the cell is primitive, and there are no obvious systematic absences in $hk0$ or $0kl$ terms. There is only one $h0l$ term (in which $k+l=2n$), making no conclusion possible from these; in the cases where $0k0$ and $00l$ terms have k and l odd, acceptable duplicate indices are available, again making conclusions impossible.

Data for β-$(NH_4)_2HPO_4$ were given by Smith, Lehr & Brown (1957): $a=8{\cdot}03$, $b=6{\cdot}68$, $c=11{\cdot}02$ Å; $\beta=113°38'$; 4 molecules per unit-cell, calculated density 1·61 g.cm^{-3}. It is to be noted that $c\sin\beta=10{\cdot}09$ Å, which compares with 10·78 Å for the a axis of the α form, suggesting that this direction may remain common to both forms, merely expanding slightly. If the α form had 8 molecules per unit cell, the calculated density would be 1·25 g.cm^{-3}. The ratio of low-temperature-form density to high temperature-form density is then 1·29, which compares with ratios of 1·24 and 1·20 for NH_4Br and NH_4Cl respectively.

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Effect of wavelength on the sign of the photo-elastic constant (P_{11}-P_{12}) of crystals of sodium-chloride structure.

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A new method is presented for calculating the reversal wavelength at which the strain optical constant $(P_{11}-P_{12})$ for alkali halides of sodium-chloride structure changes sign. Calculated absolute strain optical constants, their ratios and the strain polarizability constants of rubidium halides are given.

Bansigir & Iyengar (1961*a*) developed a theory of piezo-optic birefringence in cubic crystals of sodium chloride structure. The expressions obtained were:

$$(n^3/2)(P_{11}-P_{12})=3M-(1+\sigma)A \tag{1}$$

$$(n^3/2)(P_{11}+2P_{12})=(3L-A)(1-2\sigma) \tag{2}$$

and

$$(n^3/6)(P_{11}+2P_{12})=L(1-\lambda_0) \tag{3}$$

where

$$\lambda_0=2\sigma+A(1-2\sigma)/3L$$

$$M=(n^2-1)^2(n^2+5)/45n,$$

$$L=(n^2-1)(n^2+2)/6n$$

and

$$A=\frac{(n^2+2)^2(n^2+5)}{54n}\left[1{\cdot}458+2{\cdot}9005\,\beta\left(\frac{1}{f_1}+\frac{1}{f_2}\right)\right]\times\theta^2-\frac{(n^2-1)(n^2+2)(n^2+5)}{18n}\left[2{\cdot}916+4{\cdot}2083\,\frac{\beta}{f_1}+7{\cdot}5927\,\frac{\beta}{f_2}\,\theta\right]+\frac{(n^2-1)^2(n^2+5)}{3n}\left[0{\cdot}2711+1{\cdot}6922\,\frac{\beta}{f_2}\right].$$

P_{11} and P_{12} are the strain-optical constants, n the refractive index, σ Poisson's ratio, β the number of valence electrons, f_1, f_2 the oscillator strengths, $\theta=\alpha_j/r^3$ (α_j is the polarizability of the jth ion and r is the interionic distance) and λ_0 is the strain polarizability constant.

Using these expressions, Bansigir & Iyengar (1961*b*) calculated the wavelengths at which the photo-elastic constant $(P_{11}-P_{12})$ changes sign for KCl, KBr and KI crystals. The method adopted is based on an empirical relation that α_j/α varies linearly with $1/\lambda^2$ in the visible region (α is the sum of the polarizabilities of the two types of ion and λ is the wavelength of light). If this empirical relation is used, one has to evaluate α_j/α for a large number of wavelengths from the observed photo-elastic constants $(P_{11}-P_{12})$.

In this note a new method is given by which one can calculate the reversal wavelength at which $(P_{11}-P_{12})$ changes sign, *i.e.* from a positive value to a negative value. In order to calculate the wavelength at which $(P_{11}-P_{12})$ is equal to zero, equations (1) and (2) can be expressed in the following form:

$$x^3+ax^2+bx+c=0 \tag{3}$$

where

$$a=\frac{45}{2}\left(\frac{1+\sigma}{1-2\sigma}\right)P_{12}-\frac{15}{2}(1+\sigma)+3$$

$$b=-\frac{15}{2}(1+\sigma)+9$$

$$c=15\,(1+\sigma)+5$$

and $x=n^2$ (where n is the refractive index of the crystalline medium for which $(P_{11}-P_{12})$ is equal to zero).

Therefore x or n can be evaluated if we know the Poisson's ratio and the photo-elastic constant P_{12} for the wavelength at which $(P_{11}-P_{12})$ is equal to zero. For KCl, KBr and KI these wavelengths lie in the ultraviolet region (Srinivasan, 1959).

It is observed (Rahman & Iyengar 1966; Bansigir & Iyengar, 1961*b*) that the variation of the photo-elastic constant P_{12} is less than 5% for the entire wavelength range (from ultraviolet to the visible region). In view of this observation, one can evaluate the value of P_{12} approximately in the ultraviolet region from the observed value of P_{12} in the visible region. P_{12} of KCl, KBr, KI, RbCl, RbBr, and RbI in the ultraviolet region have been calculated by reducing the observed value at 5890 Å by 5%. Using these reduced values of P_{12}, refractive indices at the reversal wavelengths have been calculated and given in Table 1. Since dispersion data for KCl, KBr, KI and RbCl (Gyulai, 1927), RbBr and RbI (Kublitzky, 1932) are

available, the reversal wavelengths for these alkali halides have been calculated from the known refractive indices and given in Table 1, along with the observed ones (Srinivasan, 1959). It is found that the agreement is satisfactory.

Table 1. *Refractive indices and reversal wavelengths at which* $(P_{11}-P_{12})=0$.

Crystal	Refractive index, n	Reversal wavelength, λ Calculated	Observed
KCl	1·584	2548 Å	2550 Å
KBr	1·690	2712	2760
KI	1·768	3370	3380
RbCl	1·693	2092	—
RbBr	1·681	2690	—
RbI	1·824	2938	—

Absolute strain optical constants P_{11} and P_{12}, their ratios and strain polarizability constants of rubidium halides have been calculated from the experimental data (Narasimha Murthy, 1960) and expressions 1, 2 and 3. Values thus obtained are given in Table 2.

Table 2. P_{11}, P_{12}, P_{12}/P_{11} *and* λ_0.

Crystals	P_{11}	P_{12}	P_{12}/P_{11}	λ_0
RbCl	0·288	0·172	0·597	0·3946
RbBr	0·293	0·185	0·631	0·4089
RbI	0·262	0·167	0·637	0·4412

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The crystal and molecular structure of phophorus tricyanide. Erratum.

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Corrections to *Acta Cryst.* **17**, 1134 (1964).

It has been brought to our attention by Dr Tor Bjorvatten that there is an error in the text of our article on the structure of $P(CN)_3$ (Emerson & Britton, 1964). On p. 1138 at the top of column 1, sentence 2 reads: 'The C–N–P angles for these atoms are 116°, 122° and 116°, ...'. The cited angles should read 155°, 148° and 154°. The significance of these angles lay in their departure from 180°, and our conclusions about the structure are still valid. We wish to thank Dr Bjorvatten for bringing this error to our attention.

Reference

EMERSON, K. & BRITTON, D. (1964). *Acta Cryst.* **17**, 1134.