Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4,6-Bis[4-(benzylsulfanyl)styryl]-2-(methylsulfanyl)pyrimidine

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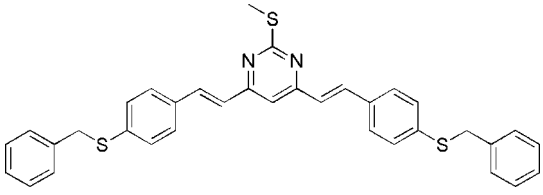
Received 14 November 2007; accepted 2 December 2007

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.046; $wR$ factor = 0.129; data-to-parameter ratio = 14.4.

The title compound, $C_{35}H_{30}N_2S_3$, has been synthesized by a solvent-free reaction. The molecule exhibits an *E*,*E* configuration, the benzene rings and pyrimidine rings being located on the opposite sides of the C=C bonds. The centroid–centroid separation of 3.5808 (17) Å indicates the existence of $\pi$–$\pi$ stacking between nearly parallel pyrimidine and benzene rings of adjacent molecules.

## Related literature

For details of the applications of conjugated organic molecules, see: Frederiksen *et al.* (2001); Zhao *et al.* (1995). For heterocycle-based two-photon absorbing chromophores exhibiting large TPA cross-sections, see: Huang *et al.* (2003).



## Experimental

### Crystal data

$C_{35}H_{30}N_2S_3$
$M_r$ = 574.79
Triclinic, $P\overline{1}$
$a$ = 7.199 (1) Å
$b$ = 10.1694 (15) Å
$c$ = 21.161 (2) Å
$\alpha$ = 77.412 (1)°
$\beta$ = 88.425 (3)°
$\gamma$ = 81.129 (2)°
$V$ = 1493.8 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 298 (2) K
0.50 × 0.38 × 0.31 mm

### Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.875, $T_{max}$ = 0.920
7820 measured reflections
5185 independent reflections
3229 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.129
$S$ = 1.04
5185 reflections
361 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

This work was supported by the Education Committee of Anhui Province, China (KJ2007B089). We thank Professor D.-Q. Wang of Liao Cheng University for assistance with the crystal structure determination.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2372).

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# supporting information

*Acta Cryst.* (2008). E**64**, o257 [https://doi.org/10.1107/S1600536807065063]

## 4,6-Bis[4-(benzylsulfanyl)styryl]-2-(methylsulfanyl)pyrimidine

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### S1. Comment

Two-photon absorption (TPA) processes in conjugated organic molecules have aroused considerable attention due to their potential applications in optical data storage, three-dimension fluorescence imaging, photodynamic therapy, two-photon upconversion lasing and three-dimension lithographic microfabrication (Frederiksen *et al.*, 2001; Zhao *et al.*, 1995). A sustained level of fundamental research over the past ten years has left organic nonlinear optical (NLO) well positioned to make a technological impact in a variety of disciplines. Some studies showed that the heterocycle-based two-photon absorbing chromophores exhibit large TPA cross-sections (Huang *et al.*, 2003). As part of our ongoing investigtion on heterocycle-based two-photon absorbing chromophores, the title compound has been prepared and its crystal structure is presented here.

The molecule structure is shown in Fig. 1. Bond lengths and angles are normal. The C7-containing and C22-containing benzene rings are nearly coplanar with the pyrimidine ring, dihedral angles being 8.59 (2)° and 8.40 (2)°, respectively. In the crystal structure, $\pi$-$\pi$ stacking is observed between nearly parallel pyrimidine and C10$^{i}$-containing benzene rings as shown in Fig. 2 [symmetry code: (i) 1 + *x*,*y*,*z*]; the dihedral angle and centroid-to-centroid separation being 8.69 (13)° and 3.5808 (17) Å, respectively.

### S2. Experimental

At room temperature, t-BuOK (5.6 g, 50 mmol) was placed into a dry mortar and milled to very small, then 2-thiomethyl-4,6-dimethylpyrimidine (1.54 g, 10 mmol) and 4-benzylthiobenzalaldehyde (4.56 g, 20 mmol) were added and mixed. The mixture was milled vigorously for about 20 min. The mixture became sticky and then continuously milled for 10 min. After completion of the reaction (monitored by TLC), the mixture was dispersed in 100 ml me thanol. The residual solid was filtered and recrystallized from anhydrous dichloromethane/methanol solution, to give microcrystals (2.87 g, yield 50%). Single crystals suitable for X-ray analysis were obtained by slow evaporation from a dichloromethane/2-propanol (3:1) solution.

