

The crystalline structure of zircon.

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I. *Introduction*.—In a paper recently published by Prof. Vegard¹ is contained an analysis of the structure of the zircon group of crystals, which belong to the tetragonal holohedral class, the axial ratio being approximately $a : c = 1 : 0.656$.

As the present work was completed when the above paper appeared, it is interesting to find that the principal deductions concerning the structure of zircon, $ZrSiO_4$, are confirmatory. The parametral values are, however, slightly different. This difference, though small in itself, is found to introduce larger discrepancies between the observed and calculated intensities of reflection.

According to Groth,² zircon belongs to the ditetragonal-bipyramidal class. The axial ratio, determined by Kupffer,³ is $a : c = 1 : 0.640373$.

II. *The space-group of zircon*.—A natural specimen from the Urals was employed for observations with the ionization spectrometer. This crystal, of yellowish-brown tint and measuring $15 \times 12 \times 8$ mm., was found by hydrostatic weighing to possess a density of 4.63. Natural faces (111), (110), (100), and (221) were well developed; (001) was absent. Smaller crystals of pyramidal habit, of which the locality was not known, were used for investigation by the Debye-Scherrer method. These were of a dark-brown colour and all approximately of the same size ($4 \times 2 \times 2$ mm.). The density, determined hydrostatically, was 4.67.

A determination of the dimensions of the unit cell was made with the spectrometer, using molybdenum K_α -radiation. This gave:—

$$a = 9.30 \text{ \AA}, c = 5.93 \text{ \AA}, c/a = 0.638.$$

Vegard treats the structure as a face-centred one. In order that the comparison between the two sets of results may be facilitated, the crystal is also considered here to be face-centred.

¹ L. Vegard, *Phil. Mag.*, 1926, ser. 7, vol. 1, p. 1151.

² P. Groth, *Chemische Krystallographie*, 1906, vol. 1, p. 92.

³ A. T. Kupffer, *Preisschrift über genaue Messung der Winkel an Krystallen*. Berlin, 1825, p. 66.

There are eight molecules $ZrSiO_4$ in the unit cell, the calculated density being 4.68, while the value given by Groth is 4.70.¹

Inspection of a Debye powder photograph, supplemented by data from spectrometer surveys, gave results which may be summarized thus:

- (hhl) is halved if $(h+l)$ is odd.
- (hkl) is halved if $(h+k)$, or $(k+l)$, or $(h+l)$ is odd.
- ($hk0$) is halved if $(h+k)$ is even; quartered if odd.
- ($0kl$) is halved if $(k+l)$ is even; quartered if odd.

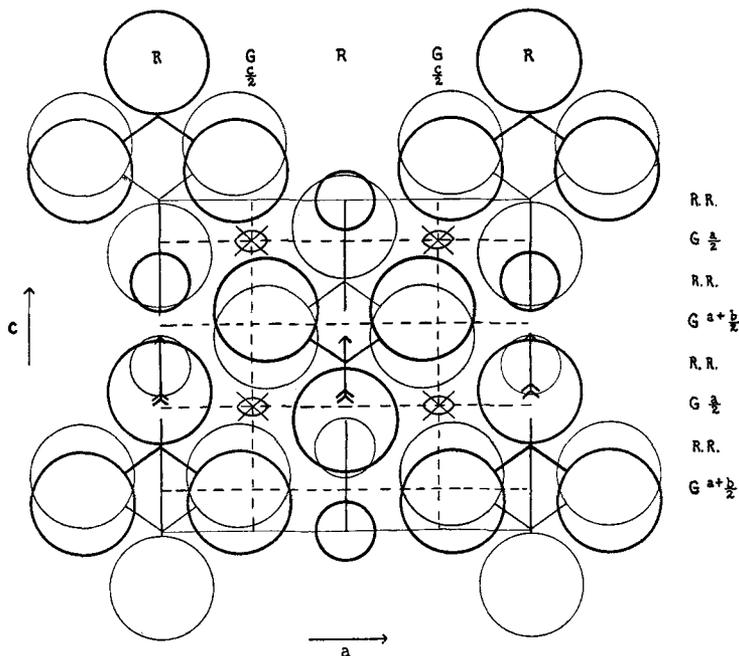


FIG. 1. Structure of zircon, showing the positions of the atoms in the reflection plane (110). The large circles represent oxygen atoms, the small ones zirconiums. Silicon atoms (not shown) lie at the centres of tetrahedral groups of oxygens. Atoms represented by thin lines lie in the reflection plane immediately below the plane containing atoms shown by thick lines.

