is 30·3°, while the angle between the plane passing through C(1), C(2) and C(3), and the one containing the atoms N, C(1) and C(2) is 73·7° (70° in copper β-alanine hexahydrate; Tomita, 1961).

(b) *Crystal structure*

The projection of the structure along the c axis is shown in Fig. 2. The nickel β-alanine dihydrate units are held together in a stable layer structure parallel to the (100) plane by the following bonds:

O(1)(x, y, z)–O(3)$(x, y, z-1)$	2·71 ± 0·03 Å
N (x, y, z)–O(3)$(\bar{x}, \bar{y}, 1-z)$	3·12 ± 0·04 Å
O(2)(x, y, z)–O(3)$(\bar{x}, 1-y, \bar{z})$	2·63 ± 0·03 Å
N (x, y, z)–O(2)$(x, y-1, z)$	3·11 ± 0·04 Å

The hydrogen atoms of the water molecule make the two hydrogen bonds O(3)–O(1) and O(3)–O(2). If the N–H and N–C bonds about the nitrogen atom are assumed to be coplanar and to make angles of about 120° with each other, the possible hydrogen bonds with the nitrogen atom would also be expected to be roughly coplanar with the C–N bond and to make angles of the order of 120° with it. The angles between the C(1)–N bond and the contacts N–O(2) (3·11 Å), N–O(3) (3·12 Å) and N–O(3) (2·96 Å) are 103·3 ± 1·7°, 147·6 ± 1·9° and 100·6 ± 1·7° respectively; further the C(1)–N bond and the two N–O(3) contacts are coplanar within about 15° (Fig. 2). It seems therefore that either the two N–O(3) contacts are the possible hydrogen bonds or the contact N–O(2) is a possible hydrogen bond. The angles between the possible hydrogen bonds around the water oxygen atom O(3) are: 140·7 ± 1·2° between O(3)–O(1) (2·71 Å) and O(3)–O(2) (2·63 Å); 123·7 ± 1·1° between O(3)–O(1) (2·71 Å) and O(3)–N (2·96 Å); 60·7 ± 0·8° between O(3)–O(1) (2·71 Å) and O(3)–N (3·12 Å); 118·5 ± 1·1° between O(3)–O(2) (2·63 Å) and O(3)–N (3·12 Å); 67·3 ± 0·9° between O(3)–O(2) (2·63 Å) and O(3)–N (2·96 Å); and 108·4 ± 1·0° between O(3)–N (3·12 Å) and O(3)–N (2·96 Å).

The stacking of the layers normal to the (100) plane is governed by the van der Waals bonds of the type CH_2–CH_2 and CH_2–O, as shown in Fig. 2. It is thus clear that the crystal structure of nickel β-alanine dihydrate is similar to the structures of nickel glycine dihydrate (Stosick, 1945), bis-(β-aminobutyrato)copper(II) dihydrate (Bryan, Poljak & Tomita, 1961) and copper proline dihydrate (Mathieson & Welsh, 1952).

The B values of the atoms for the $0kl$ reflexions are in general smaller than those for the $hk0$ and $h0l$ reflexions, thereby indicating, as expected, larger thermal vibration amplitudes normal to the layers of molecules.

References

Bryan, R. F., Poljak, R. J. & Tomita, K. (1961). *Acta Cryst.* **14**, 1125.

Darlow, S. F. (1960). *Acta Cryst.* **13**, 683.

Lipson, H. & Cochran, W. (1953). *The Determination of Crystal Structures*, pp. 288, 309. London: Bell.

Mathieson, A. McL. & Welsh, H. K. (1952). *Acta Cryst.* **5**, 599.

McWeeny, R. (1951). *Acta Cryst.* **4**, 513.

Noguchi, T. (1962). *Bull. Chem. Soc. Japan*, **35**, 99.

Orgel, L. E. (1952). *J. Chem. Soc.* p. 4756.

Orgel, L. E. & Dunitz, J. D. (1957). *Nature, Lond.* **179**, 462.

Stosick, A. J. (1945). *J. Amer. Chem. Soc.* **67**, 365.

Thomas, L. H. & Umeda, K. (1957). *J. Chem. Phys.* **26**, 293.

Tomita, K. (1961). *Bull. Chem. Soc. Japan*, **34**, 297.

Wilson, A. J. C. (1942). *Nature, Lond.* **150**, 152.

Acta Cryst. (1964). **17**, 28

Variation with Temperature of the Elastic Compliances of Potassium Iodide

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The thermo-elastic behaviour of a single crystal of potassium iodide has been investigated, from the boiling point of liquid oxygen to 300 °C. The composite piezoelectric oscillator method is the experimental technique employed. The compliances S_{11} and S_{44} increase with temperature, whereas the non-diagonal constant S_{12} decreases with temperature.