### S3. Refinement

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C).

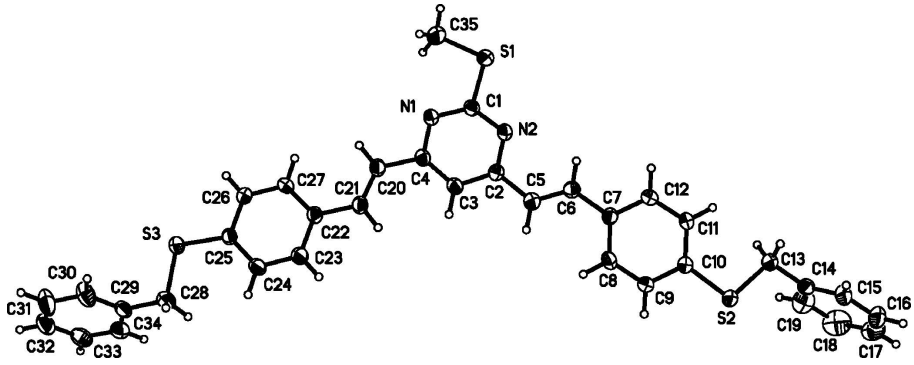


**Figure 1**

The molecular structure of the title compound with 30% probability displacement ellipsoids for non-H atoms.

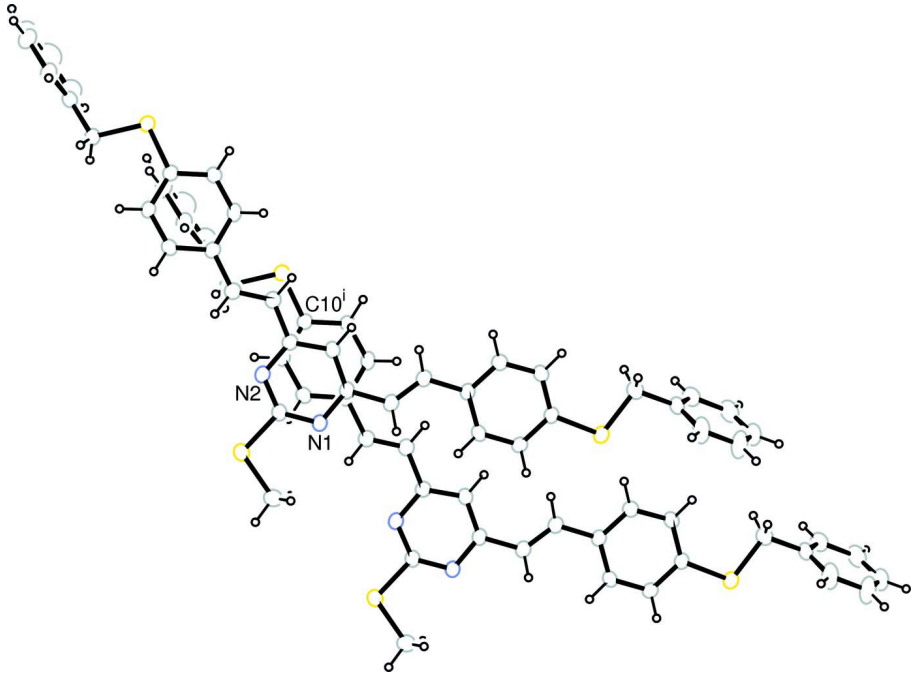


**Figure 2**

A diagram showing $\pi$-$\pi$ stacking [symmetry code: (i) 1 + $x$,$y$,$z$].

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*Crystal data*

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$\beta$ = 88.425 (3)°
$\gamma$ = 81.129 (2)°
$V$ = 1493.8 (3) Å$^3$
$Z$ = 2
$F$(000) = 604
$D_x$ = 1.278 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2350 reflections
$\theta$ = 2.5–25.8°
$\mu$ = 0.28 mm$^{-1}$
$T$ = 298 K
Block, red
0.50 × 0.38 × 0.31 mm

*Data collection*

Bruker SMART CCD area detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.875, $T_{max}$ = 0.920
7820 measured reflections
5185 independent reflections
3229 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.0°
$h$ = −8→8
$k$ = −12→9
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.129
$S$ = 1.04
5185 reflections
361 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.0894P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