Assuming that the crystal is holohedral, the space-group is D_{4h}^{20} . The tables of symmetry elements given by Niggli and Wyckoff refer to

¹ Although zirecons range from 4.0 to 4.7 in density (Min. Mag., 1904, vol. 14, p. 48).

the body-centred lattice. These can be transformed, in order to be applicable to the face-centred lattice, by rotating the body-centred lattice through an angle $\pi/4$ about the c -axis.

There are two sets of pure reflection planes $(110)_{\frac{1}{4}}$ $(110)_{\frac{3}{4}}$ and $(\bar{1}\bar{1}0)_{\frac{1}{4}}$

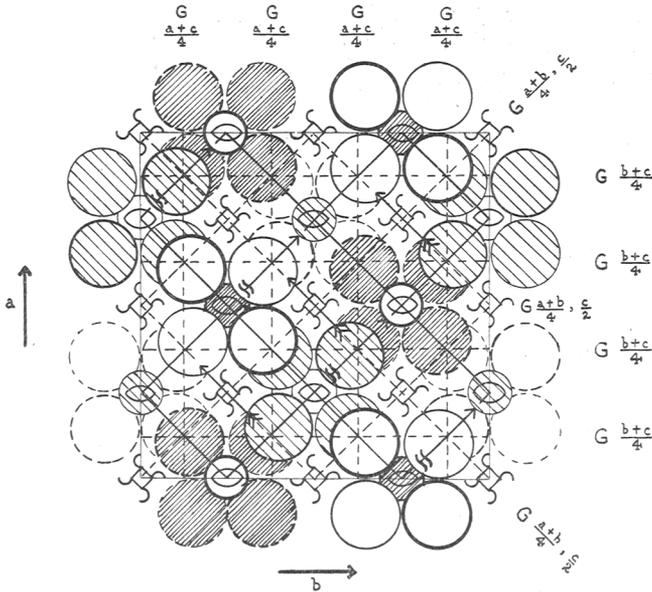


FIG. 2. Structure of zircon. The atoms in the (001) planes are represented in increasing values of c in the following manner: (a) Continuous circles, unshaded. (b) Continuous circles, shaded lightly from left to right downwards. (c) Dotted circles, shaded from right to left downwards. (d) Dotted circles, unshaded. In each tetrahedron, the pair of oxygen atoms thickly outlined lies above the pair thinly outlined. The large circles represent oxygen atoms and the small circles zirconium atoms, the silicons not being shown.

$(\bar{1}\bar{1}0)_{\frac{3}{4}}$, and two sets of rotation reflection planes $(001)_0$ $(001)_{\frac{1}{2}}$, $(001)_{\frac{1}{4}}$ $(001)_{\frac{3}{4}}$. Glide-planes have the following positions:

$$\begin{aligned} (001)_{\frac{1}{8}} (001)_{\frac{3}{8}} (001)_{\frac{5}{8}} (001)_{\frac{7}{8}} & \text{--- Translation } \frac{a}{4}, \frac{b}{4} \\ (110)_0 (\bar{1}\bar{1}0)_0 (110)_{\frac{1}{2}} (\bar{1}\bar{1}0)_{\frac{1}{2}} & \text{--- Translation } \frac{a+b}{4}, \frac{c}{2} \\ (100)_{\frac{1}{8}} (100)_{\frac{3}{8}} (100)_{\frac{5}{8}} (100)_{\frac{7}{8}} & \text{--- Translation } \frac{a}{4}, \frac{c}{4} \\ (010)_{\frac{1}{8}} (010)_{\frac{3}{8}} (010)_{\frac{5}{8}} (010)_{\frac{7}{8}} & \text{--- Translation } \frac{b}{4}, \frac{c}{4} \end{aligned}$$

III. *The arrangement of the atoms.*—Symmetry considerations show that, in order to limit the number of atoms to eight in the unit cell, the silicon atoms, and also the zirconium atoms, must lie on the axes of intersection of the two sets of reflection planes,

$$(110)_{\frac{1}{4}}, (\bar{1}\bar{1}0)_{\frac{1}{4}}; (110)_{\frac{3}{4}}, (\bar{1}\bar{1}0)_{\frac{3}{4}}.$$

