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1-(4-Chlorophenyl)-2-[(3-phenyl-isoquinolin-1-yl)sulfanyl]ethanone

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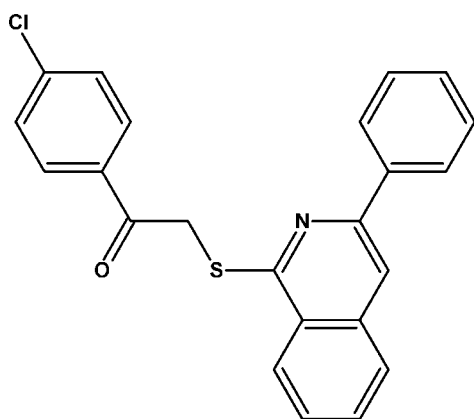
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.071; wR factor = 0.125; data-to-parameter ratio = 13.7.

The title compound, $\text{C}_{23}\text{H}_{16}\text{ClNOS}$, exhibits dihedral angles of 11.73 (1) and 66.07 (1)°, respectively, between the mean plane of the isoquinoline system and the attached phenyl ring, and between the isoquinoline system and the chlorophenyl ring. The dihedral angle between the phenyl and chlorophenyl rings is 54.66 (1)°.

Related literature

For general background, see: Cremlyn *et al.* (1996); Carreno (1995); Kondo *et al.* (2000); Mosberg & Omnaas (1985); McReynolds *et al.* (2004). For related crystal structures, see: Hathwar *et al.* (2008); Manivel *et al.* (2009).



Experimental

Crystal data

$\text{C}_{23}\text{H}_{16}\text{ClNOS}$
 $M_r = 389.89$
 Orthorhombic, $Pbca$
 $a = 9.5874$ (14) Å
 $b = 17.888$ (3) Å
 $c = 22.025$ (3) Å
 $V = 3777.3$ (10) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.33$ mm⁻¹
 $T = 290$ (2) K
 $0.26 \times 0.20 \times 0.14$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.901$, $T_{\max} = 0.956$
 25674 measured reflections
 3332 independent reflections
 1915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.116$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.071$
 $wR(F^2) = 0.125$
 $S = 1.04$
 3332 reflections
 244 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.23$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2532).

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supplementary materials

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1-(4-Chlorophenyl)-2-[(3-phenylisoquinolin-1-yl)sulfanyl]ethanone

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Comment

Organic thioethers are useful synthetic intermediates, key reagents in organic synthesis, bio-organic, medicinal, and heterocyclic chemistry (Cremlyn, 1996 and McReynolds *et al.*, 2004). They are also useful as heteroatomic functional groups in organic synthesis, for example, chiral sulphoxides can be generated by the oxidation of thioethers which are useful as auxiliaries in asymmetric syntheses (Carreno, 1995). Many syntheses have been reported for the preparation of thioethers in literature (Kondo *et al.*, 2000) whereas commonly used method is the alkylation of thiols (Mosberg *et al.*, 1985 and references there in).

The compound (I) forms the dihedral angles of 11.73 (1)° and 66.07 (1)° between mean plane of isoquinoline moiety and phenyl ring and mean plane of isoquinoline moiety and chlorophenyl ring respectively. The crystal packing is stabilized by C—H...O inter molecular Hydrogen bonds (Figure 2).

Experimental

3-Phenylisoquinoline-1-thiol and 2-bromo-1-(4-chlorophenyl)ethanone were mixed in the ratio 1:1.05 equivalents with ethanol in a round bottom flask. Then it was heated under nitrogen atmosphere on an oil bath at 323 K. After 2 h, the products were filtered and dissolved in chloroform. Further, it was washed with water, dried and concentrated. The single-crystal for X-ray structure analysis was obtained from ether solution by slow evaporation.

Refinement

All the H atoms in (I) were positioned geometrically and refined using a riding model with C—H bond lengths of 0.93 Å and 0.97 Å for aromatic and for methylene H atoms respectively and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for all carbon bound H atoms.

Figures

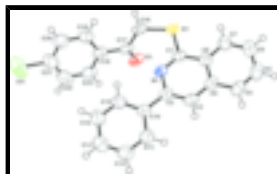


Fig. 1. ORTEP diagram of the asymmetric unit of (I) with 50% probability displacement ellipsoids.