Introduction

The alkali halides constitute an important group among the cubic crystals. The physical properties, especially the elastic behaviour, of this group have been extensively studied, perhaps because of the simplicity of their structure. The effects of temperature on the elastic constants of potassium chloride and potassium bromide have been investigated by Durand (1936), Galt (1948), and Subrahmanyam (1958). In the case of potassium iodide the elastic constants at laboratory temperature were determined by

Bridgman (1929) and Huntington (1947). The thermal variation of the elastic constants of potassium iodide have been recently studied by Norwood & Briscoe (1958) in the range 4 °K to 300 °K, using pulse technique. In the present investigation, the elastic compliances (S_{ij}) of potassium iodide have been determined from the boiling point of liquid oxygen (−183 °C) to 300 °C.

Experimental

The present study is concerned with two directions in the cubic lattice, namely [100] and [110].

Along the [100] direction,

$$1/Y = S_{11} \quad \text{and} \quad 1/G = 4S_{44}$$

and along the [110] direction,

$$1/Y = \tfrac{1}{2}[S_{11}+S_{12}+2S_{44}] \quad \text{and} \quad 1/G = [S_{11}-S_{12}+2S_{44}]$$

where Y and G are the Young's modulus and rigidity modulus along these directions respectively, and S_{11}, S_{12} and $4S_{44}$ are the principal elastic compliances of the crystal, as represented in Wooster's notation (1938). Both the modes in the [100] direction are used to determine S_{11} and $4S_{44}$; and the torsional mode in the direction [110] has been used to evaluate the non-diagonal constant, S_{12}.

The experimental method employed is the composite oscillator method described in detail in our previous papers (Jayarama Reddy & Subrahmanyam, 1959). All the sections are cut from a large clear crystal. The densities of the specimens are determined at the laboratory temperature employing hydrostatic methods. The lengths and densities of these sections at other temperatures are calculated from the thermal expansion data of Pathak & Pandya (1960) and Yates & Panter (1962). An electric furnace, in which the temperature could be varied by adjusting the current by means of a Variac, has been used for the study above the laboratory temperature up to 300 °C. For the study below 0 °C, a special calorimeter and a cryostatic system have been designed and perfected so that the temperature in the cryostat could be held to within ±5 °C for more than two hours at any temperature. The composite oscillator is sealed and lowered into the cryostat. The cryostat is maintained at the desired temperature for more than an hour so that the oscillator could attain the same steady temperature. Measurements have been made at a series of such temperatures down to −183 °C. A copper–constantan thermocouple, calibrated and converted into a direct reading thermometer, has been used for the measurement of temperature.

Results and discussion

The actual measurements made on the bars at the laboratory temperature are given in Table 1, along with other relevant data.

Measurements on bars 1 and 2 directly give S_{11} and $4S_{44}$ as 36·90 and 240·0 respectively. On combining these with the measurements on bars, we obtain S_{12} as −5·10. The full set of elastic compliances at 30 °C are $S_{11} = 36{\cdot}90 \times 10^{-13}$, $4S_{44} = 240{\cdot}0 \times 10^{-13}$ and $S_{12} = -5{\cdot}10 \times 10^{-13}$, all in units of $\text{cm}^2.\text{dyne}^{-1}$. The author's values are compared with those of previous workers in Table 2. The compliances (S) are converted into stiffness constants (C) for purpose of comparison.

It is seen that, in general, the agreement with the results of previous workers is good.

The directly determined effective longitudinal and torsional constants along the [100] direction (S_{11} and S_{44} respectively) are plotted against temperature in Fig. 1. The variation of S_{11} is roughly linear throughout the temperature range of investigation. S_{44} is almost constant in the range below 0 °C, whereas its variation is very much greater than that of S_{11} above laboratory temperature. This is in perfect agreement with the behaviour of other alkali halides. The stiffness con-

Table 1. *Measurements on bars at laboratory temperature*

Direction	Length	Frequency	Mode	Effective compliance	
[100]	1·080 cm	136·24 kc/s	L	S_{11}	$36{\cdot}9 \times 10^{-13}$ cm^2.dyne^{-1}
[100]	0·530	108·95	T	$4S_{44}$	$240{\cdot}0 \times 10^{-13}$
[110]	0·685	102·20	T	$(S_{11}-S_{12}+2S_{44})$	$162{\cdot}0 \times 10^{-13}$

Table 2. *Comparison of results obtained by various workers*

S_{ij} are expressed in units of 10^{-13} cm^2.dyne^{-1}, and C_{ij} are expressed in units of 10^{11} dynes.cm^{-2}

