The title compound, C\textsubscript{20}H\textsubscript{19}N\textsubscript{3}S\textsubscript{2}, crystallized as a cis–trans conformer in which the quinoline ring system is cis across the C–S bond but adopts a trans geometry with respect to the C–N bond. The compound exists in the thione form with the presence of a C=S bond.

Related literature

The dithiocarbazate ligand used to prepare the title compound is \textit{S}-quinolin-2-ylmethyl dithiocarbazate. This compound was prepared as described by How \textit{et al.} (2007). Interatomic parameters for similar compounds are reported by Chan \textit{et al.} (2003), Khoo \textit{et al.} (2005) and How \textit{et al.} (2007).

Experimental

Crystal data

\[
\begin{align*}
\text{C}_{20}\text{H}_{19}\text{N}_{3}\text{S}_{2} & \quad M = 365.52 \\
M & = 365.52 \\
\text{Triclinic, } & \alpha = 7.7423 (2) \ \text{Å} \\
\beta & = 8.1250 (13)^{c} \\
x & = 8.2816 (2) \ \text{Å} \\
y & = 8.57886 (13)^{c} \\
z & = 2 \\
V & = 876.70 (4) \ \text{Å}^{3} \\
T & = 150 \ \text{K} \\
\end{align*}
\]

Refinement

\[
\begin{align*}
\text{min} & = 0.79, \text{max} = 0.98 \\
\sigma(C–C) & = 0.002 \ \text{Å} \\
\text{R} & = 0.095; \text{data-to-parameter ratio} = 18.4. \\
\end{align*}
\]

\[
\begin{align*}
\mu & = 0.31 \ \text{mm}^{-1} \quad T = 150 \ \text{K} \\
\text{wR} = 0.095 \\
\end{align*}
\]

\[
\begin{align*}
\text{S} & = 0.93 \\
\text{S} & = 0.93 \\
\text{4155 reflections} & = 0.061 \\
226 parameters & \\
\text{H-atom parameters constrained} & \Delta \rho_{\text{max}} = 0.52 \ \text{e Å}^{-3} \\
\text{H-atom parameters constrained} & \Delta \rho_{\text{min}} = -0.45 \ \text{e Å}^{-3} \\
\text{4155 independent reflections} & \overline{\Delta \rho_{\text{max}}} = 0.095 \\
\text{4155 reflections} & \overline{\Delta \rho_{\text{min}}} = 0.095 \\
\text{4155 reflections with } I > 2\sigma(I) & \overline{\Delta \rho_{\text{max}}} = 0.095 \\
\text{4155 reflections with } I > 2\sigma(I) & \overline{\Delta \rho_{\text{min}}} = 0.095 \\
\end{align*}
\]

\table{Table 1}{Selected geometric parameters (Å, °).}{
\begin{tabular}{lll}
\hline
C9—N10 & 1.352 (2) & N10—N11 & 1.3803 (19) \\
C9—S21 & 1.6593 (17) & \text{C9—N10—N11} & 117.61 (13) \\
S8—C9—S21 & 1.352 (2) & \text{S8—C9—S21} & 126.92 (10) \\
N10—N11 & 1.3803 (19) & \text{N10—N11} & 117.61 (13) \\
N10—C9—S21 & 120.76 (13) & \text{N10—C9—S21} & 120.76 (12) \\
\hline
\end{tabular}
\}

\small
\text{FNFH gratefully acknowledges MOSTI, Malaysia, for an attachment grant under an NSF scholarship, and the Chemical Crystallography Laboratory, Oxford University, for instrumental facilities.}

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2012).

References


supplementary materials
2-Quinolylmethyl N’-[1-(m-tolyl)ethylidene]hydrazinecarbodithioate

F. N.-F. How, D. J. Watkin, K. A. Crouse and M. I. M. Tahir

Comment

S-quinolin-2-ylmethyl dithiocarbazate, a new dithiocarbazate derivative has been introduced. This dithiocarbazate derivative ligand contains a quinoline ring [How, et al., 2007]. This new ligand were used to synthesized new Schiff bases. It is likely that these compound will be of interest for further research.

The C9—N10 bond [1.352 (2) Å] is comparable with the literature value and showed a double-bond character. [1.342 (2) Å; Chan et al., 2003] and [1.343 (3) Å; Khoo et al., 2005]. The C=S bond is 1.6593 (17) Å, which is shorter than in S-quinolin-2-ylmethyl dithiocarbazate [1.6804 (14) Å; How, et al., 2007] but comparable with Schiff bases derived from S-benzyldithiocarbazate. [1.6503 (17) Å; Chan et al., 2003] and [1.664 (2) Å; Khoo et al., 2005]

The molecule contains three planar fragments viz. the quinoline ring, dithiocarbazate moiety and the benzyl group. [Fig. 1.]. The dihedral angle between the planar quinoline ring and the dithiocarbazate moiety is 103.7°. The dihedral angle between the dithiocarbazate moiety with the benzyl group is 17.2°.