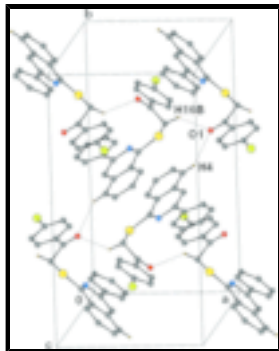


Fig. 2. The crystal packing diagram of (I). The dotted lines indicate intermolecular C—H...O hydrogen bonds. All H atoms have been omitted for clarity.

1-(4-Chlorophenyl)-2-[(3-phenylisoquinolin-1-yl)sulfanyl]ethanone

Crystal data

C₂₃H₁₆ClNOS

M_r = 389.89

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

a = 9.5874 (14) Å

b = 17.888 (3) Å

c = 22.025 (3) Å

V = 3777.3 (10) Å³

Z = 8

*F*₀₀₀ = 1616

D_x = 1.371 Mg m⁻³

Mo *K*α radiation

λ = 0.71073 Å

Cell parameters from 871 reflections

θ = 1.9–25.0°

μ = 0.33 mm⁻¹

T = 290 (2) K

Rod, colourless

0.26 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 290(2) K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

T_{min} = 0.901, *T_{max}* = 0.956

25674 measured reflections

3332 independent reflections

1915 reflections with *I* > 2σ(*I*)

R_{int} = 0.116

θ_{max} = 25.0°

θ_{min} = 1.9°

h = -11→11

k = -21→21

l = -24→26

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.071

wR(*F*²) = 0.125

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0308P)^2 + 0.7191P]$$

where *P* = (*F_o*² + 2*F_c*²)/3

| | |
|--|--|
| $S = 1.04$ | $(\Delta/\sigma)_{\max} < 0.001$ |
| 3332 reflections | $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$ |
| 244 parameters | $\Delta\rho_{\min} = -0.23 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|--------------|---------------|----------------------------------|
| C11 | -0.16890 (17) | 0.07371 (9) | 0.25163 (6) | 0.1375 (6) |
| S1 | -0.09127 (10) | 0.34062 (5) | -0.06818 (5) | 0.0545 (3) |
| O1 | 0.0295 (2) | 0.19469 (13) | -0.02148 (12) | 0.0588 (7) |
| N1 | 0.0851 (3) | 0.36685 (14) | 0.02265 (13) | 0.0406 (7) |
| C1 | 0.0416 (3) | 0.39062 (18) | -0.03051 (16) | 0.0401 (9) |
| C2 | 0.1941 (3) | 0.40302 (18) | 0.05067 (15) | 0.0390 (9) |
| C3 | 0.2597 (4) | 0.46147 (19) | 0.02355 (16) | 0.0460 (9) |
| H3 | 0.3348 | 0.4841 | 0.0430 | 0.055* |
| C4 | 0.2805 (4) | 0.54850 (19) | -0.06405 (19) | 0.0554 (10) |
| H4 | 0.3564 | 0.5724 | -0.0463 | 0.067* |
| C5 | 0.2337 (5) | 0.5720 (2) | -0.1189 (2) | 0.0644 (12) |
| H5 | 0.2784 | 0.6111 | -0.1387 | 0.077* |
| C6 | 0.1184 (5) | 0.5375 (2) | -0.14581 (18) | 0.0665 (12) |
| H6 | 0.0862 | 0.5543 | -0.1832 | 0.080* |
| C7 | 0.0532 (4) | 0.47981 (19) | -0.11778 (17) | 0.0570 (11) |
| H7 | -0.0237 | 0.4575 | -0.1360 | 0.068* |
| C8 | 0.1007 (4) | 0.45349 (17) | -0.06155 (16) | 0.0410 (8) |
| C9 | 0.2160 (4) | 0.48838 (17) | -0.03338 (16) | 0.0428 (9) |
| C10 | 0.2362 (4) | 0.3727 (2) | 0.11049 (16) | 0.0439 (9) |
| C11 | 0.3618 (4) | 0.3927 (2) | 0.13781 (17) | 0.0656 (12) |
| H11 | 0.4201 | 0.4267 | 0.1184 | 0.079* |
| C12 | 0.4012 (5) | 0.3632 (3) | 0.19275 (19) | 0.0801 (13) |
| H12 | 0.4854 | 0.3779 | 0.2100 | 0.096* |
| C13 | 0.3193 (5) | 0.3129 (3) | 0.22247 (19) | 0.0778 (13) |
| H13 | 0.3463 | 0.2933 | 0.2598 | 0.093* |
| C14 | 0.1957 (5) | 0.2919 (2) | 0.19589 (19) | 0.0748 (13) |
| H14 | 0.1390 | 0.2570 | 0.2152 | 0.090* |

