1,3,5-Tris(chloromethyl)benzene

Jeffrey C. Bryan,* Michael N. Burnett and Richard A. Sachleben

Chemical and Analytical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA
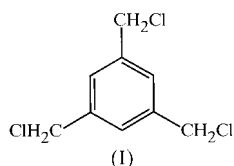Correspondence e-mail: bryanjc@ornl.gov

Data validation number: IUC0000073

The title compound, $C_9H_9Cl_3$, is being used as a platform for new tripodal receptors. Two molecules make up the asymmetric unit; weak intermolecular hydrogen bonding is observed between methylene H atoms and the chlorine of an adjacent molecule. There are also $C—H\cdots\pi$ interactions.

Comment

Two molecules make up the asymmetric unit of the title compound, (I). Weak intermolecular hydrogen bonding is observed (full details in Table 1) between a methylene H atom H18B and chlorine Cl4 of an adjacent molecule. There are also $C—H\cdots\pi$ interactions with $H\cdots$ring-centroid separations of 3.07–3.31 Å (Table 1).

(I)

Experimental

The title compound was prepared following literature methods (Cochrane *et al.*, 1968) and was recrystallized from toluene.

Crystal data

$C_9H_9Cl_3$	$Z = 4$
$M_r = 223.51$	$D_x = 1.474$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.7124\ (12)$ Å	Cell parameters from 25
$b = 9.0659\ (5)$ Å	reflections
$c = 12.7901\ (15)$ Å	$\theta = 10.4–14.9°$
$\alpha = 87.537\ (8)°$	$\mu = 0.85$ mm^{-1}
$\beta = 86.992\ (10)°$	$T = 163\ (2)$ K
$\gamma = 87.873\ (8)°$	Fragment, colourless
$V = 1007.3\ (2)$ Å^3	$0.30 \times 0.30 \times 0.25$ mm

Data collection

Nonius CAD-4 diffractometer	$R_{int} = 0.025$
$\omega–\theta$ scans	$\theta_{max} = 26.0°$
Absorption correction: ψ scan	$h = -9 \rightarrow 10$
(Siemens, 1994)	$k = -11 \rightarrow 11$
$T_{min} = 0.722$, $T_{max} = 0.809$	$l = -15 \rightarrow 15$
6800 measured reflections	3 standard reflections
3943 independent reflections	frequency: 120 min
3047 reflections with $I > 2\sigma(I)$	intensity decay: 1%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0424P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.032$	$+ 0.2112P]$
$wR(F^2) = 0.088$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.041$	$(\Delta/\sigma)_{max} = 0.001$
3943 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
217 parameters	$\Delta\rho_{min} = -0.34$ e Å^{-3}
H-atom parameters constrained	

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C18—H18$B\cdots$Cl4^i	0.99	2.72	3.682 (2)	163
C7—H7$A\cdots$CG1^{ii}	0.99	3.07	3.509 (2)	108
C7—H7$B\cdots$CG1^{ii}	0.99	3.12	3.509 (2)	105
C17—H17$A\cdots$CG2^{iii}	0.99	3.31	3.729 (2)	107

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

Data collection: *CAD-4-PC* (Nonius, 1993); cell refinement: *CAD-4-PC* (Nonius, 1993); data reduction: *XCAD*4 (Harms, 1995); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); software used to prepare material for publication: *SHELXTL* (Siemens, 1994).

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