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# 7′-Phenyl-1′,3′,5′,6′,7′,7a′-hexahydrodipiro[acenaphthylene-1,5′-pyrrolo[1,2-*c*]thiazole-6′,2″-indane]-2,1″(1*H*)-dione

**Ang Chee Wei,[a] Mohamed Ashraf Ali,[a] Tan Soo Choon,[a] Suhana Arshad[b] and Ibrahim Abdul Razak[b]*‡**

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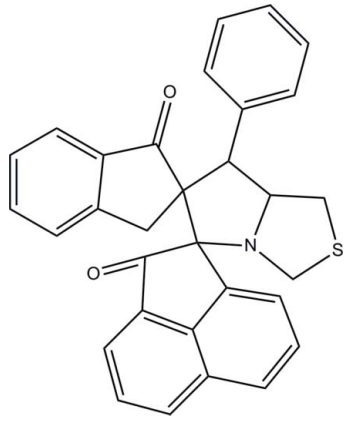
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.051; $wR$ factor = 0.124; data-to-parameter ratio = 31.8.

In the title compound, $C_{31}H_{23}NO_2S$, the pyrrolidine ring adopts an envelope conformation (with the spiro C atom as the flap), while the thiazolidine ring and the two cyclopentane rings adopt twisted conformations. The mean plane through the hexahydropyrrolo[1,2-*c*]thiazole ring [r.m.s deviation = 0.400 (1) Å] forms dihedral angles of 76.83 (4), 80.70 (5) and 79.00 (4)° with the benzene ring and the mean planes of the dihydroacenaphthylene and the dihydroindene rings, respectively. In the crystal, molecules are linked by C—H···O hydrogen bonds into sheets lying parallel to the *bc* plane. One of the ketone O atoms accepts three such bonds. Weak C—H···$\pi$ interactions are also observed.

## Related literature

For related structures, see: Wei *et al.* (2011*a*,*b*, 2012). For ring conformations, see: Cremer & Pople (1975). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

$C_{31}H_{23}NO_2S$
$M_r$ = 473.56
Monoclinic, $P2_1/c$
$a$ = 8.4054 (1) Å
$b$ = 11.3716 (1) Å
$c$ = 23.5194 (2) Å
$\beta$ = 92.259 (1)°
$V$ = 2246.30 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 100 K
0.30 × 0.18 × 0.16 mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.949, $T_{max}$ = 0.972
39597 measured reflections
10047 independent reflections
7694 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.124
$S$ = 1.03
10047 reflections
316 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C2–C6/C11 and C15–C20 rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C4—H4*A*···O1$^{i}$ | 0.95 | 2.58 | 3.2598 (14) | 129 |
| C23—H23*A*···O1$^{ii}$ | 1.00 | 2.46 | 3.4180 (14) | 160 |
| C31—H31*A*···O1$^{ii}$ | 0.95 | 2.56 | 3.4434 (14) | 155 |
| C7—H7*A*···O2$^{iii}$ | 0.95 | 2.54 | 3.4111 (14) | 152 |
| C18—H18*A*···*Cg*1$^{iv}$ | 0.95 | 2.91 | 3.5502 (14) | 126 |
| C25—H25*A*···*Cg*2$^{v}$ | 0.99 | 2.68 | 3.5182 (13) | 142 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6700).

## References

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Wei, A. C., Ali, M. A., Choon, T. S., Razak, I. A. & Arshad, S. (2012). *Acta Cryst.* E**68**, o560–o561.

# supplementary materials

*Acta Cryst.* (2012). E**68**, o1265–o1266 [doi:10.1107/S1600536812013293]

# 7′-Phenyl-1′,3′,5′,6′,7′,7a′-hexahydrodipiro[acenaphthylene-1,5′-pyrrolo[1,2-*c*]thiazole-6′,2″-indane]-2,1″(1*H*)-dione

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## Comment

As part of our ongoing search to prepare heterocyclic compounds with potential antitubercular activity (Wei *et al.*, 2011*a*,*b*), we have synthesized the title compound as described below.

In the molecular structure (Fig 1), the pyrrolidine ring (N1/C12/C13/C22/C23) is in envelope conformation (Cremer & Pople, 1975) [puckering parameters, Q= 0.4480 (11) Å and $\varphi$= 68.75 (14)° with atom C13 at the flap]. Meanwhile, the thiazolidine ring and the two cyclopentane rings (S1/N1/C23–C25, C1/C2/C10–C12 & C13–C15/C20/C21) are twisted about C25–S1 bond [puckering parameters, Q= 0.3450 (11) Å and $\varphi$= 339.37 (19)°], C12–C1 bond [puckering parameters, Q= 0.1209 (11) Å and $\varphi$= 167.0 (5)°] and C13–S14 bond [puckering parameters, Q= 0.2875 (11) Å and $\varphi$= 190.5 (2)°], respectively, adopting half-chair conformation. In addition, the dihedral angles between the mean plane through the hexahydropyrrolo [1,2-*c*]thiazole ring (S1/N1/C12/C13/C22–C25) [r.m.s deviation of 0.400 (1) Å] with the benzene ring (C26–C31) and the mean planes of the dihydroacenaphthylene and the dihydro-indene rings (C1–C10/C12 & C13–C21) are 76.83 (4), 80.70 (5) and 79.00 (4)°, respectively. The bond lengths and angles are within normal ranges and comparable to the related structure (Wei, *et al.*, 2011*b*; Wei, *et al.*, 2012).