supplementary materials

| | | | | |
|------|-------------|--------------|---------------|-------------|
| C15 | 0.1543 (4) | 0.3218 (2) | 0.14102 (17) | 0.0594 (11) |
| H15 | 0.0694 | 0.3072 | 0.1243 | 0.071* |
| C16 | -0.1538 (3) | 0.28339 (18) | -0.00757 (16) | 0.0486 (10) |
| H16A | -0.1685 | 0.3150 | 0.0276 | 0.058* |
| H16B | -0.2440 | 0.2634 | -0.0193 | 0.058* |
| C17 | -0.0618 (4) | 0.21887 (18) | 0.01117 (18) | 0.0454 (10) |
| C18 | -0.0910 (4) | 0.18457 (17) | 0.07171 (18) | 0.0470 (9) |
| C19 | -0.2116 (4) | 0.1996 (2) | 0.10416 (18) | 0.0529 (10) |
| H19 | -0.2767 | 0.2330 | 0.0885 | 0.064* |
| C20 | -0.2360 (4) | 0.1656 (3) | 0.15937 (19) | 0.0693 (12) |
| H20 | -0.3179 | 0.1754 | 0.1806 | 0.083* |
| C21 | -0.1389 (6) | 0.1174 (3) | 0.18275 (19) | 0.0769 (13) |
| C22 | -0.0177 (5) | 0.1022 (2) | 0.1514 (2) | 0.0762 (13) |
| H22 | 0.0480 | 0.0695 | 0.1675 | 0.091* |
| C23 | 0.0055 (4) | 0.1354 (2) | 0.0962 (2) | 0.0630 (11) |
| H23 | 0.0869 | 0.1249 | 0.0750 | 0.076* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| C11 | 0.1541 (14) | 0.1891 (16) | 0.0694 (9) | -0.0056 (13) | -0.0200 (9) | 0.0362 (10) |
| S1 | 0.0462 (6) | 0.0542 (5) | 0.0632 (7) | -0.0085 (5) | -0.0116 (6) | -0.0032 (5) |
| O1 | 0.0391 (15) | 0.0504 (15) | 0.087 (2) | 0.0030 (12) | 0.0112 (15) | -0.0136 (14) |
| N1 | 0.0357 (17) | 0.0379 (15) | 0.0481 (19) | -0.0030 (14) | 0.0007 (16) | -0.0072 (14) |
| C1 | 0.032 (2) | 0.038 (2) | 0.050 (2) | 0.0031 (16) | 0.0014 (18) | -0.0074 (18) |
| C2 | 0.036 (2) | 0.037 (2) | 0.045 (2) | 0.0020 (17) | 0.0029 (17) | -0.0125 (17) |
| C3 | 0.044 (2) | 0.040 (2) | 0.054 (2) | -0.0063 (17) | -0.005 (2) | -0.0126 (19) |
| C4 | 0.055 (3) | 0.040 (2) | 0.071 (3) | -0.0047 (19) | 0.010 (2) | -0.005 (2) |
| C5 | 0.074 (3) | 0.043 (2) | 0.076 (3) | -0.001 (2) | 0.017 (3) | 0.006 (2) |
| C6 | 0.084 (3) | 0.058 (3) | 0.058 (3) | 0.005 (2) | 0.003 (3) | 0.011 (2) |
| C7 | 0.060 (3) | 0.048 (2) | 0.063 (3) | 0.000 (2) | -0.004 (2) | 0.003 (2) |
| C8 | 0.042 (2) | 0.0353 (18) | 0.046 (2) | 0.0077 (17) | 0.0068 (19) | -0.0053 (18) |
| C9 | 0.043 (2) | 0.0303 (19) | 0.055 (2) | -0.0010 (17) | 0.007 (2) | -0.0096 (18) |
| C10 | 0.040 (2) | 0.047 (2) | 0.045 (2) | -0.0009 (18) | 0.001 (2) | -0.0121 (19) |
| C11 | 0.057 (3) | 0.087 (3) | 0.054 (3) | -0.015 (2) | -0.002 (2) | 0.004 (2) |
| C12 | 0.064 (3) | 0.119 (4) | 0.057 (3) | -0.018 (3) | -0.013 (3) | 0.003 (3) |
| C13 | 0.082 (4) | 0.101 (4) | 0.050 (3) | -0.005 (3) | -0.010 (3) | 0.006 (3) |
| C14 | 0.084 (3) | 0.078 (3) | 0.063 (3) | -0.016 (3) | -0.009 (3) | 0.019 (3) |
| C15 | 0.060 (3) | 0.059 (3) | 0.058 (3) | -0.009 (2) | -0.011 (2) | 0.005 (2) |
| C16 | 0.033 (2) | 0.044 (2) | 0.068 (3) | -0.0058 (17) | -0.0008 (19) | -0.0072 (19) |
| C17 | 0.031 (2) | 0.0346 (19) | 0.071 (3) | -0.0067 (17) | -0.005 (2) | -0.011 (2) |
| C18 | 0.039 (2) | 0.0350 (18) | 0.067 (3) | -0.0037 (18) | -0.005 (2) | -0.012 (2) |
| C19 | 0.047 (3) | 0.053 (2) | 0.058 (3) | -0.002 (2) | -0.008 (2) | -0.008 (2) |
| C20 | 0.059 (3) | 0.091 (3) | 0.058 (3) | -0.009 (3) | -0.006 (3) | -0.013 (3) |
| C21 | 0.084 (4) | 0.090 (3) | 0.057 (3) | -0.012 (3) | -0.019 (3) | -0.003 (3) |
| C22 | 0.077 (4) | 0.062 (3) | 0.090 (4) | 0.004 (3) | -0.030 (3) | 0.007 (3) |
| C23 | 0.050 (3) | 0.050 (2) | 0.089 (3) | 0.002 (2) | -0.008 (2) | -0.001 (2) |