*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 $F^2 > \sigma(F^2)$ 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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.57325 (12) | 0.40771 (8) | 0.15862 (4) | 0.0709 (3) |
| S2 | −0.76178 (11) | 1.09386 (8) | 0.14193 (4) | 0.0630 (3) |
| S3 | 1.42863 (10) | 0.70995 (8) | 0.54464 (4) | 0.0593 (2) |
| N1 | 0.6566 (3) | 0.5069 (2) | 0.25966 (10) | 0.0453 (5) |
| N2 | 0.3517 (3) | 0.5797 (2) | 0.21019 (10) | 0.0477 (6) |
| C1 | 0.5236 (4) | 0.5089 (3) | 0.21646 (12) | 0.0461 (7) |
| C2 | 0.3081 (4) | 0.6646 (3) | 0.25115 (12) | 0.0437 (6) |
| C3 | 0.4379 (4) | 0.6735 (3) | 0.29656 (12) | 0.0472 (7) |
| H3 | 0.4085 | 0.7335 | 0.3241 | 0.057* |
| C4 | 0.6107 (4) | 0.5926 (3) | 0.30053 (12) | 0.0435 (6) |
| C5 | 0.1233 (4) | 0.7484 (3) | 0.24433 (13) | 0.0525 (7) |
| H5 | 0.0955 | 0.8108 | 0.2708 | 0.063* |
| C6 | −0.0066 (4) | 0.7414 (3) | 0.20317 (13) | 0.0487 (7) |
| H6 | 0.0239 | 0.6759 | 0.1785 | 0.058* |
| C7 | −0.1931 (4) | 0.8236 (3) | 0.19117 (12) | 0.0449 (7) |
| C8 | −0.2598 (4) | 0.9304 (3) | 0.22157 (13) | 0.0553 (8) |

| | | | | |
|---|---|---|---|---|
| H8 | −0.1856 | 0.9487 | 0.2529 | 0.066* |
| C9 | −0.4317 (4) | 1.0091 (3) | 0.20649 (13) | 0.0535 (8) |
| H9 | −0.4712 | 1.0804 | 0.2272 | 0.064* |
| C10 | −0.5476 (4) | 0.9832 (3) | 0.16040 (13) | 0.0468 (7) |
| C11 | −0.4868 (4) | 0.8747 (3) | 0.13147 (13) | 0.0496 (7) |
| H11 | −0.5639 | 0.8539 | 0.1016 | 0.060* |
| C12 | −0.3126 (4) | 0.7972 (3) | 0.14656 (12) | 0.0487 (7) |
| H12 | −0.2740 | 0.7252 | 0.1263 | 0.058* |
| C13 | −0.8416 (4) | 1.0492 (3) | 0.06998 (14) | 0.0627 (9) |
| H13A | −0.7393 | 1.0448 | 0.0393 | 0.075* |
| H13B | −0.8820 | 0.9604 | 0.0813 | 0.075* |
| C14 | −1.0021 (4) | 1.1548 (3) | 0.03979 (13) | 0.0518 (7) |
| C15 | −1.1850 (4) | 1.1341 (3) | 0.05280 (14) | 0.0610 (8) |
