Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

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Electronic paper
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2-Chloro-3-morpholino-1,4-naphthoquinone

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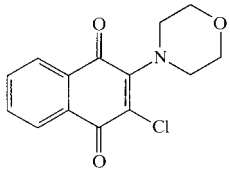
Received 28 September 2000
Accepted 9 October 2000

Data validation number: IUC0000289

The structure of the title compound, $C_{14}H_{12}ClNO_3$, (I), comprises essentially planar molecules stacked parallel to the *a* axis. C—H···O hydrogen-bonding interactions exist to both naphthoquinone O atoms and the Cl atom, but not to the morpholine O atom.



(I)

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.

Crystal data

$C_{14}H_{12}ClNO_3$
M_r = 277.70
Triclinic, $P\overline{1}$
a = 5.0386 (1) Å
b = 10.3948 (2) Å
c = 12.7421 (3) Å
α = 67.2038 (12)°
β = 84.4066 (10)°
γ = 81.2678 (12)°
V = 607.56 (2) Å^3
Z = 2
D_x = 1.518 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4135 reflections
θ = 2.91–27.48°
μ = 0.317 mm^{-1}
T = 150 (2) K
Plate, red
0.40 × 0.20 × 0.08 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.884, T_{max} = 0.977
6621 measured reflections
2761 independent reflections
2449 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.53°
$h = -6 \rightarrow 6$
$k = -13 \rightarrow 13$
$l = -15 \rightarrow 16$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.142
S = 1.160
2761 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1000P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O4^{i}	0.95	2.41	3.2914 (18)	155
C33—H122···O4^{ii}	0.99	2.56	3.3692 (19)	139
C36—H142···Cl2	0.99	2.61	3.1439 (14)	114
C36—H142···O1^{iii}	0.99	2.56	3.2246 (17)	125

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

All H atoms were included in the refinement at calculated positions as riding, with the C—H distance set to 0.95 (for aryl H atoms) or 0.99 Å (for CH_2).

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

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