	0.9900	C34—C35	1.387 (3)
C8—C11	1.529 (2)	C34—H34A	0.9500
C8—C31	1.540 (2)	C35—C36	1.390 (2)
C8—C21	1.547 (2)	C35—H35A	0.9500
C11—C12	1.388 (2)	C36—H36A	0.9500
C11—C16	1.407 (2)		
C7—S1—C8	102.65 (7)	C12—C11—C8	122.58 (14)
C1—N1—C6	118.26 (13)	C16—C11—C8	119.53 (14)
C1—N2—C2	118.85 (13)	C13—C12—C11	121.21 (15)
C1—N2—C3	120.79 (13)	C13—C12—H12A	119.4
C2—N2—C3	115.29 (13)	C11—C12—H12A	119.4
C1—N3—C4	117.09 (13)	C14—C13—C12	120.73 (17)
C1—N3—C5	116.23 (13)	C14—C13—H13A	119.6
C4—N3—C5	113.03 (15)	C12—C13—H13A	119.6
N1—C1—N3	120.10 (14)	C13—C14—C15	118.89 (18)
N1—C1—N2	125.31 (14)	C13—C14—H14A	120.6
N3—C1—N2	114.51 (13)	C15—C14—H14A	120.6
N2—C2—H2A	109.5	C16—C15—C14	120.48 (16)
N2—C2—H2B	109.5	C16—C15—H15A	119.8
H2A—C2—H2B	109.5	C14—C15—H15A	119.8
N2—C2—H2C	109.5	C15—C16—C11	121.08 (16)
H2A—C2—H2C	109.5	C15—C16—H16A	119.5
H2B—C2—H2C	109.5	C11—C16—H16A	119.5
N2—C3—H3A	109.5	C26—C21—C22	118.52 (14)
N2—C3—H3B	109.5	C26—C21—C8	123.04 (14)
H3A—C3—H3B	109.5	C22—C21—C8	118.44 (14)
N2—C3—H3C	109.5	C23—C22—C21	120.84 (16)
H3A—C3—H3C	109.5	C23—C22—H22A	119.6
H3B—C3—H3C	109.5	C21—C22—H22A	119.6
N3—C4—H4A	109.5	C24—C23—C22	120.29 (17)
N3—C4—H4B	109.5	C24—C23—H23A	119.9
H4A—C4—H4B	109.5	C22—C23—H23A	119.9
N3—C4—H4C	109.5	C25—C24—C23	119.57 (15)
H4A—C4—H4C	109.5	C25—C24—H24A	120.2
H4B—C4—H4C	109.5	C23—C24—H24A	120.2
N3—C5—H5A	109.5	C24—C25—C26	120.45 (16)
N3—C5—H5B	109.5	C24—C25—H25A	119.8
H5A—C5—H5B	109.5	C26—C25—H25A	119.8
N3—C5—H5C	109.5	C21—C26—C25	120.32 (16)