The crystal packing is shown in Fig. 2. The molecules are linked into sheets lying parallel to *bc*-plane *via* C7—H7A···O2, C4—H4A···O1, C23—H23A···O1 and C31—H31A···O1 (Table 1) hydrogen bonds. The crystal structure also features C18—H18A···*Cg*1 and C25—H25A···*Cg*2 (Table 1) interactions (*Cg*1 and *Cg*2 are the centroids of the C2–C6/C11 and C15–C20 rings, respectively).

## Experimental

A mixture of (*E*)-(2-benzylidene)-2,3-dihydro-1*H*-indene-1-one (0.001 mol), acenaphthenequinone (0.001 mol) and thiazolidine-4-carboxylic acid (0.002 mol) (1:1:2) were dissolved in methanol (10 ml) and refluxed for 4 h. After completion of the reaction as evident from TLC, the excess solvent was evaporated slowly and the product was separated and recrystallized from methanol to reveal the title compound as yellow crystals.

## Refinement

All H atoms were positioned geometrically (C–H = 0.95 and 1.00 Å) and refined using a riding model with $U_{iso}$(H) = 1.2 $U_{eq}$(C).

## Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication:

*SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

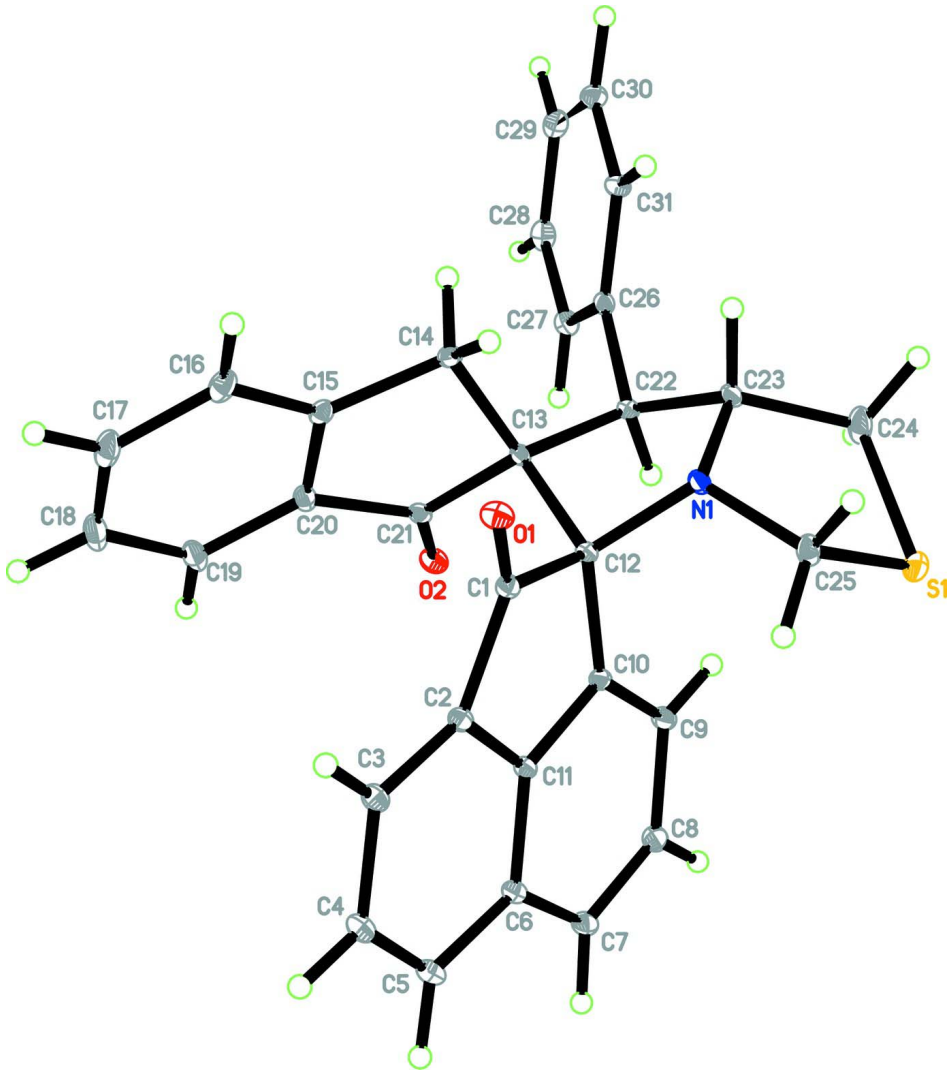


**Figure 1**

The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

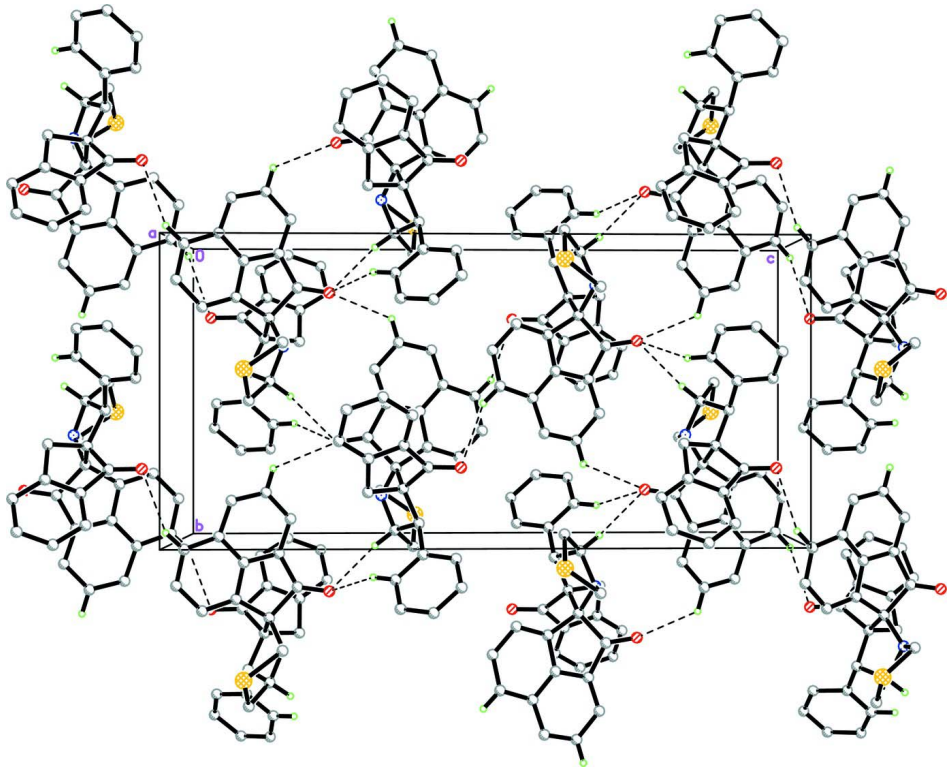

**Figure 2**

The crystal packing of the title compound. The H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

### 7′-Phenyl-1′,3′,5′,6′,7′,7a′-hexahydrodipiro[acenaphthene-1,5′- pyrrolo[1,2-*c*]thiazole-6′,2′′-indane]-2,1′′(1*H*)-dione

*Crystal data*

$C_{31}H_{23}NO_2S$
$M_r = 473.56$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.4054$ (1) Å
$b = 11.3716$ (1) Å
$c = 23.5194$ (2) Å
$\beta = 92.259$ (1)°
$V = 2246.30$ (4) Å$^3$
$Z = 4$
$F(000) = 992$
$D_x = 1.400$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9949 reflections
$\theta = 2.5$–35.2°
$\mu = 0.18$ mm$^{-1}$
$T = 100$ K
Block, yellow
0.30 × 0.18 × 0.16 mm

*Data collection*

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.949$, $T_{max} = 0.972$
