

$C_6S_2[CN]Cl_3$ *hP78*(176) $P6_3/m-h^{13}$ **$C_7Cl_3NS_2$ [1]**

Structural features: Planar $C_6S_2Cl_3CN$ molecules (a C_5 pentagon sharing an edge with a C_3S_2 pentagon, one Cl bonded to each non-bridging C of the former, a CN unit bonded to the non-bridging C of the latter) arranged in layers perpendicular to [001].

Rakitin O.A. et al. (1996) [1]

 $C_7Cl_3NS_2$ $a = 1.557$, $c = 0.6815$ nm, $c/a = 0.438$, $V = 1.4308$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	6 <i>h</i>	<i>m..</i>	0.0	0.3546	$\frac{1}{4}$		coplanar triangle C ₃
C2	6 <i>h</i>	<i>m..</i>	0.0264	0.2764	$\frac{1}{4}$		coplanar triangle C ₂ S
C3	6 <i>h</i>	<i>m..</i>	0.0721	0.5375	$\frac{1}{4}$		non-colinear NC
C4	6 <i>h</i>	<i>m..</i>	0.0779	0.4485	$\frac{1}{4}$		coplanar triangle C ₂ S
Cl5	6 <i>h</i>	<i>m..</i>	0.1448	0.0725	$\frac{1}{4}$		single atom C
S6	6 <i>h</i>	<i>m..</i>	0.1512	0.315	$\frac{1}{4}$		non-colinear CS
S7	6 <i>h</i>	<i>m..</i>	0.1962	0.4644	$\frac{1}{4}$		non-colinear CS
C8	6 <i>h</i>	<i>m..</i>	0.2466	0.0587	$\frac{1}{4}$		coplanar triangle C ₂ Cl
C9	6 <i>h</i>	<i>m..</i>	0.3478	0.1409	$\frac{1}{4}$		coplanar triangle C ₂ Cl
Cl10	6 <i>h</i>	<i>m..</i>	0.3766	0.2613	$\frac{1}{4}$		single atom C
N11	6 <i>h</i>	<i>m..</i>	0.3896	0.4618	$\frac{1}{4}$		single atom C
C12	6 <i>h</i>	<i>m..</i>	0.4124	0.1056	$\frac{1}{4}$		coplanar triangle C ₂ Cl
Cl13	6 <i>h</i>	<i>m..</i>	0.5393	0.1741	$\frac{1}{4}$		single atom C

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.032$

Remarks: 4,5,6-trichlorocyclopenta-1,2-dithiole-3-carbonitrile.

References: [1] Rakitin O.A., Rees C.W., Williams D.J., Torroba T. (1996), J. Org. Chem. 61, 9178-9185.