Geometric parameters (Å, °)

| | | | |
|-----------|-------------|---------------|-----------|
| C11—C21 | 1.731 (4) | C11—C12 | 1.373 (5) |
| S1—C1 | 1.764 (3) | C11—H11 | 0.9300 |
| S1—C16 | 1.786 (3) | C12—C13 | 1.362 (5) |
| O1—C17 | 1.212 (4) | C12—H12 | 0.9300 |
| N1—C1 | 1.314 (4) | C13—C14 | 1.374 (5) |
| N1—C2 | 1.375 (4) | C13—H13 | 0.9300 |
| C1—C8 | 1.433 (4) | C14—C15 | 1.379 (5) |
| C2—C3 | 1.359 (4) | C14—H14 | 0.9300 |
| C2—C10 | 1.481 (4) | C15—H15 | 0.9300 |
| C3—C9 | 1.407 (4) | C16—C17 | 1.510 (4) |
| C3—H3 | 0.9300 | C16—H16A | 0.9700 |
| C4—C5 | 1.355 (5) | C16—H16B | 0.9700 |
| C4—C9 | 1.412 (4) | C17—C18 | 1.494 (5) |
| C4—H4 | 0.9300 | C18—C23 | 1.385 (5) |
| C5—C6 | 1.398 (5) | C18—C19 | 1.385 (5) |
| C5—H5 | 0.9300 | C19—C20 | 1.380 (5) |
| C6—C7 | 1.355 (5) | C19—H19 | 0.9300 |
| C6—H6 | 0.9300 | C20—C21 | 1.369 (6) |
| C7—C8 | 1.401 (4) | C20—H20 | 0.9300 |
| C7—H7 | 0.9300 | C21—C22 | 1.380 (6) |
| C8—C9 | 1.413 (4) | C22—C23 | 1.371 (5) |
| C10—C15 | 1.378 (4) | C22—H22 | 0.9300 |
| C10—C11 | 1.392 (5) | C23—H23 | 0.9300 |
| C1—S1—C16 | 100.46 (17) | C11—C12—H12 | 119.4 |
| C1—N1—C2 | 119.3 (3) | C12—C13—C14 | 118.2 (4) |
| N1—C1—C8 | 123.6 (3) | C12—C13—H13 | 120.9 |
| N1—C1—S1 | 119.0 (3) | C14—C13—H13 | 120.9 |
| C8—C1—S1 | 117.3 (3) | C13—C14—C15 | 121.0 (4) |
| C3—C2—N1 | 121.1 (3) | C13—C14—H14 | 119.5 |
| C3—C2—C10 | 123.1 (3) | C15—C14—H14 | 119.5 |
| N1—C2—C10 | 115.8 (3) | C10—C15—C14 | 121.3 (4) |
| C2—C3—C9 | 121.2 (3) | C10—C15—H15 | 119.4 |
| C2—C3—H3 | 119.4 | C14—C15—H15 | 119.4 |
| C9—C3—H3 | 119.4 | C17—C16—S1 | 116.5 (2) |
| C5—C4—C9 | 121.1 (4) | C17—C16—H16A | 108.2 |
| C5—C4—H4 | 119.4 | S1—C16—H16A | 108.2 |
| C9—C4—H4 | 119.4 | C17—C16—H16B | 108.2 |
| C4—C5—C6 | 120.3 (4) | S1—C16—H16B | 108.2 |
| C4—C5—H5 | 119.9 | H16A—C16—H16B | 107.3 |
| C6—C5—H5 | 119.9 | O1—C17—C18 | 121.2 (3) |
| C7—C6—C5 | 120.5 (4) | O1—C17—C16 | 122.2 (3) |
| C7—C6—H6 | 119.8 | C18—C17—C16 | 116.6 (3) |
| C5—C6—H6 | 119.8 | C23—C18—C19 | 118.6 (4) |
| C6—C7—C8 | 120.6 (4) | C23—C18—C17 | 118.9 (4) |
| C6—C7—H7 | 119.7 | C19—C18—C17 | 122.5 (3) |
| C8—C7—H7 | 119.7 | C20—C19—C18 | 120.7 (4) |

