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(*SR*)-5-(2,6-Dichlorophenyl)-3-(2-naphthyl)-1-phenyl-2-pyrazoline trichloromethane hemisolvate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.005 Å
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.138
Data-to-parameter ratio = 12.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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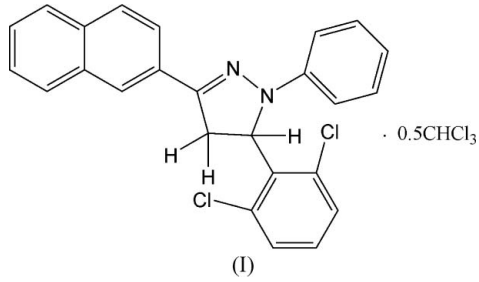
In the title compound, $C_{25}H_{18}Cl_2N_2\cdot0.5CHCl_3$, the mean planes of the dichlorobenzene ring, the phenyl ring, and the naphthalene ring system make dihedral angles of 85.1 (3), 7.2 (3) and 3.2 (3)°, respectively, with the mean plane of the pyrazoline ring. A disordered solvent molecule completes the structure.

Comment

The title compound, (I) (Fig. 1), was prepared and structurally characterized as part of our ongoing studies (Lu *et al.*, 2006) of pyrazoline derivatives.



(I)

As shown in Fig. 1, there is one molecule in the asymmetric unit, together with a disordered trichloromethane solvent molecule. The molecule of (I) is chiral; in the arbitrarily chosen asymmetric unit, C7 has an *S* configuration, but crystal symmetry generates a racemic mixture.

In the main molecule, the mean planes of the C1–C6 (*A*) and C20–C25 (*B*) benzene rings and the C10–C19 naphthalene ring system make dihedral angles of 85.1 (3), 7.2 (3) and 3.2 (3)°, respectively, with the mean plane of the N1–C9 pyrazoline ring. Rings *A* and *B* are inclined to each other at an angle of 91.7 (3)° and the dihedral angle between the naphthalene ring system and ring *A* is 87.8 (3)°.

A $CHCl_3$ solvent molecule, positionally disordered about an inversion centre, completes the structure of (I).

Experimental

A mixture of 3-(2,6-dichlorophenyl)-1-(2-naphthyl)prop-2-en-1-one (5.0 mmol), phenylhydrazine (25.0 mmol) and acetic acid (30 ml) was heated under reflux for 5 h, then poured on to crushed ice. The precipitate was separated by filtration, washed with water and crystallized from trichloromethane–methanol (1:1 *v*/*v*) to obtain the product (m.p. 442–443 K). The product (50 mg) was dissolved in a mixture of trichloromethane (10 ml) and methanol (10 ml) and the solution was kept at room temperature for 10 d. Natural evaporation of the solution gave colourless crystals of (I) suitable for X-ray crystallographic analysis.

Crystal data

$C_{25}H_{18}Cl_2N_2\cdot 0.5CHCl_3$
$M_r = 477.00$
Monoclinic, $P2_1/c$
$a = 14.494$ (3) Å
$b = 10.616$ (2) Å
$c = 15.573$ (3) Å
$\beta = 107.910$ (4)°
$V = 2280.1$ (8) Å^3
$Z = 2$
$D_x = 1.390$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.48$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.28 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.878$, $T_{max} = 0.911$
11344 measured reflections
4032 independent reflections
2298 reflections with $I > 2\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.138$
$S = 1.02$
4032 reflections
334 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.7045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}

All H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$. The $CHCl_3$ solvent molecule lies close to an inversion centre and was refined with 0.5 site occupancy for all atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

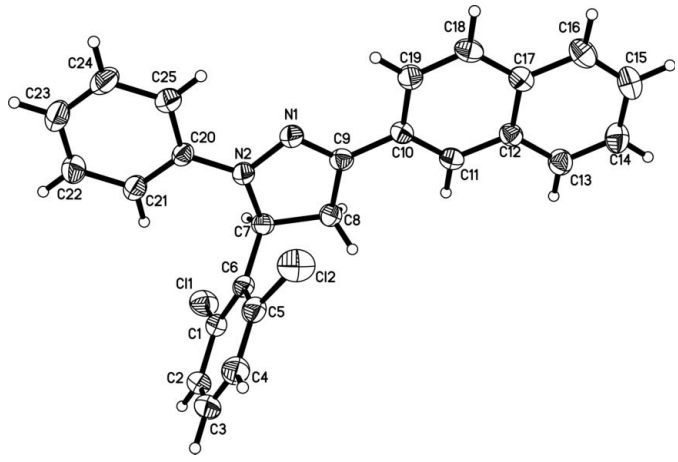


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The disordered trichloromethane molecule is not shown.

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