Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,6-Dichloro-2-methylthio-5-phenylpyrimidine

Daniel E. Lynch[a]* and Ian McClenaghan[b]†

[a]School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and [b]Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England

† E-mail: 106355.1670@CompuServe.com.

Correspondence e-mail: apx106@coventry.ac.uk

Received 13 February 2001
Accepted 14 February 2001
Online 28 February 2001

Key indicators

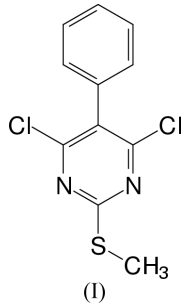
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.086
Data-to-parameter ratio = 17.8

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, $C_{11}H_8Cl_2N_2S$, comprises two unique molecules with the dihedral angles between the two linked rings for each molecule being 77.1 (1) and 78.4 (1)°. Only one C—H···X short contact exists from an aromatic C—H group to a Cl atom.

Comment

The title compound, (I), is an analogue of 4,6-dichloro-2-methylthiopyrimidine (dcmtp; Lynch & McClenaghan, 2000). In dcmtp, the Cl atoms are displaced by nucleophiles first, before the methylthio group, although the second Cl atom is much less reactive than the first. In terms of substituent effects, the presence of the phenyl ring in (I) should increase the activity of the Cl atoms, but as found for 4,6-dichloro-2-amino-5-phenylpyrimidine, nucleophilic displacement of the first Cl atom takes a reaction time of hours, whereas that of the second takes days. This rate difference may be due to steric effects, thus we have instigated a series of studies to examine the structural changes that the phenyl ring imposes on the nucleophilic substituents of several different analogues of (I), including the 2-amino series. Here we report the single-crystal structure of (I) as our point of reference for further derivatized compounds in the 2-methylthio series.



(I)

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) formed when the reaction solution ($POCl_3$) was poured into excess water.

Crystal data

$C_{11}H_8Cl_2N_2S$
M_r = 271.15
Orthorhombic, $P2_12_12_1$
a = 7.467 (2) Å
b = 16.217 (3) Å
c = 19.318 (4) Å
V = 2339.1 (8) Å^3
Z = 8
D_x = 1.540 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9258 reflections
θ = 1.0–27.5°
μ = 0.70 mm^{-1}
T = 150 (2) K
Prism, colourless
0.28 × 0.24 × 0.20 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.827, T_{max} = 0.872
11 464 measured reflections
5186 independent reflections
4655 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.5°
$h = -9 \rightarrow 9$
$k = -19 \rightarrow 20$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.087
S = 1.06
5186 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0400P)^2 + 0.3307P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = −0.04 (5)

Table 1
Selected geometric parameters (°).

N1*A*—C2*A*—S21*A*—C22*A*	3.7 (2)	N1*B*—C2*B*—S21*B*—C22*B*	3.4 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22*B*—H22*B*···Cl4*B*^{i}	0.98	2.76	3.452 (3)	128

Symmetry code: (i) $\frac{3}{2} - x, 1 - y, \frac{1}{2} + z$.

All H atoms were included in the refinement at calculated positions as riding models with C—H distances set to 0.95 (Ar-H) and 0.98 Å (CH_3). The number of Friedel pairs is 2167.

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); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

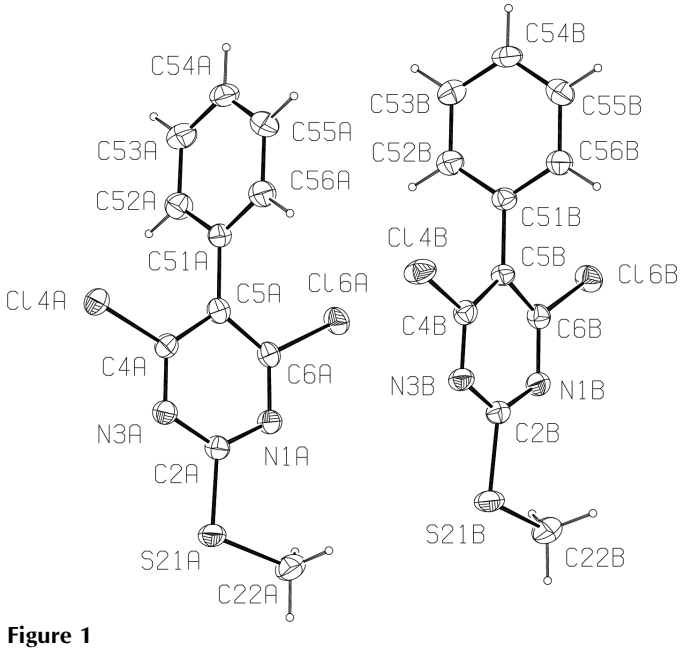


Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 50% probability ellipsoids.

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

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Lynch, D. E. & McClenaghan, I. (2000). *Acta Cryst.* C**56**, e536.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1997). *PLATON*97. Version of May 1997. University of Utrecht, The Netherlands.