supplementary materials

| | | | |
|---------------|------------|-----------------|------------|
| C7—C8—C9 | 119.6 (3) | C20—C19—H19 | 119.6 |
| C7—C8—C1 | 123.8 (3) | C18—C19—H19 | 119.6 |
| C9—C8—C1 | 116.5 (3) | C21—C20—C19 | 119.6 (4) |
| C3—C9—C4 | 123.8 (3) | C21—C20—H20 | 120.2 |
| C3—C9—C8 | 118.2 (3) | C19—C20—H20 | 120.2 |
| C4—C9—C8 | 118.0 (3) | C20—C21—C22 | 120.6 (4) |
| C15—C10—C11 | 116.9 (4) | C20—C21—C11 | 120.1 (4) |
| C15—C10—C2 | 121.4 (3) | C22—C21—C11 | 119.3 (4) |
| C11—C10—C2 | 121.8 (3) | C23—C22—C21 | 119.7 (4) |
| C12—C11—C10 | 121.3 (4) | C23—C22—H22 | 120.2 |
| C12—C11—H11 | 119.3 | C21—C22—H22 | 120.2 |
| C10—C11—H11 | 119.3 | C22—C23—C18 | 120.8 (4) |
| C13—C12—C11 | 121.3 (4) | C22—C23—H23 | 119.6 |
| C13—C12—H12 | 119.4 | C18—C23—H23 | 119.6 |
| C2—N1—C1—C8 | -0.6 (4) | C3—C2—C10—C11 | -12.3 (5) |
| C2—N1—C1—S1 | 176.3 (2) | N1—C2—C10—C11 | 165.9 (3) |
| C16—S1—C1—N1 | 14.4 (3) | C15—C10—C11—C12 | -0.4 (6) |
| C16—S1—C1—C8 | -168.5 (2) | C2—C10—C11—C12 | -178.8 (4) |
| C1—N1—C2—C3 | -1.8 (4) | C10—C11—C12—C13 | 0.4 (7) |
| C1—N1—C2—C10 | 179.9 (3) | C11—C12—C13—C14 | 0.3 (7) |
| N1—C2—C3—C9 | 1.8 (5) | C12—C13—C14—C15 | -1.0 (7) |
| C10—C2—C3—C9 | 180.0 (3) | C11—C10—C15—C14 | -0.3 (6) |
| C9—C4—C5—C6 | 1.0 (6) | C2—C10—C15—C14 | 178.1 (3) |
| C4—C5—C6—C7 | -0.8 (6) | C13—C14—C15—C10 | 1.0 (6) |
| C5—C6—C7—C8 | -0.3 (6) | C1—S1—C16—C17 | -73.9 (3) |
| C6—C7—C8—C9 | 1.2 (5) | S1—C16—C17—O1 | -18.5 (4) |
| C6—C7—C8—C1 | -176.9 (3) | S1—C16—C17—C18 | 163.1 (2) |
| N1—C1—C8—C7 | -178.9 (3) | O1—C17—C18—C23 | 13.8 (5) |
| S1—C1—C8—C7 | 4.2 (4) | C16—C17—C18—C23 | -167.7 (3) |
| N1—C1—C8—C9 | 2.9 (5) | O1—C17—C18—C19 | -165.7 (3) |
| S1—C1—C8—C9 | -174.0 (2) | C16—C17—C18—C19 | 12.8 (4) |
| C2—C3—C9—C4 | -179.5 (3) | C23—C18—C19—C20 | -0.8 (5) |
| C2—C3—C9—C8 | 0.7 (5) | C17—C18—C19—C20 | 178.7 (3) |
| C5—C4—C9—C3 | -180.0 (3) | C18—C19—C20—C21 | 1.0 (6) |
| C5—C4—C9—C8 | -0.2 (5) | C19—C20—C21—C22 | -0.5 (6) |
| C7—C8—C9—C3 | 178.9 (3) | C19—C20—C21—C11 | -179.4 (3) |
| C1—C8—C9—C3 | -2.8 (4) | C20—C21—C22—C23 | -0.2 (6) |
| C7—C8—C9—C4 | -0.9 (4) | C11—C21—C22—C23 | 178.7 (3) |
| C1—C8—C9—C4 | 177.3 (3) | C21—C22—C23—C18 | 0.4 (6) |
| C3—C2—C10—C15 | 169.4 (3) | C19—C18—C23—C22 | 0.1 (5) |
| N1—C2—C10—C15 | -12.4 (4) | C17—C18—C23—C22 | -179.4 (3) |

