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A co-crystal of 1,10-phenanthroline and chloroform

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.119
Data-to-parameter ratio = 13.1

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

The structure of the title compound, $C_{12}H_8N_2{\cdot}CHCl_3$, shows a bifurcated C—H···N hydrogen bond.

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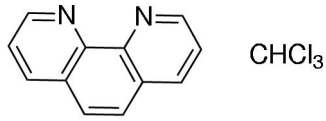
Comment

The aim of our research is the cocrystallization of two small organic compounds in order to examine the hydrogen bonds formed between hydrogen-bond acceptors and hydrogen-bond donors. In this work, we wanted to cocrystallize phenanthroline and 2,3-dimethylbutane-2,3-diol in chloroform. Unfortunately, we obtained a cocrystal of phenanthroline with its chloroform solvent.



(I)

A perspective view of the title compound is shown in Fig. 1. The structure is composed of discrete phenanthroline and chloroform molecules. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 1.7 plus one update; Mogul Version 1.0; Allen, 2002). There is a bifurcated hydrogen bond from the chloroform H atom to the two phenanthroline N atoms (Table 1).

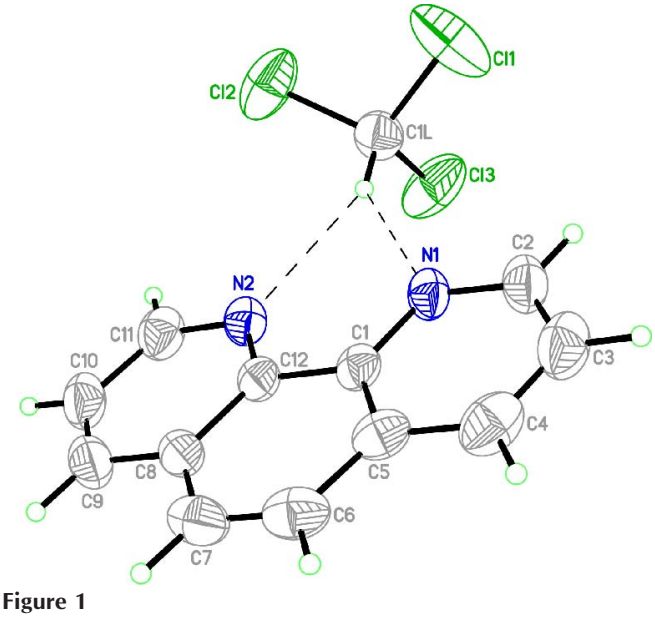


Figure 1
Perspective view of the title compound, with the atom numbering; displacement ellipsoids are at the 50% probability level. The minor minor component of the disordered Cl atoms has been omitted for clarity. Dashed lines indicate hydrogen bonds.

Experimental

Phenanthroline (0.018 g, 0.1 mmol) and the molar equivalent of 2,3-dimethylbutane-2,3-diol were dissolved in chloroform (0.3 ml), and the vial was sealed. The sample was set aside at room temperature. After three weeks, crystals of the title compound were obtained.

Crystal data

$C_{12}H_8N_2{\cdot}CHCl_3$
M_r = 299.57
Monoclinic, $P2_1/c$
a = 9.7350 (7) Å
b = 10.9349 (10) Å
c = 13.0522 (10) Å
β = 103.544 (6)°
V = 1350.8 (2) Å^3
Z = 4
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 13 605 reflections
θ = 3.5–25.7°
μ = 0.66 mm^{-1}
T = 173 (2) K
Block, colourless
0.40 × 0.20 × 0.15 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.778, T_{max} = 0.908
18 069 measured reflections
2533 independent reflections
1927 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 25.7°
$h = -11 \rightarrow 11$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.119
S = 1.02
2533 reflections
193 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.3494P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.027 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1*L*—H1*L*···N1	1.00	2.29	3.175 (3)	146
C1*L*—H1*L*···N2	1.00	2.39	3.225 (3)	141

H atoms were located in a difference map and refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C)] using a riding model, with C—H = 0.95 and 1.00 Å for $C_{aromatic}$ and $C_{tertiary}$, respectively. The chloroform molecule is disordered over two distinct positions about the C—H vector. The site occupation factor of the major occupied site refined to 0.68 (1). Bond lengths and angles of the two disordered conformations were restrained to be equal.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *PLATON* (Spek, 2003) and *SHELXL97*.

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