39597 measured reflections
10047 independent reflections
7694 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 35.3°$, $\theta_{min} = 2.0°$
$h = -13 \rightarrow 13$
$k = -18 \rightarrow 14$
$l = -38 \rightarrow 28$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.124$
$S = 1.03$
10047 reflections
316 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
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.9508P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**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 | 0.86000 (4) | 0.42837 (3) | 0.121701 (14) | 0.01913 (7) |
| O1 | 0.48435 (10) | 0.17004 (8) | 0.24386 (3) | 0.01480 (15) |
| O2 | 0.24182 (10) | 0.24847 (8) | 0.04159 (3) | 0.01487 (16) |
| N1 | 0.60468 (11) | 0.35224 (8) | 0.17368 (4) | 0.01107 (16) |
| C1 | 0.49807 (12) | 0.15401 (9) | 0.19309 (4) | 0.01060 (17) |
| C2 | 0.51959 (12) | 0.04064 (9) | 0.16415 (4) | 0.01095 (18) |
| C3 | 0.50561 (13) | −0.07416 (10) | 0.18207 (5) | 0.01361 (19) |
| H3A | 0.4668 | −0.0923 | 0.2184 | 0.016* |
| C4 | 0.55106 (14) | −0.16396 (10) | 0.14435 (5) | 0.0159 (2) |
| H4A | 0.5401 | −0.2437 | 0.1556 | 0.019* |
| C5 | 0.61100 (14) | −0.13945 (10) | 0.09164 (5) | 0.0153 (2) |
| H5A | 0.6423 | −0.2022 | 0.0679 | 0.018* |
| C6 | 0.62624 (13) | −0.02169 (10) | 0.07274 (5) | 0.01244 (18) |
| C7 | 0.68707 (13) | 0.01653 (10) | 0.02044 (5) | 0.0147 (2) |
| H7A | 0.7235 | −0.0392 | −0.0062 | 0.018* |
| C8 | 0.69293 (14) | 0.13492 (10) | 0.00849 (5) | 0.0147 (2) |
| H8A | 0.7345 | 0.1592 | −0.0266 | 0.018* |
| C9 | 0.63933 (13) | 0.22232 (10) | 0.04655 (5) | 0.01278 (18) |
| H9A | 0.6441 | 0.3032 | 0.0367 | 0.015* |
| C10 | 0.58047 (12) | 0.18838 (9) | 0.09778 (4) | 0.01008 (17) |
| C11 | 0.57568 (12) | 0.06664 (9) | 0.10990 (4) | 0.01046 (17) |
| C12 | 0.51304 (12) | 0.25553 (9) | 0.14809 (4) | 0.00966 (17) |
| C13 | 0.34938 (12) | 0.32033 (9) | 0.13396 (4) | 0.00936 (17) |
| C14 | 0.25058 (12) | 0.32869 (10) | 0.18797 (4) | 0.01128 (18) |