| H15 | −1.2083 | 1.0543 | 0.0808 | 0.073* |
| C16 | −1.3336 (5) | 1.2288 (4) | 0.02532 (19) | 0.0816 (11) |
| H16 | −1.4562 | 1.2134 | 0.0352 | 0.098* |
| C17 | −1.3021 (7) | 1.3434 (5) | −0.01566 (19) | 0.0933 (14) |
| H17 | −1.4033 | 1.4061 | −0.0351 | 0.112* |
| C18 | −1.1220 (8) | 1.3695 (4) | −0.02939 (19) | 0.1124 (15) |
| H18 | −1.1011 | 1.4499 | −0.0574 | 0.135* |
| C19 | −0.9702 (5) | 1.2737 (4) | −0.00067 (17) | 0.0872 (11) |
| H19 | −0.8477 | 1.2910 | −0.0091 | 0.105* |
| C20 | 0.7619 (4) | 0.5923 (3) | 0.34563 (12) | 0.0481 (7) |
| H20 | 0.8696 | 0.5292 | 0.3446 | 0.058* |
| C21 | 0.7625 (4) | 0.6709 (3) | 0.38730 (12) | 0.0486 (7) |
| H21 | 0.6516 | 0.7290 | 0.3911 | 0.058* |
| C22 | 0.9207 (4) | 0.6763 (3) | 0.42844 (12) | 0.0442 (6) |
| C23 | 0.8985 (4) | 0.7586 (3) | 0.47332 (13) | 0.0556 (8) |
| H23 | 0.7807 | 0.8077 | 0.4779 | 0.067* |
| C24 | 1.0456 (4) | 0.7700 (3) | 0.51137 (13) | 0.0553 (8) |
| H24 | 1.0254 | 0.8246 | 0.5416 | 0.066* |
| C25 | 1.2236 (4) | 0.6999 (3) | 0.50432 (12) | 0.0437 (6) |
| C26 | 1.2470 (4) | 0.6161 (3) | 0.45996 (12) | 0.0502 (7) |
| H26 | 1.3648 | 0.5673 | 0.4549 | 0.060* |
| C27 | 1.0977 (4) | 0.6045 (3) | 0.42341 (13) | 0.0505 (7) |
| H27 | 1.1165 | 0.5468 | 0.3945 | 0.061* |
| C28 | 1.3614 (4) | 0.8283 (3) | 0.59547 (16) | 0.0743 (10) |
| H28A | 1.2957 | 0.9133 | 0.5703 | 0.089* |
| H28B | 1.2786 | 0.7914 | 0.6295 | 0.089* |
| C29 | 1.5394 (4) | 0.8521 (3) | 0.62436 (14) | 0.0545 (8) |
| C30 | 1.6381 (5) | 0.7501 (4) | 0.66976 (15) | 0.0777 (10) |
| H30 | 1.5944 | 0.6669 | 0.6825 | 0.093* |
| C31 | 1.8009 (6) | 0.7694 (4) | 0.69664 (17) | 0.0919 (12) |
| H31 | 1.8660 | 0.6999 | 0.7278 | 0.110* |
| C32 | 1.8670 (5) | 0.8905 (4) | 0.67762 (17) | 0.0742 (10) |
| H32 | 1.9762 | 0.9038 | 0.6962 | 0.089* |
| C33 | 1.7747 (5) | 0.9907 (3) | 0.63203 (16) | 0.0704 (9) |
| H33 | 1.8214 | 1.0726 | 0.6186 | 0.085* |

