

be $B_N > B_C > B_{Co}$, but because of the limited sensitivity of this experiment to temperature effects it seems that $B_C = B_{Co}$.

The prototype of this structure elpasolite, K_2NaAlF_6 , was originally studied by powder techniques (Menzer, 1932; Frondel, 1948; Steward & Rooksby, 1953). According to these workers the crystal belongs to the $Pa\bar{3}$ (T_h^9) space group. However, more recently Helmholz (1959) and Helmholz, Guzzo & Sanders (1961) assigned to this crystal the $Fm\bar{3}m$ (O_h^2) space group, after a single-crystal study. There are now available several more examples of members of this isostructural family, e.g. K_2NaGaF_6 (Helmholz, 1959), K_2NaCrF_6 and K_2NaFeF_6 (Knox & Mitchell, 1961), K_2NaTiF_6 (Bright & Wurm, 1958) and the current work on $Cs_2LiCo(CN)_6$, all having the $Fm\bar{3}m$ space group. In addition, the e.p.r. studies of FeF_6^{3-} and CrF_6^{3-} doped in K_2NaGaF_6 (Helmholz, 1959; Helmholz, Guzzo & Sanders, 1961) and $Cr(CN)_6^{3-}$ in $Cs_2LiCo(CN)_6$ (to be published) showed no evidence of any distortion of the octahedral complexes. Evidence of a reversible transition, which could be ascribed to misalignment of the complex axes with respect to those of the unit cell, were found in our e.p.r. work on $Cr(CN)_6^{3-}$ in $Cs_2LiCo(CN)_6$ at about 70°K. We feel that this work should be emphasized since it seems that the remarks of Helmholz, Guzzo & Sanders (1961) on the elpasolite structure have been overlooked.

The author would like to acknowledge the help and guidance received from Professor L. Helmholz of the Washington University Chemistry Department.

References

- BARKHATOV, V. (1942). *Acta Physicochimica USSR*, **16**, 123.
 BARKHATOV, V. & ZHDANOV, M. (1942). *Acta Physicochimica USSR*, **16**, 42.
 BRIGHT, N. F. M. & WURM, J. G. (1958). *Canad. J. Chem.* **36**, 615.
 CURRY, N. A. & RUNCIMAN, W. A. (1959). *Acta Cryst.* **12**, 674.
 FRONDEL, C. (1948). *Amer. Min.* **33**, 84.
 HELMHOLZ, L. (1959). *J. Chem. Phys.* **31**, 172.
 HELMHOLZ, L., GUZZO, A. V. & SANDERS, R. N. (1961). *J. Chem. Phys.* **35**, 1349.
International Tables for X-Ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.
 KNOX, K. & MITCHELL, D. W. (1961). *J. Inorg. Nucl. Chem.* **21**, 253.
 MENZER, G. (1932). *Fortschr. Min.* **17**, 439.
 MEYER, V. J. & CHAO, P. (1937). *Zeit. anorg. allg. Chemie*, **232**, 238.
 STEWARD, E. G. & ROOKSBY, H. P. (1953). *Acta Cryst.* **6**, 49.

Acta Cryst. (1969). B25, 162

Crystallographic data for carbazole, indole and phenanthridine. BY P. T. CLARKE and J. M. SPINK, *National Physical Laboratory, Teddington, Middlesex, England*

(Received 5 August 1968)

Carbazole, indole and phenanthridine are shown to be orthorhombic with four molecules in the unit cell. The first two have space groups $Pna2_1$ (or $Pnma$) and $Pna2_1$ (or $Pnma$), and the last one $P2_12_12_1$.

As part of a series of studies of the electro-optic properties of some heterocyclic molecules we have determined crystallographic constants (Table 1) for carbazole, indole and phenanthridine. The X-ray data were obtained from oscillation and Weissenberg photographs with Cu $K\alpha$ radiations. The densities were determined by flotation; the instrument produced by Crystal Structures Ltd was used to test for the piezoelectric effect. In the cases of indole and carbazole the non-centrosymmetric space group $Pna2_1$ is

preferred to the alternative centrosymmetric possibility $Pnma$ despite the lack of any detectable piezoelectric effect since the symmetry requirements imposed by $Pnma$ would lead to improbable packing arrangements. All cell dimensions are accurate to about 0.4%. No further crystallographic studies of these compounds are contemplated.

This work forms part of the programme of the Division of Molecular Science at the National Physical Laboratory.

Table 1. *Crystallographic data for carbazole, indole and phenanthridine*

	Carbazole	Indole	Phenanthridine
Empirical formula	$C_{12}H_9N$	C_8H_7N	$C_{13}H_9N$
Molecular weight	167.21	117.15	179.21
Solvent	Ethanol	Cyclohexane	Cyclohexane and ethanol
Habit	Thin plates	Thin plates	Flat needles
Piezoelectric effect	Nil	Nil	Nil
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Systematic absences	$0kl, k+l \neq 2n$ $h0l, h \neq 2n$	$0kl, k+l \neq 2n$ $h0l, h \neq 2n$	$h00, h \neq 2n$ $0k0, k \neq 2n$ $00l, l \neq 2n$
Space group	$Pna2_1$ (or $Pnma$)	$Pna2_1$ (or $Pnma$)	$P2_12_12_1$
Molecules per unit cell	4	4	4
Cell dimensions			
a (Å)	5.73	14.89	11.72
b (Å)	19.27	7.87	16.41
c (Å)	7.82	5.64	4.97
V (Å ³)	825.3	660.7	955.9
Density (observed)	1.285	1.188	1.19
Density (calculated)	1.30	1.19	1.24