| | | | | |
|---|---|---|---|---|
| H14A | 0.3205 | 0.3309 | 0.2228 | 0.014* |
| H14B | 0.1818 | 0.3994 | 0.1869 | 0.014* |
| C15 | 0.15252 (12) | 0.21773 (10) | 0.18530 (5) | 0.01242 (18) |
| C16 | 0.07876 (14) | 0.15873 (11) | 0.22895 (5) | 0.0173 (2) |
| H16A | 0.0894 | 0.1859 | 0.2671 | 0.021* |
| C17 | −0.01086 (15) | 0.05901 (12) | 0.21539 (6) | 0.0217 (2) |
| H17A | −0.0608 | 0.0174 | 0.2448 | 0.026* |
| C18 | −0.02897 (15) | 0.01885 (12) | 0.15930 (6) | 0.0221 (2) |
| H18A | −0.0930 | −0.0483 | 0.1510 | 0.027* |
| C19 | 0.04614 (14) | 0.07663 (11) | 0.11552 (6) | 0.0176 (2) |
| H19A | 0.0346 | 0.0501 | 0.0773 | 0.021* |
| C20 | 0.13885 (13) | 0.17474 (10) | 0.12972 (5) | 0.01284 (18) |
| C21 | 0.24112 (12) | 0.24687 (9) | 0.09327 (4) | 0.01074 (17) |
| C22 | 0.40993 (12) | 0.43806 (9) | 0.10995 (4) | 0.01032 (17) |
| H22A | 0.4528 | 0.4210 | 0.0717 | 0.012* |
| C23 | 0.55326 (12) | 0.46704 (10) | 0.15034 (5) | 0.01232 (18) |
| H23A | 0.5157 | 0.5170 | 0.1821 | 0.015* |
| C24 | 0.69479 (14) | 0.52975 (11) | 0.12283 (6) | 0.0225 (3) |
| H24A | 0.7256 | 0.6006 | 0.1451 | 0.027* |
| H24B | 0.6638 | 0.5545 | 0.0836 | 0.027* |
| C25 | 0.77507 (13) | 0.34147 (11) | 0.17878 (5) | 0.0159 (2) |
| H25A | 0.8066 | 0.2580 | 0.1753 | 0.019* |
| H25B | 0.8146 | 0.3710 | 0.2163 | 0.019* |
| C26 | 0.28586 (12) | 0.53385 (9) | 0.10170 (4) | 0.01095 (17) |
| C27 | 0.20247 (13) | 0.54334 (10) | 0.04912 (5) | 0.01402 (19) |
| H27A | 0.2268 | 0.4909 | 0.0192 | 0.017* |
| C28 | 0.08491 (14) | 0.62787 (11) | 0.03980 (5) | 0.0170 (2) |
| H28A | 0.0287 | 0.6319 | 0.0040 | 0.020* |
| C29 | 0.04933 (14) | 0.70648 (11) | 0.08275 (5) | 0.0176 (2) |
| H29A | −0.0311 | 0.7643 | 0.0765 | 0.021* |
| C30 | 0.13264 (14) | 0.69968 (10) | 0.13495 (5) | 0.0163 (2) |
| H30A | 0.1102 | 0.7540 | 0.1642 | 0.020* |
| C31 | 0.24880 (13) | 0.61373 (10) | 0.14462 (5) | 0.01328 (19) |
| H31A | 0.3035 | 0.6092 | 0.1807 | 0.016* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.01378 (12) | 0.01626 (14) | 0.02775 (15) | −0.00203 (10) | 0.00564 (10) | 0.00049 (11) |
| O1 | 0.0201 (4) | 0.0142 (4) | 0.0101 (3) | 0.0016 (3) | 0.0005 (3) | 0.0002 (3) |
| O2 | 0.0185 (4) | 0.0146 (4) | 0.0114 (3) | −0.0002 (3) | −0.0016 (3) | −0.0021 (3) |
| N1 | 0.0106 (4) | 0.0089 (4) | 0.0135 (4) | −0.0008 (3) | −0.0017 (3) | −0.0008 (3) |
| C1 | 0.0104 (4) | 0.0104 (4) | 0.0110 (4) | 0.0011 (3) | −0.0002 (3) | 0.0010 (3) |
| C2 | 0.0123 (4) | 0.0094 (4) | 0.0111 (4) | 0.0004 (3) | −0.0002 (3) | 0.0004 (3) |
| C3 | 0.0159 (4) | 0.0113 (5) | 0.0136 (4) | −0.0005 (4) | 0.0000 (3) | 0.0014 (4) |
| C4 | 0.0202 (5) | 0.0095 (5) | 0.0180 (5) | −0.0007 (4) | 0.0002 (4) | 0.0012 (4) |
| C5 | 0.0185 (5) | 0.0104 (5) | 0.0169 (5) | 0.0005 (4) | 0.0000 (4) | −0.0019 (4) |
| C6 | 0.0142 (4) | 0.0098 (4) | 0.0133 (4) | 0.0003 (4) | 0.0004 (3) | −0.0017 (3) |
| C7 | 0.0168 (5) | 0.0139 (5) | 0.0138 (4) | −0.0009 (4) | 0.0031 (4) | −0.0041 (4) |
| C8 | 0.0170 (5) | 0.0149 (5) | 0.0123 (4) | −0.0019 (4) | 0.0041 (4) | −0.0016 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0154 (4) | 0.0109 (4) | 0.0123 (4) | −0.0006 (4) | 0.0031 (3) | −0.0001 (3) |