| | | | | |
|---|---|---|---|---|
| C34 | 1.6106 (5) | 0.9720 (3) | 0.60510 (15) | 0.0682 (9) |
| H34 | 1.5477 | 1.0417 | 0.5735 | 0.082* |
| C35 | 0.8140 (5) | 0.3378 (4) | 0.17513 (18) | 0.0965 (13) |
| H35A | 0.8879 | 0.4104 | 0.1698 | 0.145* |
| H35B | 0.8570 | 0.2800 | 0.1457 | 0.145* |
| H35C | 0.8268 | 0.2855 | 0.2188 | 0.145* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0735 (6) | 0.0698 (6) | 0.0726 (6) | 0.0162 (4) | −0.0277 (5) | −0.0374 (4) |
| S2 | 0.0491 (5) | 0.0758 (6) | 0.0681 (5) | 0.0111 (4) | −0.0168 (4) | −0.0363 (4) |
| S3 | 0.0447 (4) | 0.0671 (5) | 0.0722 (5) | −0.0031 (4) | −0.0138 (4) | −0.0303 (4) |
| N1 | 0.0461 (14) | 0.0443 (13) | 0.0459 (13) | −0.0042 (11) | −0.0087 (11) | −0.0113 (10) |
| N2 | 0.0471 (14) | 0.0467 (13) | 0.0490 (13) | −0.0035 (11) | −0.0109 (11) | −0.0110 (11) |
| C1 | 0.0542 (18) | 0.0397 (15) | 0.0435 (15) | −0.0052 (13) | −0.0100 (14) | −0.0072 (12) |
| C2 | 0.0426 (16) | 0.0443 (16) | 0.0426 (15) | −0.0047 (13) | −0.0023 (13) | −0.0070 (13) |
| C3 | 0.0478 (17) | 0.0544 (17) | 0.0422 (15) | −0.0073 (14) | −0.0027 (13) | −0.0166 (13) |
| C4 | 0.0466 (17) | 0.0442 (16) | 0.0394 (14) | −0.0096 (13) | −0.0053 (13) | −0.0057 (12) |
| C5 | 0.0501 (18) | 0.0574 (18) | 0.0514 (17) | −0.0041 (14) | −0.0055 (14) | −0.0166 (14) |
| C6 | 0.0493 (17) | 0.0429 (16) | 0.0535 (17) | −0.0063 (13) | −0.0037 (14) | −0.0098 (13) |
| C7 | 0.0419 (16) | 0.0429 (16) | 0.0487 (16) | −0.0062 (13) | −0.0044 (13) | −0.0072 (13) |
| C8 | 0.0550 (19) | 0.0578 (18) | 0.0567 (18) | −0.0080 (15) | −0.0181 (15) | −0.0182 (15) |
| C9 | 0.0514 (18) | 0.0501 (17) | 0.0628 (19) | 0.0007 (14) | −0.0109 (15) | −0.0250 (14) |
| C10 | 0.0417 (16) | 0.0492 (16) | 0.0503 (16) | −0.0036 (13) | −0.0047 (13) | −0.0141 (13) |
| C11 | 0.0428 (17) | 0.0546 (17) | 0.0551 (17) | −0.0064 (14) | −0.0102 (13) | −0.0189 (14) |
| C12 | 0.0518 (18) | 0.0462 (16) | 0.0519 (17) | −0.0067 (14) | −0.0030 (14) | −0.0192 (13) |
| C13 | 0.0527 (19) | 0.074 (2) | 0.066 (2) | 0.0063 (16) | −0.0156 (15) | −0.0344 (17) |
| C14 | 0.0540 (19) | 0.062 (2) | 0.0413 (16) | 0.0007 (15) | −0.0049 (14) | −0.0207 (15) |
| C15 | 0.054 (2) | 0.069 (2) | 0.0616 (19) | −0.0117 (17) | −0.0106 (16) | −0.0160 (16) |
| C16 | 0.056 (2) | 0.106 (3) | 0.084 (3) | 0.006 (2) | −0.019 (2) | −0.034 (2) |
| C17 | 0.110 (4) | 0.091 (3) | 0.066 (3) | 0.033 (3) | −0.032 (3) | −0.020 (2) |
| C18 | 0.153 (5) | 0.090 (3) | 0.074 (3) | −0.005 (3) | 0.002 (3) | 0.015 (2) |
| C19 | 0.083 (3) | 0.102 (3) | 0.070 (2) | −0.015 (2) | 0.012 (2) | −0.006 (2) |
| C20 | 0.0444 (17) | 0.0530 (17) | 0.0465 (16) | −0.0057 (13) | −0.0058 (13) | −0.0099 (13) |
| C21 | 0.0403 (16) | 0.0590 (18) | 0.0472 (16) | −0.0062 (14) | −0.0029 (13) | −0.0138 (14) |
| C22 | 0.0383 (15) | 0.0511 (16) | 0.0454 (16) | −0.0102 (13) | −0.0017 (12) | −0.0122 (13) |
| C23 | 0.0405 (17) | 0.071 (2) | 0.0616 (18) | −0.0047 (15) | −0.0001 (14) | −0.0299 (16) |
