Acta Cryst. (1963) **16**, 1258

Bond lengths and angles in $AgSCN.P(CH_2.CH_2.CH_3)_3$.

By CARLO PANATTONI and EDOARDO FRASSON,
Centro di Strutturistica Chimica del C.N.R., Padova, Italy

(*Received* 4 *March* 1963 *and in revised form* 1 *April* 1963)

The complex $AgSCN.P(CH_2.CH_2.CH_3)_3$ belongs to the space group $P2_1/c$. Lattice constants:

$$a = 6{\cdot}32 \pm 0{\cdot}02,\ b = 14{\cdot}00 \pm 0{\cdot}05,\ c = 18{\cdot}24 \pm 0{\cdot}07\ \text{Å};$$
$$\beta = 114° \pm 10';\ Z = 4\ .$$

The steric characteristics of the molecule were described in preliminary papers (Panattoni & Frasson, 1960; Turco, Panattoni & Frasson, 1960). A complete description is now reported. The reliability factor is $R = 0{\cdot}10$ for $0kl$ reflexions and $R = 0{\cdot}11$ for $h0l$ reflexions. Table 1 shows atomic coordinates with standard deviations calculated by Cruickshank's method (1949). Values of σ were calculated for the well resolved atoms, neglecting some overlapping carbon atoms of propyl chains for which it was not possible to calculate the form of the maximum of electron density. Fig. 1 shows a perspective of a pair of molecules. In this figure the propyl groups are neglected. In Table 2 bond lengths and angles are listed.

Table 1. *Atomic coordinates with standard deviations*

	x/a	y/b	z/c	$\sigma(x)$ (Å)	$\sigma(y)$ (Å)	$\sigma(z)$ (Å)
Ag	+0·0260	+0·5700	+0·4195	0·0037	0·0033	0·0038
S	+0·2730	−0·0805	+0·0890	0·011	0·014	0·012
P	+0·2110	+0·2140	+0·1380	0·015	0·009	0·021
N	+0·3090	−0·5100	+0·3990	0·024	0·060	0·063
C(1)	+0·2340	+0·2810	+0·0620	0·080	0·036	0·060
C(2)	+0·3420	+0·2410	+0·0030	0·050	0·061	0·084
C(3)	+0·4190	+0·2080	+0·4431	0·048	0·060	0·058
C(4)	+0·4900	+0·6860	+0·2920	0·080	0·066	0·073
C(5)	+0·4431	+0·6270	+0·2320	0·080	0·027	0·049
C(6)	+0·3333	+0·6060	+0·1610	0·080	0·042	0·063
C(7)	+0·2490	+0·3120	+0·1831	0·080	0·085	0·059
C(8)	+0·0813	+0·3670	+0·2020	0·075	0·090	0·065
C(9)	+0·1220	−0·0670	+0·3150	0·057	0·090	0·073
C(10)	+0·4700	−0·0150	+0·0800	0·058	0·090	0·090

Fourier synthesis, structure factors, bond lengths and angles were calculated with an electronic computer (Olivetti Elea 6001), with programs elaborated in our laboratory with the help of the technical personnel of the C.E.C.S. and Olivetti S.p.A. whose assistance we gratefully acknowledge.

Table 2. *Bond lengths and angles*

Ag–S	2·83	±0·02 Å	C(1)–C(2)	1·59	±0·15 Å
Ag–S′	2·88	±0·02	C(2)–C(3)	1·55	±0·15
Ag–P	2·48	±0·03	C(4)–C(5)	1·50	±0·16
Ag–N	2·10	±0·10	C(5)–C(6)	1·50	±0·14
N–C(10)	1·42	±0·18	C(7)–C(8)	1·45	±0·19
C(10)–S	1·81	±0·14	C(8)–C(9)	1·55	±0·19
P–C(1)	1·71	±0·11			
P–C(4)	1·84	±0·13	Average		
P–C(7)	1·73	±0·14	C–C	1·53	
Average					
P–C	1·76				
∠ S–Ag–S′	93° 30′		∠ S′–Ag–P	104° 50′	
Ag–S′–Ag	86° 40′		P–Ag–N	130° 00′	
S–Ag–N	108° 00′		Ag–P–C(1)	109° 40′	
Ag–N–C(10)	165° 20′		Ag–P–C(4)	110° 00′	
N–C(10)–S′	155° 20′		Ag–P–C(7)	112° 40′	
C(10)–S′–Ag	91° 00′		Average		
			Ag–P–C	110° 46′	

References

CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* **2**, 65.

PANATTONI, C. & FRASSON, E. (1960). *Acta Cryst.* **13**, 1027.

TURCO, A., PANATTONI, C. & FRASSON, E. (1960). *Nature, Lond.* **187**, 772.

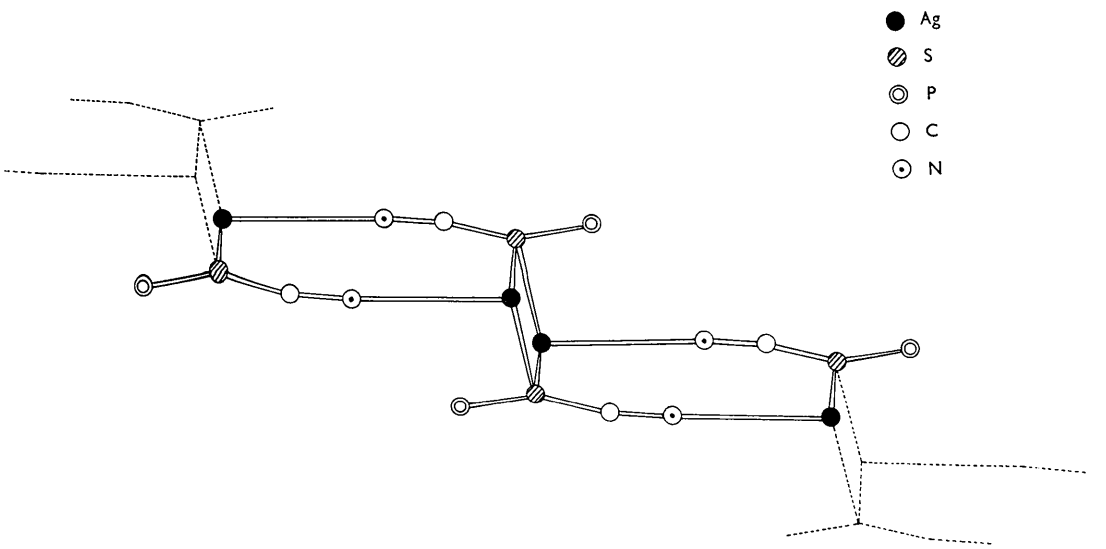

Fig. 1. A perspective view of the molecular chain of $AgSCN.P(C_3H_7)_3$. The propyl radicals are neglected.