Bond angle N11—N10—C9 [117.61 (13)°] is slightly shorter than other Schiff bases. [119.20 (14)°; Chan et al., 2003] and [119.35 (17)°; Khoo et al., 2005]. However, S21—C9—S8 [126.92 (10)°] is slightly longer. [125.60 (10)°; Chan et al., 2003] and [125.22 (12)°; Khoo et al., 2005]. This is due to the twisting of both benzyl ring and the quinoline ring for stabilization.

The isolated molecule is L shaped [Fig. 2.]. Viewed along the a axis, the molecule packed in hearing-bone columns with pairs of quinoline rings residues lying parallel [Fig. 3.] and overlapping (mean separation 3.4 Å), corresponding to a reasonably strong π-π interaction between the quinoline rings. [Fig. 4.] Pairs of methyl benzyl residues are also almost parallell (mean separation 3.7 Å), but there is no overlap between the aromatic moieties. The moiety C7/S8/C9/N10/N11/C12/S21 behaves as a rigid group (TLS R-factor= 0.085).

Experimental

S-quinolin-2-ylmethyl dithiocarbazate (0.02 mol) [How, et al., 2007] was dissolved in hot absolute ethanol (30 ml) with dropwise addition of equimolar amount of 3-methylacetophenone. The mixture was left heated with stirring to reduce half the volume. Precipitate formed were filtered and washed with a little ice-cold ethanol. The crude yellow product was re-crystallized from ethanol. Yellow single crystals were formed upon slow evaporation of an ethanol solution. (Yield = 70%, M.p = 437.7–438.5 K)

Refinement

The H atoms were all located in a difference map, but those attached to carbon atoms were repositioned geometrically. The H atoms were initially refined with soft restraints on the bond lengths and angles to regularize their geometry (C—H in the range 0.93–0.98, N—H in the range 0.86–0.89 Å) and $U_{iso}(H)$ (in the range 1.2–1.5 times $U_{eq}$ of the parent atom), after
which the positions were refined with riding constraints. The other atoms were refined with anisotropic atomic displacement parameters.

**Figures**

Fig. 1. The title compound with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

Fig. 2. The packing diagram of the molecules viewed along the $a$ axis.

Fig. 3. The quinoline rings are parallel to each other.

Fig. 4. The overlapping of the quinoline rings due to the $\pi-\pi$ interaction.
2-Quinolylmethyl \(N'\)-[1-(\(m\)-tolyl)ethylidene]hydrazinecarbodithioate

Crystal data

C\(_{20}\)H\(_{19}\)N\(_3\)S\(_2\)  
\(F_{000} = 384\)

\(M_r = 365.52\)

Triclinic, \(P\bar{T}\)

\(a = 7.7423\) (2) \(\AA\)

\(b = 8.2816\) (2) \(\AA\)

\(c = 14.0409\) (4) \(\AA\)

\(\alpha = 81.2501\) (13)\(^{\circ}\)

\(\beta = 80.5729\) (13)\(^{\circ}\)

\(\gamma = 85.7886\) (13)\(^{\circ}\)

\(V = 876.70\) (4) \(\AA^3\)

\(Z = 2\)

Melting point: 438.5 K

\(\lambda = 0.71073\) \(\AA\)

Cell parameters from 3785 reflections

\(\mu = 0.31\) mm\(^{-1}\)

\(T = 150\) K

Plate, yellow

Data collection

Nonius KappaCCD diffractometer

4155 reflections with \(I > -3\sigma(I)\)

Monochromator: graphite

\(R_{int} = 0.043\)

\(T = 150\) K

\(\theta_{max} = 27.9^{\circ}\)

\(\omega\) scans

Absorption correction: multi-scan

DENZO/SCALEPACK; Otwinowski & Minor, 1997

\(h = -9 \rightarrow 10\)

\(T_{min} = 0.79, T_{max} = 0.98\)

14454 measured reflections

\(I = -18 \rightarrow 18\)

14155 independent reflections

Refinement

Refinement on \(F^2\)

Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full

H-atom parameters constrained

Method = Modified Sheldrick

\(R[F^2 > 2\sigma(F^2)] = 0.061\)

\(wR(F^2) = 0.095\)

\((\Delta/\sigma)_{max} = 0.0003\)

\(S = 0.93\)

4155 reflections

\(\Delta \rho_{max} = 0.52\) e \(\AA^{-3}\)

226 parameters

\(\Delta \rho_{min} = -0.45\) e \(\AA^{-3}\)

Primary atom site location: structure-invariant direct methods

Extinction correction: None
### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

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**Atomic displacement parameters (Å\(^2\))**

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supplementary materials

Fig. 2
Fig. 3
supplementary materials

Fig. 4