| C24 | 0.0461 (18) | 0.071 (2) | 0.0581 (18) | −0.0081 (15) | 0.0002 (14) | −0.0339 (15) |
| C25 | 0.0427 (16) | 0.0449 (16) | 0.0439 (15) | −0.0073 (13) | −0.0057 (12) | −0.0094 (13) |
| C26 | 0.0423 (16) | 0.0544 (17) | 0.0535 (17) | 0.0021 (14) | −0.0070 (13) | −0.0167 (14) |
| C27 | 0.0536 (18) | 0.0534 (18) | 0.0495 (16) | −0.0038 (14) | −0.0067 (14) | −0.0238 (14) |
| C28 | 0.055 (2) | 0.094 (3) | 0.088 (2) | −0.0027 (18) | −0.0088 (18) | −0.053 (2) |
| C29 | 0.0501 (18) | 0.068 (2) | 0.0533 (18) | −0.0103 (16) | −0.0037 (14) | −0.0294 (16) |
| C30 | 0.100 (3) | 0.076 (2) | 0.063 (2) | −0.042 (2) | −0.020 (2) | −0.0031 (18) |
| C31 | 0.110 (3) | 0.091 (3) | 0.074 (2) | −0.029 (3) | −0.044 (2) | −0.001 (2) |
| C32 | 0.066 (2) | 0.094 (3) | 0.075 (2) | −0.024 (2) | −0.0118 (19) | −0.036 (2) |
| C33 | 0.085 (3) | 0.065 (2) | 0.074 (2) | −0.034 (2) | 0.005 (2) | −0.0270 (19) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C34 | 0.085 (3) | 0.0491 (19) | 0.073 (2) | −0.0029 (18) | −0.0146 (19) | −0.0211 (16) |
| C35 | 0.080 (3) | 0.110 (3) | 0.106 (3) | 0.032 (2) | −0.030 (2) | −0.066 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.760 (3) | C16—H16 | 0.9300 |
| S1—C35 | 1.782 (3) | C17—C18 | 1.374 (6) |
| S2—C10 | 1.761 (3) | C17—H17 | 0.9300 |
| S2—C13 | 1.812 (3) | C18—C19 | 1.401 (5) |
| S3—C25 | 1.753 (3) | C18—H18 | 0.9300 |
| S3—C28 | 1.788 (3) | C19—H19 | 0.9300 |
| N1—C1 | 1.336 (3) | C20—C21 | 1.314 (3) |
| N1—C4 | 1.357 (3) | C20—H20 | 0.9300 |
| N2—C1 | 1.327 (3) | C21—C22 | 1.467 (3) |
| N2—C2 | 1.350 (3) | C21—H21 | 0.9300 |
| C2—C3 | 1.385 (3) | C22—C27 | 1.381 (3) |
| C2—C5 | 1.457 (3) | C22—C23 | 1.387 (3) |
| C3—C4 | 1.376 (3) | C23—C24 | 1.381 (3) |
| C3—H3 | 0.9300 | C23—H23 | 0.9300 |
| C4—C20 | 1.466 (3) | C24—C25 | 1.388 (3) |
| C5—C6 | 1.316 (3) | C24—H24 | 0.9300 |
| C5—H5 | 0.9300 | C25—C26 | 1.390 (3) |
| C6—C7 | 1.465 (3) | C26—C27 | 1.375 (3) |
| C6—H6 | 0.9300 | C26—H26 | 0.9300 |
| C7—C12 | 1.389 (3) | C27—H27 | 0.9300 |
| C7—C8 | 1.397 (3) | C28—C29 | 1.509 (4) |
| C8—C9 | 1.370 (4) | C28—H28A | 0.9700 |
| C8—H8 | 0.9300 | C28—H28B | 0.9700 |
| C9—C10 | 1.394 (3) | C29—C30 | 1.371 (4) |
| C9—H9 | 0.9300 | C29—C34 | 1.371 (4) |
| C10—C11 | 1.383 (3) | C30—C31 | 1.376 (4) |
| C11—C12 | 1.380 (3) | C30—H30 | 0.9300 |
| C11—H11 | 0.9300 | C31—C32 | 1.363 (5) |
| C12—H12 | 0.9300 | C31—H31 | 0.9300 |
| C13—C14 | 1.502 (4) | C32—C33 | 1.345 (4) |
| C13—H13A | 0.9700 | C32—H32 | 0.9300 |
| C13—H13B | 0.9700 | C33—C34 | 1.382 (4) |
| C14—C19 | 1.369 (4) | C33—H33 | 0.9300 |
| C14—C15 | 1.376 (4) | C34—H34 | 0.9300 |
| C15—C16 | 1.372 (4) | C35—H35A | 0.9600 |
| C15—H15 | 0.9300 | C35—H35B | 0.9600 |
| C16—C17 | 1.339 (5) | C35—H35C | 0.9600 |
| | | | |
| C1—S1—C35 | 102.24 (14) | C17—C18—H18 | 120.3 |
| C10—S2—C13 | 102.92 (12) | C19—C18—H18 | 120.3 |
| C25—S3—C28 | 106.17 (13) | C14—C19—C18 | 120.0 (4) |
| C1—N1—C4 | 115.2 (2) | C14—C19—H19 | 120.0 |
| C1—N2—C2 | 115.8 (2) | C18—C19—H19 | 120.0 |