H5A—C5—H5C	109.5	C21—C26—H26A	119.8
H5B—C5—H5C	109.5	C25—C26—H26A	119.8
N1—C6—C7	111.05 (13)	C36—C31—C32	118.41 (14)
N1—C6—H6A	109.4	C36—C31—C8	120.00 (14)
C7—C6—H6A	109.4	C32—C31—C8	121.49 (15)
N1—C6—H6B	109.4	C33—C32—C31	120.45 (16)
C7—C6—H6B	109.4	C33—C32—H32A	119.8
H6A—C6—H6B	108.0	C31—C32—H32A	119.8
C6—C7—S1	110.18 (12)	C34—C33—C32	120.67 (16)
C6—C7—H7A	109.6	C34—C33—H33A	119.7
S1—C7—H7A	109.6	C32—C33—H33A	119.7
C6—C7—H7B	109.6	C33—C34—C35	119.27 (15)
S1—C7—H7B	109.6	C33—C34—H34A	120.4
H7A—C7—H7B	108.1	C35—C34—H34A	120.4
C11—C8—C31	113.75 (12)	C34—C35—C36	120.37 (17)
C11—C8—C21	112.13 (12)	C34—C35—H35A	119.8
C31—C8—C21	107.10 (12)	C36—C35—H35A	119.8
C11—C8—S1	106.62 (10)	C35—C36—C31	120.80 (15)
C31—C8—S1	104.56 (10)	C35—C36—H36A	119.6
C21—C8—S1	112.52 (10)	C31—C36—H36A	119.6
C12—C11—C16	117.61 (16)		
C6—N1—C1—N3	−167.11 (14)	C8—C11—C16—C15	174.43 (14)
C6—N1—C1—N2	9.7 (2)	C11—C8—C21—C26	109.61 (17)
C4—N3—C1—N1	10.9 (2)	C31—C8—C21—C26	−124.93 (16)
C5—N3—C1—N1	−126.98 (16)	S1—C8—C21—C26	−10.6 (2)
C4—N3—C1—N2	−166.20 (15)	C11—C8—C21—C22	−70.47 (18)
C5—N3—C1—N2	55.91 (19)	C31—C8—C21—C22	54.98 (19)
C2—N2—C1—N1	61.4 (2)	S1—C8—C21—C22	169.34 (13)
C3—N2—C1—N1	−144.98 (17)	C26—C21—C22—C23	−0.4 (3)
C2—N2—C1—N3	−121.68 (16)	C8—C21—C22—C23	179.65 (15)
C3—N2—C1—N3	32.0 (2)	C21—C22—C23—C24	−0.7 (3)
C1—N1—C6—C7	140.92 (15)	C22—C23—C24—C25	1.2 (3)
N1—C6—C7—S1	66.04 (15)	C23—C24—C25—C26	−0.5 (3)
C8—S1—C7—C6	−166.43 (10)	C22—C21—C26—C25	1.1 (2)
C7—S1—C8—C11	−43.94 (11)	C8—C21—C26—C25	−179.03 (15)
C7—S1—C8—C31	−164.72 (10)	C24—C25—C26—C21	−0.6 (3)
C7—S1—C8—C21	79.39 (12)	C11—C8—C31—C36	−163.15 (13)
C31—C8—C11—C12	−131.94 (14)	C21—C8—C31—C36	72.38 (16)
C21—C8—C11—C12	−10.2 (2)	S1—C8—C31—C36	−47.22 (15)
S1—C8—C11—C12	113.35 (14)	C11—C8—C31—C32	20.51 (19)
C31—C8—C11—C16	54.32 (18)	C21—C8—C31—C32	−103.96 (16)
C21—C8—C11—C16	176.04 (13)	S1—C8—C31—C32	136.43 (12)
S1—C8—C11—C16	−60.39 (15)	C36—C31—C32—C33	1.2 (2)
C16—C11—C12—C13	−0.2 (2)	C8—C31—C32—C33	177.56 (14)
C8—C11—C12—C13	−174.07 (14)	C31—C32—C33—C34	0.4 (2)
C11—C12—C13—C14	−0.5 (3)	C32—C33—C34—C35	−0.9 (2)
C12—C13—C14—C15	1.0 (3)	C33—C34—C35—C36	−0.1 (2)
C13—C14—C15—C16	−0.8 (3)	C34—C35—C36—C31	1.7 (2)
C14—C15—C16—C11	0.2 (2)	C32—C31—C36—C35	−2.2 (2)

C12—C11—C16—C15	0.4 (2)	C8—C31—C36—C35	−178.63 (14)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C25—H25A···S1^{i}	0.95	2.95	3.7995 (18)	149

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

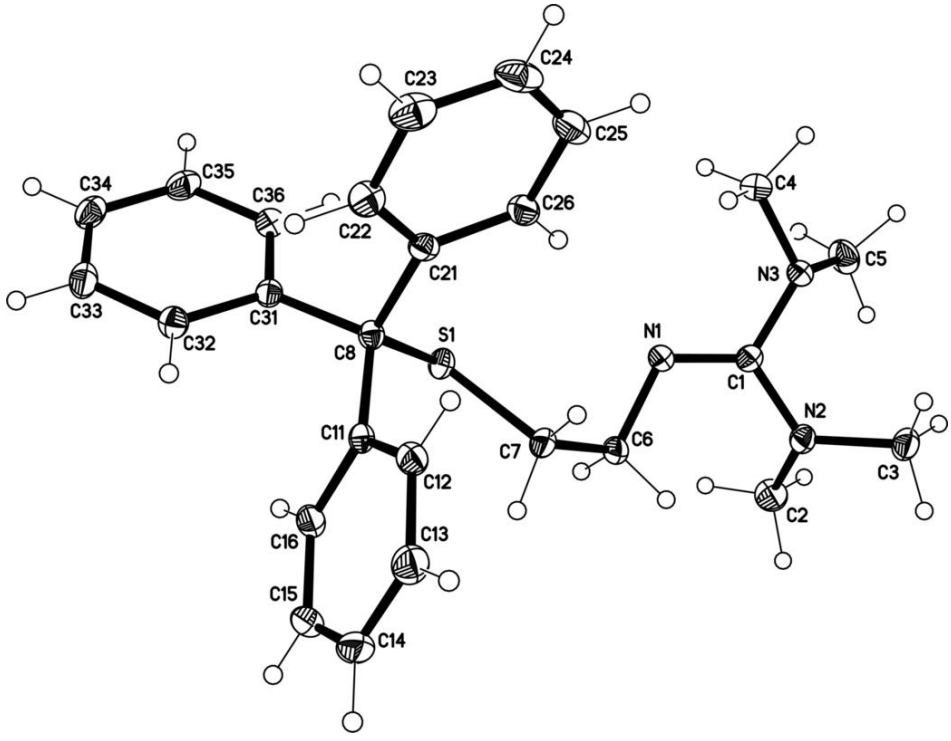
C24
C23
C25
C35
C34
C36
C4
C22
C26
C5
N3
C21
C33
C31
C32
C8
S1
N1
C1
N2
C11
C7
C6
C12
C3
C2
C16
C13
C15
C14

Fig. 2