| C10 | 0.0106 (4) | 0.0090 (4) | 0.0107 (4) | 0.0006 (3) | 0.0009 (3) | −0.0001 (3) |
| C11 | 0.0112 (4) | 0.0087 (4) | 0.0114 (4) | 0.0000 (3) | 0.0004 (3) | −0.0001 (3) |
| C12 | 0.0109 (4) | 0.0084 (4) | 0.0097 (4) | −0.0002 (3) | 0.0004 (3) | −0.0001 (3) |
| C13 | 0.0098 (4) | 0.0088 (4) | 0.0095 (4) | −0.0005 (3) | 0.0000 (3) | −0.0009 (3) |
| C14 | 0.0118 (4) | 0.0108 (4) | 0.0113 (4) | 0.0008 (3) | 0.0020 (3) | −0.0005 (3) |
| C15 | 0.0099 (4) | 0.0128 (5) | 0.0146 (4) | 0.0021 (4) | 0.0015 (3) | 0.0024 (4) |
| C16 | 0.0146 (5) | 0.0194 (6) | 0.0183 (5) | 0.0016 (4) | 0.0043 (4) | 0.0062 (4) |
| C17 | 0.0147 (5) | 0.0195 (6) | 0.0310 (6) | −0.0005 (4) | 0.0044 (4) | 0.0122 (5) |
| C18 | 0.0149 (5) | 0.0151 (5) | 0.0362 (7) | −0.0035 (4) | −0.0012 (5) | 0.0064 (5) |
| C19 | 0.0148 (5) | 0.0127 (5) | 0.0251 (6) | −0.0027 (4) | −0.0031 (4) | 0.0012 (4) |
| C20 | 0.0116 (4) | 0.0112 (5) | 0.0156 (5) | −0.0006 (4) | −0.0007 (3) | 0.0012 (4) |
| C21 | 0.0109 (4) | 0.0083 (4) | 0.0128 (4) | 0.0013 (3) | −0.0014 (3) | −0.0006 (3) |
| C22 | 0.0116 (4) | 0.0086 (4) | 0.0108 (4) | 0.0000 (3) | 0.0004 (3) | −0.0005 (3) |
| C23 | 0.0116 (4) | 0.0083 (4) | 0.0169 (5) | 0.0001 (3) | −0.0016 (3) | −0.0017 (4) |
| C24 | 0.0140 (5) | 0.0142 (5) | 0.0390 (7) | −0.0026 (4) | −0.0021 (5) | 0.0093 (5) |
| C25 | 0.0122 (4) | 0.0133 (5) | 0.0219 (5) | −0.0007 (4) | −0.0038 (4) | 0.0025 (4) |
| C26 | 0.0111 (4) | 0.0092 (4) | 0.0125 (4) | −0.0005 (3) | 0.0003 (3) | 0.0011 (3) |
| C27 | 0.0156 (4) | 0.0132 (5) | 0.0132 (4) | −0.0006 (4) | −0.0007 (3) | 0.0019 (4) |
| C28 | 0.0153 (5) | 0.0166 (5) | 0.0188 (5) | −0.0007 (4) | −0.0029 (4) | 0.0065 (4) |
| C29 | 0.0139 (5) | 0.0131 (5) | 0.0260 (6) | 0.0023 (4) | 0.0018 (4) | 0.0068 (4) |
| C30 | 0.0164 (5) | 0.0114 (5) | 0.0215 (5) | 0.0024 (4) | 0.0042 (4) | 0.0004 (4) |
| C31 | 0.0147 (4) | 0.0105 (5) | 0.0146 (4) | 0.0013 (4) | 0.0007 (3) | −0.0005 (4) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| S1—C24 | 1.8058 (13) | C14—H14B | 0.9900 |
| S1—C25 | 1.8340 (12) | C15—C16 | 1.3923 (15) |
| O1—C1 | 1.2178 (12) | C15—C20 | 1.3961 (16) |
| O2—C21 | 1.2159 (13) | C16—C17 | 1.3914 (19) |
| N1—C25 | 1.4377 (14) | C16—H16A | 0.9500 |
| N1—C12 | 1.4589 (14) | C17—C18 | 1.398 (2) |
| N1—C23 | 1.4743 (14) | C17—H17A | 0.9500 |
| C1—C2 | 1.4724 (15) | C18—C19 | 1.3936 (18) |
| C1—C12 | 1.5745 (15) | C18—H18A | 0.9500 |
| C2—C3 | 1.3782 (15) | C19—C20 | 1.3939 (16) |
| C2—C11 | 1.4090 (14) | C19—H19A | 0.9500 |
| C3—C4 | 1.4151 (16) | C20—C21 | 1.4849 (15) |
| C3—H3A | 0.9500 | C22—C26 | 1.5152 (15) |
| C4—C5 | 1.3849 (16) | C22—C23 | 1.5403 (15) |
| C4—H4A | 0.9500 | C22—H22A | 1.0000 |
| C5—C6 | 1.4184 (16) | C23—C24 | 1.5502 (16) |
| C5—H5A | 0.9500 | C23—H23A | 1.0000 |
| C6—C11 | 1.4080 (15) | C24—H24A | 0.9900 |
| C6—C7 | 1.4187 (15) | C24—H24B | 0.9900 |
| C7—C8 | 1.3766 (17) | C25—H25A | 0.9900 |
| C7—H7A | 0.9500 | C25—H25B | 0.9900 |
| C8—C9 | 1.4227 (15) | C26—C27 | 1.4014 (15) |
| C8—H8A | 0.9500 | C26—C31 | 1.4021 (15) |
| C9—C10 | 1.3757 (14) | C27—C28 | 1.3898 (16) |