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| N2—C1—N1 | 128.4 (2) | C21—C20—C4 | 127.4 (3) |
| N2—C1—S1 | 112.86 (18) | C21—C20—H20 | 116.3 |
| N1—C1—S1 | 118.8 (2) | C4—C20—H20 | 116.3 |
| N2—C2—C3 | 120.5 (2) | C20—C21—C22 | 126.5 (3) |
| N2—C2—C5 | 117.6 (2) | C20—C21—H21 | 116.7 |
| C3—C2—C5 | 121.8 (2) | C22—C21—H21 | 116.7 |
| C4—C3—C2 | 119.3 (2) | C27—C22—C23 | 117.0 (2) |
| C4—C3—H3 | 120.3 | C27—C22—C21 | 122.5 (2) |
| C2—C3—H3 | 120.3 | C23—C22—C21 | 120.5 (2) |
| N1—C4—C3 | 120.8 (2) | C24—C23—C22 | 122.2 (3) |
| N1—C4—C20 | 114.0 (2) | C24—C23—H23 | 118.9 |
| C3—C4—C20 | 125.2 (2) | C22—C23—H23 | 118.9 |
| C6—C5—C2 | 124.2 (2) | C23—C24—C25 | 119.9 (2) |
| C6—C5—H5 | 117.9 | C23—C24—H24 | 120.1 |
| C2—C5—H5 | 117.9 | C25—C24—H24 | 120.1 |
| C5—C6—C7 | 128.3 (3) | C24—C25—C26 | 118.4 (2) |
| C5—C6—H6 | 115.8 | C24—C25—S3 | 126.20 (19) |
| C7—C6—H6 | 115.8 | C26—C25—S3 | 115.4 (2) |
| C12—C7—C8 | 116.8 (2) | C27—C26—C25 | 120.7 (2) |
| C12—C7—C6 | 119.4 (2) | C27—C26—H26 | 119.7 |
| C8—C7—C6 | 123.9 (2) | C25—C26—H26 | 119.7 |
| C9—C8—C7 | 121.9 (2) | C26—C27—C22 | 121.8 (2) |
| C9—C8—H8 | 119.1 | C26—C27—H27 | 119.1 |
| C7—C8—H8 | 119.1 | C22—C27—H27 | 119.1 |
| C8—C9—C10 | 120.5 (2) | C29—C28—S3 | 107.2 (2) |
| C8—C9—H9 | 119.8 | C29—C28—H28A | 110.3 |
| C10—C9—H9 | 119.8 | S3—C28—H28A | 110.3 |
| C11—C10—C9 | 118.5 (2) | C29—C28—H28B | 110.3 |
| C11—C10—S2 | 124.3 (2) | S3—C28—H28B | 110.3 |
| C9—C10—S2 | 117.21 (19) | H28A—C28—H28B | 108.5 |
| C12—C11—C10 | 120.5 (2) | C30—C29—C34 | 118.2 (3) |
| C12—C11—H11 | 119.8 | C30—C29—C28 | 119.7 (3) |
| C10—C11—H11 | 119.8 | C34—C29—C28 | 122.1 (3) |
| C11—C12—C7 | 121.9 (2) | C29—C30—C31 | 120.8 (3) |
| C11—C12—H12 | 119.0 | C29—C30—H30 | 119.6 |
| C7—C12—H12 | 119.0 | C31—C30—H30 | 119.6 |
| C14—C13—S2 | 109.33 (18) | C32—C31—C30 | 120.0 (3) |
| C14—C13—H13A | 109.8 | C32—C31—H31 | 120.0 |
| S2—C13—H13A | 109.8 | C30—C31—H31 | 120.0 |
| C14—C13—H13B | 109.8 | C33—C32—C31 | 120.2 (3) |
| S2—C13—H13B | 109.8 | C33—C32—H32 | 119.9 |
| H13A—C13—H13B | 108.3 | C31—C32—H32 | 119.9 |
| C19—C14—C15 | 118.6 (3) | C32—C33—C34 | 120.0 (3) |
| C19—C14—C13 | 120.9 (3) | C32—C33—H33 | 120.0 |
| C15—C14—C13 | 120.5 (3) | C34—C33—H33 | 120.0 |
| C16—C15—C14 | 121.4 (3) | C29—C34—C33 | 120.8 (3) |
| C16—C15—H15 | 119.3 | C29—C34—H34 | 119.6 |
| C14—C15—H15 | 119.3 | C33—C34—H34 | 119.6 |