Compliance or stiffness	Bridgman	Huntington	Norwood & Briscoe (27 °C)	Spangenberg & Haussühl (22 °C)	Present authors (30 °C)
S_{11}	39·2	—	38·73	—	36·9
C_{11}	2·66	2·69	2·71	2·775	2·80
$4S_{44}$	238·0	—	274·7	—	240·0
C_{44}	0·41	0·36	0·36	0·38	0·42
S_{12}	−5·4	—	−5·52	—	−5·1
C_{12}	0·43	—	0·45	0·47	0·45

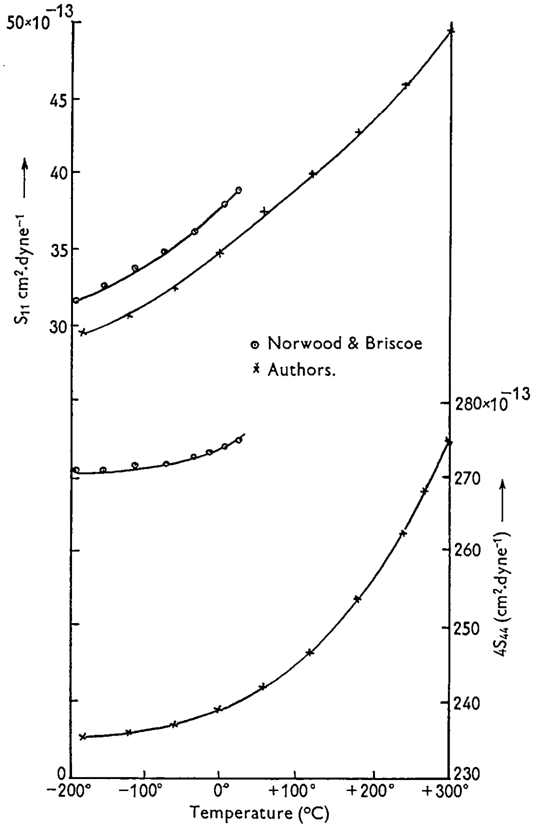

Fig. 1. Temperature dependence of S_{11} and $4S_{44}$.

stants (C_{ij}) determined by Norwood & Briscoe (1958) in the range −193 °C to 27 °C, have been converted into S's and plotted in Fig. 1 for comparison. Though the absolute values differ, the general variation with temperature agrees very well in both the investigations.

The values of S_{11} and S_{44} taken from smooth curves of Fig. 1, and S_{12} deduced from measurements on the bar in the [110] direction, are presented in Table 3.

Table 3. *S_{11} and S_{44} from Norwood & Briscoe's results, and S_{12} from measurements along* [110]

All in units of 10^{-13} cm².dyne⁻¹

Temperature	S_{11}	$4S_{44}$	$-S_{12}$
−180 °C	29·40	235·4	2·31
−150	30·00	235·7	2·62
−120	30·65	236·0	2·96
−90	31·60	236·3	3·31
−60	32·40	236·9	3·70
−30	33·49	238·0	4·05
0	34·80	239·1	4·50
+30	36·90	240·0	5·10
+60	37·51	241·8	5·80
+90	38·72	244·1	7·01
+120	40·01	246·4	7·80
+150	41·30	250·0	8·21
+180	42·82	253·6	9·42
+210	44·50	257·8	9·80
+240	45·96	262·4	9·90
+270	47·68	268·0	9·11
+300	49·51	274·8	8·62

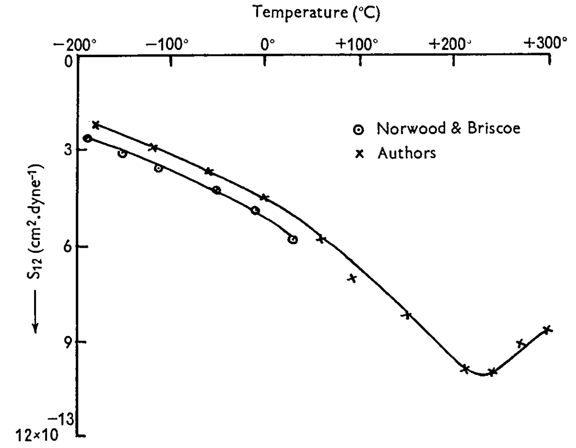

Fig. 2. Temperature dependence of S_{12}.

The non-diagonal constant S_{12} is plotted against temperature in Fig. 2. The constant decreases with temperature as in the case of potassium chloride and potassium bromide. But, above 240 °C, there is a slight increase in S_{12}. This may be due to the fact that the rates of variation of S_{11} and S_{44} above that temperature are different. In this case also, the variation with temperature agrees with that of previous workers as seen from Fig. 2.