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|---|---|---|---|
| C9—H9A | 0.9500 | C27—H27A | 0.9500 |
| C10—C11 | 1.4142 (15) | C28—C29 | 1.3903 (18) |
| C10—C12 | 1.5355 (14) | C28—H28A | 0.9500 |
| C12—C13 | 1.5842 (14) | C29—C30 | 1.3914 (18) |
| C13—C21 | 1.5405 (15) | C29—H29A | 0.9500 |
| C13—C22 | 1.5469 (15) | C30—C31 | 1.3938 (16) |
| C13—C14 | 1.5477 (14) | C30—H30A | 0.9500 |
| C14—C15 | 1.5071 (16) | C31—H31A | 0.9500 |
| C14—H14A | 0.9900 | | |

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| C24—S1—C25 | 90.66 (6) | C17—C16—H16A | 120.8 |
| C25—N1—C12 | 118.57 (9) | C15—C16—H16A | 120.8 |
| C25—N1—C23 | 112.52 (9) | C16—C17—C18 | 121.35 (11) |
| C12—N1—C23 | 111.82 (8) | C16—C17—H17A | 119.3 |
| O1—C1—C2 | 127.04 (10) | C18—C17—H17A | 119.3 |
| O1—C1—C12 | 124.22 (10) | C19—C18—C17 | 120.49 (12) |
| C2—C1—C12 | 108.47 (8) | C19—C18—H18A | 119.8 |
| C3—C2—C11 | 120.75 (10) | C17—C18—H18A | 119.8 |
| C3—C2—C1 | 132.42 (10) | C18—C19—C20 | 117.75 (12) |
| C11—C2—C1 | 106.65 (9) | C18—C19—H19A | 121.1 |
| C2—C3—C4 | 117.61 (10) | C20—C19—H19A | 121.1 |
| C2—C3—H3A | 121.2 | C19—C20—C15 | 121.95 (10) |
| C4—C3—H3A | 121.2 | C19—C20—C21 | 129.39 (11) |
| C5—C4—C3 | 122.18 (11) | C15—C20—C21 | 108.61 (9) |
| C5—C4—H4A | 118.9 | O2—C21—C20 | 127.67 (10) |
| C3—C4—H4A | 118.9 | O2—C21—C13 | 125.94 (10) |
| C4—C5—C6 | 120.74 (10) | C20—C21—C13 | 106.38 (9) |
| C4—C5—H5A | 119.6 | C26—C22—C23 | 116.28 (9) |
| C6—C5—H5A | 119.6 | C26—C22—C13 | 115.74 (8) |
| C11—C6—C5 | 116.48 (10) | C23—C22—C13 | 102.74 (8) |
| C11—C6—C7 | 116.58 (10) | C26—C22—H22A | 107.2 |
| C5—C6—C7 | 126.94 (10) | C23—C22—H22A | 107.2 |
| C8—C7—C6 | 119.58 (10) | C13—C22—H22A | 107.2 |
| C8—C7—H7A | 120.2 | N1—C23—C22 | 104.53 (8) |
| C6—C7—H7A | 120.2 | N1—C23—C24 | 110.13 (9) |
| C7—C8—C9 | 122.68 (10) | C22—C23—C24 | 115.81 (10) |
| C7—C8—H8A | 118.7 | N1—C23—H23A | 108.7 |
| C9—C8—H8A | 118.7 | C22—C23—H23A | 108.7 |
| C10—C9—C8 | 119.27 (10) | C24—C23—H23A | 108.7 |
| C10—C9—H9A | 120.4 | C23—C24—S1 | 108.40 (8) |
| C8—C9—H9A | 120.4 | C23—C24—H24A | 110.0 |
| C9—C10—C11 | 117.72 (9) | S1—C24—H24A | 110.0 |
| C9—C10—C12 | 133.78 (10) | C23—C24—H24B | 110.0 |
| C11—C10—C12 | 108.49 (8) | S1—C24—H24B | 110.0 |
| C6—C11—C2 | 122.16 (10) | H24A—C24—H24B | 108.4 |
| C6—C11—C10 | 124.16 (9) | N1—C25—S1 | 107.95 (8) |
| C2—C11—C10 | 113.65 (9) | N1—C25—H25A | 110.1 |
| N1—C12—C10 | 119.20 (8) | S1—C25—H25A | 110.1 |
| N1—C12—C1 | 109.29 (8) | N1—C25—H25B | 110.1 |