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| C17—C16—C15 | 120.0 (4) | S1—C35—H35A | 109.5 |
| C17—C16—H16 | 120.0 | S1—C35—H35B | 109.5 |
| C15—C16—H16 | 120.0 | H35A—C35—H35B | 109.5 |
| C16—C17—C18 | 120.8 (4) | S1—C35—H35C | 109.5 |
| C16—C17—H17 | 119.6 | H35A—C35—H35C | 109.5 |
| C18—C17—H17 | 119.6 | H35B—C35—H35C | 109.5 |
| C17—C18—C19 | 119.3 (4) | | |

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| C2—N2—C1—N1 | 2.8 (4) | C13—C14—C15—C16 | −179.5 (2) |
| C2—N2—C1—S1 | −176.85 (19) | C14—C15—C16—C17 | 0.8 (5) |
| C4—N1—C1—N2 | −2.8 (4) | C15—C16—C17—C18 | −1.8 (6) |
| C4—N1—C1—S1 | 176.89 (19) | C16—C17—C18—C19 | 0.9 (6) |
| C35—S1—C1—N2 | 175.6 (2) | C15—C14—C19—C18 | −1.9 (5) |
| C35—S1—C1—N1 | −4.1 (3) | C13—C14—C19—C18 | 178.6 (3) |
| C1—N2—C2—C3 | −0.5 (4) | C17—C18—C19—C14 | 1.0 (6) |
| C1—N2—C2—C5 | 177.7 (2) | N1—C4—C20—C21 | 175.0 (3) |
| N2—C2—C3—C4 | −1.4 (4) | C3—C4—C20—C21 | −3.0 (5) |
| C5—C2—C3—C4 | −179.5 (2) | C4—C20—C21—C22 | −174.9 (2) |
| C1—N1—C4—C3 | 0.4 (4) | C20—C21—C22—C27 | 5.9 (5) |
| C1—N1—C4—C20 | −177.7 (2) | C20—C21—C22—C23 | −176.1 (3) |
| C2—C3—C4—N1 | 1.4 (4) | C27—C22—C23—C24 | 0.4 (4) |
| C2—C3—C4—C20 | 179.3 (2) | C21—C22—C23—C24 | −177.7 (3) |
| N2—C2—C5—C6 | 3.6 (4) | C22—C23—C24—C25 | 1.4 (5) |
| C3—C2—C5—C6 | −178.2 (3) | C23—C24—C25—C26 | −1.9 (4) |
| C2—C5—C6—C7 | −177.8 (3) | C23—C24—C25—S3 | 175.9 (2) |
| C5—C6—C7—C12 | −178.0 (3) | C28—S3—C25—C24 | −0.3 (3) |
| C5—C6—C7—C8 | 2.8 (5) | C28—S3—C25—C26 | 177.6 (2) |
| C12—C7—C8—C9 | −2.5 (4) | C24—C25—C26—C27 | 0.8 (4) |
| C6—C7—C8—C9 | 176.7 (3) | S3—C25—C26—C27 | −177.3 (2) |
| C7—C8—C9—C10 | 1.0 (5) | C25—C26—C27—C22 | 0.9 (4) |
| C8—C9—C10—C11 | 1.3 (4) | C23—C22—C27—C26 | −1.5 (4) |
| C8—C9—C10—S2 | −177.6 (2) | C21—C22—C27—C26 | 176.6 (3) |
| C13—S2—C10—C11 | −10.8 (3) | C25—S3—C28—C29 | −173.1 (2) |
| C13—S2—C10—C9 | 168.1 (2) | S3—C28—C29—C30 | −70.1 (3) |
| C9—C10—C11—C12 | −2.1 (4) | S3—C28—C29—C34 | 107.6 (3) |
| S2—C10—C11—C12 | 176.7 (2) | C34—C29—C30—C31 | 2.0 (5) |
| C10—C11—C12—C7 | 0.5 (4) | C28—C29—C30—C31 | 179.8 (3) |
| C8—C7—C12—C11 | 1.7 (4) | C29—C30—C31—C32 | −0.8 (6) |
| C6—C7—C12—C11 | −177.5 (2) | C30—C31—C32—C33 | −0.8 (6) |
| C10—S2—C13—C14 | −168.0 (2) | C31—C32—C33—C34 | 1.1 (5) |
| S2—C13—C14—C19 | 83.3 (3) | C30—C29—C34—C33 | −1.7 (5) |
| S2—C13—C14—C15 | −96.2 (3) | C28—C29—C34—C33 | −179.5 (3) |
| C19—C14—C15—C16 | 1.1 (4) | C32—C33—C34—C29 | 0.2 (5) |