Fig. 2 shows the packing in the crystal viewed along b. The DCB molecules are packed in layers normal to c at $z=\frac{1}{4}$ and $\frac{3}{4}$. There are extensive van der Waals contacts between the molecules both within each layer and between the layers.

Biphenyl and several substituted biphenyls have previously been studied both in the gas phase and/or as solids. Only for one compound, unsubstituted biphenyl, does the conformation change drastically upon crystallization. The rings are coplanar in the solid, but twisted 42° in the gas phase (Almenningen & Bastiansen, 1958). Calculations have been performed to try to explain this difference semiquantitatively, and reasonable agreement is obtained with electron diffraction, X-ray, and thermal data (Fischer-Hjalmars, 1963; Casalone, Mariani, Mugnoli & Simonetta, 1968). The geometry of the isolated molecule is found to be mainly determined by a balance of π-electron and non-bonded energies, while in the crystal the most important forces seem to be the intermolecular $C\cdots H$ attractions.

In all substituted biphenyl compounds studied, the two rings are twisted about the central C–C bond. The angle of twist is dependent on the nature, site and size of the substituents, and values range from 33 to 86°. The C–C bridge bond in biphenyls ranges from 1·48 to 1·52 Å, but based on the quoted e.s.d.'s of all but two of the published values, there are no significant differences. There is, however, a significant difference between the C–C bonds in 2,2'-dichlorobiphenyl and DCB, the lengths being respectively 1·493 (5) and 1·522 (5) Å, with twist angles 69·2 (5)° and 86·7 (3)°. The corresponding bond is 1·4966 (25) Å in planar biphenyl. In these chlorinated compounds the lengths of the C–Cl bonds are also different: 1·748 (3) and 1·718 Å (mean value for DCB). This may indicate that a larger

proportion of the π-electrons are engaged in C–Cl interaction in DCB, which consequently leads to a lowering of the electron density in the C–C bridge, with a corresponding lengthening of the bond.

The average C–Cl bond length in DCB, 1·718 Å, is consistant with Rudman's (1971) inference from available data, that C–Cl bonds on aromatic and quinoid rings are significantly shorter when the bonds are *ortho* to each other, than when they are more widely separated or isolated.

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Sodium Thiocyanate

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Abstract. NaSCN, orthorhombic, *Pnma*, $a=13\cdot38$ (1), $b=4\cdot09$ (1), $c=5\cdot66$ (1) Å, $Z=4$. The thiocyanate group is linear and the Na$^+$ ion is octahedrally surrounded by three S and three N atoms in *fac* arrangement.

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Introduction. To assist with the interpretation of the high-pressure phase diagram of NaSCN, an approximate structure based on space-group data and packing considerations was proposed by Pistorius & Boeyens (1968). The structure was confirmed by infrared work (Iqbal, 1971) and has been discussed in at least one review (Iqbal, 1972). To prevent perpetuation

of a possibly wrong structure, the present determination was carried out.

Discussion. Needle-shaped crystals elongated along [010] were obtained from aqueous solution. Photographic examination confirmed the cell data published previously, and improved cell constants were obtained from measurements on a Stoe two-circle diffractometer with Mo radiation and a graphite-crystal incident-beam monochromator.

431 independent intensities with $2\theta \le 60°$ were recorded on the same instrument at an ω-scan rate of 4 s per 0·01°. The structure was solved by Fourier methods and refined by full-matrix least squares until all parameter shifts were less than 10% of the estimated standard deviations. R at the termination of refinement was 0·075. The final atomic and isotropic thermal parameters are listed in Table 1.*

Table 1. *Positional and isotropic thermal parameters for NaSCN*

	x	y	z	B (Å^2)
Na	0·3919 (3)	0·25	0·9337 (7)	3·02 (8)
S	0·1856 (2)	0·25	0·1137 (4)	2·65 (6)
C	0·1127 (6)	0·25	0·8758 (15)	2·42 (14)
N	0·0627 (6)	0·25	0·7066 (14)	2·99 (15)

The structure is shown in Fig. 1. All atoms occur in the mirror planes at $y/b = \frac{1}{4}, \frac{3}{4}$. The SCN ions are linear within experimental error. The bond lengths are: $d(\text{S–C}) = 1·663$ (9) and $d(\text{C–N}) = 1·168$ (18) Å. The angle at the C atom is 179·0 (8)°. The packing is essentially as proposed before, and each Na$^+$ ion is octahedrally surrounded by three S and three N atoms in *fac* arrangement as shown in Fig. 2.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31314 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.
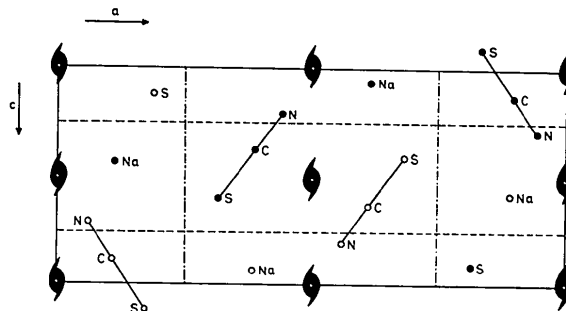

Fig. 1. The structure of NaSCN in (010) projection. Open circles represent atoms in the mirror plane at $y=\frac{1}{4}$ and solid circles atoms at $y=\frac{3}{4}$.
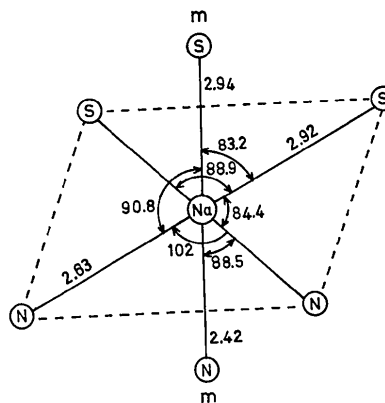

Fig. 2. Schematic drawing of the octahedral coordination sphere of a sodium ion.

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1,3,5-Triacetyl-2,4,6-hexahydro-*s*-triazine (TRAT)

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Abstract. $C_9H_{15}N_3O_3$, monoclinic, $P2_1/c$, $a=7·772$ (2), $b=15·521$ (4), $c=10·101$ (2) Å, $\beta=116·34$ (2)°, $Z=4$, $D_x=1·30$, $D_m=1·31$ g cm^{-3}, $F(000)=456$. All X-ray measurements were made with Mo $K\alpha$ radiation ($\lambda=0·71069$ Å). The structure was solved by direct methods and refined by full-matrix least-squares calculations to