The cubic compressibility evaluated from the values at 30 °C is $80{\cdot}1 \times 10^{-13}$ cm².dyne⁻¹. This is in agreement with the values $80{\cdot}7 \times 10^{-13}$ cm².dyne⁻¹ calculated from the observations of Spangenberg & Haussühl (1957).

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References

Bridgman, P. W. (1929). *Proc. Amer. Acad. Arts Sci.* **64**, 19.

Durand, M. A. (1936). *Phys. Rev.* **50**, 449.

Galt, J. K. (1948). *Phys. Rev.* **73**, 1460.

Huntington, H. B. (1947). *Phys. Rev.* **72**, 321.

Jayarama Reddy, P. & Subrahmanyam, S. V. (1959). *Proc. Indian Acad. Sci.* A, **50**, 380.

Norwood, M. H. & Briscoe, C. V. (1958). *Phys. Rev.* **112**, 45.

Pathak, P. D. & Pandya, N. V. (1960). *Indian J. Phys.* **34**, 416.

Spangenberg, K. & Haussühl, S. (1957). *Z. Kristallogr.* **109**, 422.

Subrahmanyam, S. V. (1958). *Proc. Indian Acad. Sci.* A, **47**, 25.

Wooster, W. A. (1938). *A Text book on Crystal Physics.* Cambridge University Press.

Yates, B. & Panter, C. H. (1962). *Proc. Phys. Soc.* **80**, 372.

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Temperature Dependence of Elastic Compliances of Garnet

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The effect of temperature on the elastic behaviour of garnet has been studied in the temperature range −183 °C to +300 °C. The experimental technique employed is the composite piezoelectric oscillator method. All the three constants (S_{11}, S_{12} and S_{44}) increase with temperature.

Introduction

Garnets form a series of isomorphous crystals, belonging to the cubic system. They belong to the space group *Ia*3*d*. They are alike in habit and the predominant habits are trapezohedron and dodecahedron forms. Chemical analysis reveals that they can be represented by the general formula, $R_3''R_2'''(\mathrm{SiO}_4)$ where R'' stands for Ca, Mg, Fe, Mn and R''' for Al, Fe, Cr and Ti. There are three prominent groups, having various constituents under each group (Dana & Ford, 1959). The three groups are: Group I: Aluminium garnet, Group II: Andradite and Group III: Uvarovite. Since they vary very much in composition, the physical properties vary very widely from specimen to specimen.

Experimental

The elastic behaviour of garnets is characterized by three independent elastic compliances, S_{11}, S_{12} and S_{44}. Hence, three independent measurements along three known directions are needed. The elastic stiffnesses of a number of garnets have been determined by Ramachandra Rao (1945) by the wedge method.

The specimen employed in this investigation is a well-developed natural crystal with dodecahedral habit. The faces in the zone [001] cut from the crystal are very distinct and free from twinning. The effective longitudinal and torsional compliances along the directions employed are given in Table 1.

Table 1. *Effective longitudinal and torsional compliances*

	Effective compliance	
Direction	Longitudinal	Torsional
[100]	S_{11}	$4S_{44}$
[110]	—	$(S_{11}-S_{12}+2S_{44})$

The torsional mode of a [110] rod is preferred over its longitudinal as it reduces considerably the error in evaluating S_{12}.

The experimental technique employed in the present study is the composite piezoelectric oscillator method (Jayarama Reddy & Subrahmanyam, 1959). The densities of all the sections are measured at laboratory temperature by hydrostatic methods. The lengths and densities of these sections are taken to be the same at high and low temperatures also, since their expansion is negligibly small. The high temperature furnace and the low temperature cryostat are described elsewhere (Jayarama Reddy & Bhimasenachar, 1964).

Results and discussion

The measurements made on one rectangular bar and two cylindrical rods at room temperature are given in Table 2.

Table 2. *Measurements at room temperature on one rectangular bar* (1) *and two cylindrical rods* (2, 3)

No.	Orientation of the bar	Length (cm)	Frequency (kc/s)	Mode*	Effective compliance
1	100	2·33	165·89	*L*	$3{\cdot}94\times10^{-13}$
2	100	2·27	107·13	*T*	10·04
3	110	2·01	120·77	*T*	10·10

* *L* = Longitudinal. *T* = Torsional.

From measurements on bars 1 and 2 we obtain S_{11} and $4S_{44}$ directly. The value S_{12} is deduced from the measurement on bar 3, and this works out to be $-1{\cdot}14\times10^{-13}$. Hence the three elastic compliances are $S_{11}=3{\cdot}94\times10^{-13}$, $4S_{44}=10{\cdot}04\times10^{-13}$ and $S_{12}=-1{\cdot}14\times10^{-13}$, all in units of cm^2.dyne^{-1}.