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|-------|-------------|-------------|---------------|
| C4—H4 \cdots O1 ⁱ | 0.93 | 2.51 | 3.322 (4) | 147 |
| C16—H16B \cdots O1 ⁱⁱ | 0.97 | 2.47 | 3.128 (4) | 125 |

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

Fig. 1

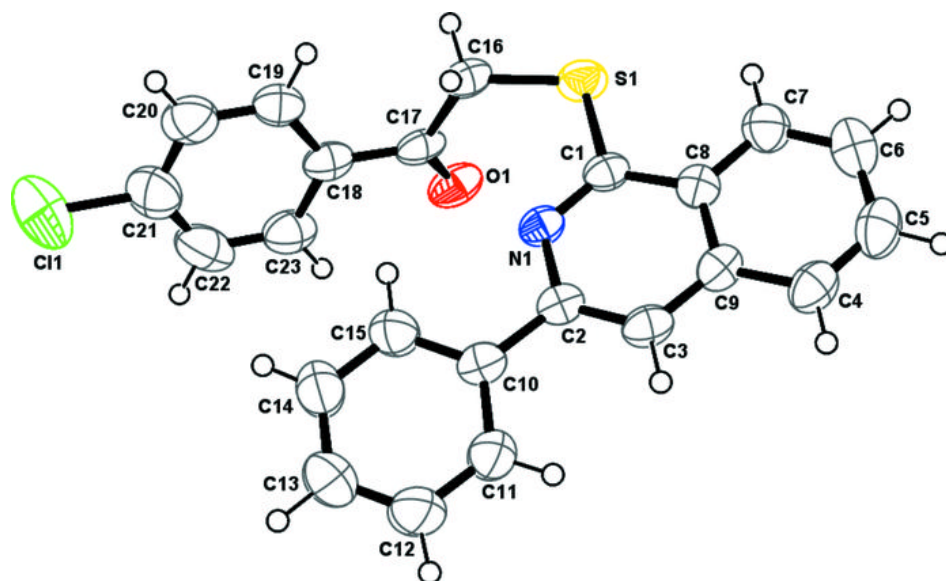


Fig. 2