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| C10—C12—C1 | 101.25 (8) | S1—C25—H25B | 110.1 |
| N1—C12—C13 | 100.13 (8) | H25A—C25—H25B | 108.4 |
| C10—C12—C13 | 114.42 (8) | C27—C26—C31 | 117.89 (10) |
| C1—C12—C13 | 112.98 (8) | C27—C26—C22 | 119.08 (9) |
| C21—C13—C22 | 115.93 (8) | C31—C26—C22 | 123.02 (10) |
| C21—C13—C14 | 102.72 (8) | C28—C27—C26 | 121.35 (11) |
| C22—C13—C14 | 116.20 (8) | C28—C27—H27A | 119.3 |
| C21—C13—C12 | 111.40 (8) | C26—C27—H27A | 119.3 |
| C22—C13—C12 | 100.58 (8) | C27—C28—C29 | 120.14 (11) |
| C14—C13—C12 | 110.24 (8) | C27—C28—H28A | 119.9 |
| C15—C14—C13 | 102.98 (8) | C29—C28—H28A | 119.9 |
| C15—C14—H14A | 111.2 | C28—C29—C30 | 119.35 (11) |
| C13—C14—H14A | 111.2 | C28—C29—H29A | 120.3 |
| C15—C14—H14B | 111.2 | C30—C29—H29A | 120.3 |
| C13—C14—H14B | 111.2 | C29—C30—C31 | 120.52 (11) |
| H14A—C14—H14B | 109.1 | C29—C30—H30A | 119.7 |
| C16—C15—C20 | 119.94 (11) | C31—C30—H30A | 119.7 |
| C16—C15—C14 | 129.15 (11) | C30—C31—C26 | 120.73 (11) |
| C20—C15—C14 | 110.90 (9) | C30—C31—H31A | 119.6 |
| C17—C16—C15 | 118.45 (12) | C26—C31—H31A | 119.6 |

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| O1—C1—C2—C3 | 11.8 (2) | C12—C13—C14—C15 | −90.66 (10) |
| C12—C1—C2—C3 | −173.99 (11) | C13—C14—C15—C16 | 158.41 (11) |
| O1—C1—C2—C11 | −163.15 (11) | C13—C14—C15—C20 | −22.15 (11) |
| C12—C1—C2—C11 | 11.09 (11) | C20—C15—C16—C17 | −1.61 (17) |
| C11—C2—C3—C4 | 0.66 (16) | C14—C15—C16—C17 | 177.78 (11) |
| C1—C2—C3—C4 | −173.68 (11) | C15—C16—C17—C18 | −0.76 (18) |
| C2—C3—C4—C5 | 1.38 (17) | C16—C17—C18—C19 | 1.58 (19) |
| C3—C4—C5—C6 | −1.31 (18) | C17—C18—C19—C20 | 0.02 (18) |
| C4—C5—C6—C11 | −0.79 (16) | C18—C19—C20—C15 | −2.44 (17) |
| C4—C5—C6—C7 | 179.17 (11) | C18—C19—C20—C21 | 174.76 (11) |
| C11—C6—C7—C8 | −0.39 (16) | C16—C15—C20—C19 | 3.28 (17) |
| C5—C6—C7—C8 | 179.66 (12) | C14—C15—C20—C19 | −176.22 (10) |
| C6—C7—C8—C9 | −0.32 (18) | C16—C15—C20—C21 | −174.43 (10) |
| C7—C8—C9—C10 | 0.68 (17) | C14—C15—C20—C21 | 6.07 (12) |
| C8—C9—C10—C11 | −0.29 (16) | C19—C20—C21—O2 | 15.01 (19) |
| C8—C9—C10—C12 | −179.68 (11) | C15—C20—C21—O2 | −167.50 (11) |
| C5—C6—C11—C2 | 2.84 (16) | C19—C20—C21—C13 | −164.61 (11) |
| C7—C6—C11—C2 | −177.12 (10) | C15—C20—C21—C13 | 12.88 (12) |
| C5—C6—C11—C10 | −179.25 (10) | C22—C13—C21—O2 | 26.92 (15) |
| C7—C6—C11—C10 | 0.79 (16) | C14—C13—C21—O2 | 154.73 (11) |
| C3—C2—C11—C6 | −2.84 (16) | C12—C13—C21—O2 | −87.27 (13) |
| C1—C2—C11—C6 | 172.80 (10) | C22—C13—C21—C20 | −153.45 (9) |
| C3—C2—C11—C10 | 179.05 (10) | C14—C13—C21—C20 | −25.64 (10) |
| C1—C2—C11—C10 | −5.31 (12) | C12—C13—C21—C20 | 92.35 (10) |
| C9—C10—C11—C6 | −0.45 (16) | C21—C13—C22—C26 | 70.82 (11) |
| C12—C10—C11—C6 | 179.09 (10) | C14—C13—C22—C26 | −49.99 (12) |
| C9—C10—C11—C2 | 177.62 (10) | C12—C13—C22—C26 | −168.95 (8) |
| C12—C10—C11—C2 | −2.84 (12) | C21—C13—C22—C23 | −161.38 (8) |

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| C25—N1—C12—C10 | −37.51 (14) | C14—C13—C22—C23 | 77.81 (10) |
| C23—N1—C12—C10 | 95.94 (11) | C12—C13—C22—C23 | −41.15 (9) |
| C25—N1—C12—C1 | 78.11 (11) | C25—N1—C23—C22 | 140.45 (9) |
| C23—N1—C12—C1 | −148.44 (8) | C12—N1—C23—C22 | 4.10 (11) |
| C25—N1—C12—C13 | −163.03 (9) | C25—N1—C23—C24 | 15.42 (13) |
| C23—N1—C12—C13 | −29.58 (10) | C12—N1—C23—C24 | −120.94 (10) |
| C9—C10—C12—N1 | −51.77 (16) | C26—C22—C23—N1 | 151.58 (9) |
| C11—C10—C12—N1 | 128.81 (10) | C13—C22—C23—N1 | 24.12 (10) |
| C9—C10—C12—C1 | −171.57 (12) | C26—C22—C23—C24 | −87.07 (12) |
| C11—C10—C12—C1 | 9.00 (10) | C13—C22—C23—C24 | 145.48 (9) |
| C9—C10—C12—C13 | 66.60 (15) | N1—C23—C24—S1 | 7.73 (12) |
| C11—C10—C12—C13 | −112.83 (10) | C22—C23—C24—S1 | −110.57 (10) |
| O1—C1—C12—N1 | 35.65 (13) | C25—S1—C24—C23 | −21.26 (10) |
| C2—C1—C12—N1 | −138.80 (9) | C12—N1—C25—S1 | 101.83 (9) |
| O1—C1—C12—C10 | 162.27 (10) | C23—N1—C25—S1 | −31.32 (11) |
| C2—C1—C12—C10 | −12.17 (10) | C24—S1—C25—N1 | 30.36 (9) |
| O1—C1—C12—C13 | −74.89 (13) | C23—C22—C26—C27 | 147.99 (10) |
| C2—C1—C12—C13 | 110.66 (9) | C13—C22—C26—C27 | −91.27 (12) |
| N1—C12—C13—C21 | 166.23 (8) | C23—C22—C26—C31 | −32.59 (14) |
| C10—C12—C13—C21 | 37.52 (11) | C13—C22—C26—C31 | 88.14 (12) |
| C1—C12—C13—C21 | −77.65 (10) | C31—C26—C27—C28 | −0.97 (16) |
| N1—C12—C13—C22 | 42.79 (9) | C22—C26—C27—C28 | 178.47 (10) |
| C10—C12—C13—C22 | −85.92 (10) | C26—C27—C28—C29 | 0.96 (17) |
| C1—C12—C13—C22 | 158.92 (8) | C27—C28—C29—C30 | 0.09 (17) |
| N1—C12—C13—C14 | −80.40 (9) | C28—C29—C30—C31 | −1.11 (17) |
| C10—C12—C13—C14 | 150.88 (9) | C29—C30—C31—C26 | 1.10 (17) |
| C1—C12—C13—C14 | 35.72 (11) | C27—C26—C31—C30 | −0.06 (16) |
| C21—C13—C14—C15 | 28.15 (10) | C22—C26—C31—C30 | −179.48 (10) |
| C22—C13—C14—C15 | 155.79 (9) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C2–C6/C11 and C15–C20 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C4—H4*A*···O1$^{i}$ | 0.95 | 2.58 | 3.2598 (14) | 129 |
| C23—H23*A*···O1$^{ii}$ | 1.00 | 2.46 | 3.4180 (14) | 160 |
| C31—H31*A*···O1$^{ii}$ | 0.95 | 2.56 | 3.4434 (14) | 155 |
| C7—H7*A*···O2$^{iii}$ | 0.95 | 2.54 | 3.4111 (14) | 152 |
| C18—H18*A*···*Cg*1$^{iv}$ | 0.95 | 2.91 | 3.5502 (14) | 126 |
| C25—H25*A*···*Cg*2$^{v}$ | 0.99 | 2.68 | 3.5182 (13) | 142 |

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, *y*+1/2, −*z*+1/2; (iii) −*x*+1, −*y*, −*z*; (iv) *x*−1, *y*, *z*; (v) *x*+1, *y*, *z*.