Disregarding for the moment the positions of these atoms along the

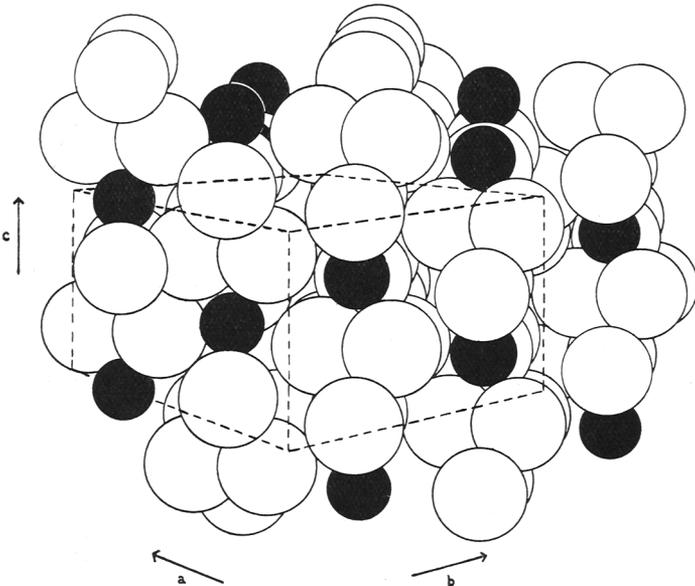


FIG. 3. The zircon structure shown spacially. The black spheres represent zirconium atoms, and the white spheres oxygen atoms grouped in tetrahedra. The silicon atoms lie at the centres of the tetrahedra, and are hidden.

vertical axes, it can be seen that the spacings (100) and (010) are quartered. To effect quartering of the other pinakoidal face, as required by symmetry considerations, the typical silicon atom on the diagonal axis $[001]_{0\frac{1}{4}}$ must be placed at one of the four positions on the axis, viz. 0 , $\frac{c}{4}$, $\frac{c}{2}$, or $\frac{3c}{4}$. The corresponding zirconium atom, lying on the same vertical axis, is placed at a distance $c/2$ from the silicon atom. That is to say, the silicons and zirconiums would form two interpenetrating face-centred lattices. The construction point may have any of the above values, for the positions of

the derived atoms are identical in the four cases, if viewed from four different construction points, surrounding a tetragonal axis.

Several arrangements of the thirty-two oxygen atoms must be considered :

(a) If an atom be placed in a general position (x, y, z) not at a symmetry centre and not on a reflection plane, symmetry operations would give sixty-four atoms to the unit. Consequently, this assemblage must be precluded.

(b) The oxygen atoms could be placed at the thirty-two symmetry centres. The amplitude of the reflected wave due to these atoms and to the Si- and Zr-atoms is:—

$$8 \cos(h+k+l) \frac{\pi}{4} \cdot [\text{Si} + (-1)^l \cdot \text{Zr} + 4 \cdot \text{O} \cdot \cos h \frac{\pi}{4} \cdot \cos k \frac{\pi}{4} \cdot \cos l \frac{\pi}{4}] \\ + 8 \sin(h+k+l) \frac{\pi}{4} \cdot [4 \cdot \text{O} \cdot \sin h \frac{\pi}{4} \cdot \sin k \frac{\pi}{4} \cdot \sin l \frac{\pi}{4}].$$

However, calculated and observed intensities are in conflict. For example, the calculated intensity of the reflection (511) is approximately twice that of the reflection (113). In the case of the observed intensity, the reverse holds.

(c) The oxygen atoms may lie on the reflection planes, but not at symmetry centres. Several sub-groupings are possible.

(1) Four oxygen atoms may be placed symmetrically round each Si-atom in a plane perpendicular to the digonal axis which passes through the Si-atom. Two arrangements would satisfy symmetry conditions. The atoms could lie either on the planes (110) and ($\bar{1}\bar{1}$ 0), or on the planes (100) and (010).

In both cases the distance between two oxygen atoms belonging to adjacent groups is so small that the atoms would penetrate considerably into each other.

The structure amplitude of the wave from atoms situated on the (110) and ($\bar{1}\bar{1}$ 0) planes is given by

$$8 \cos(h+k+l) \frac{\pi}{4} \cdot [\text{Si} + (-1)^l \cdot \text{Zr} + 4 \cdot \text{O} \cdot \cos h \theta_1 \cdot \cos k \theta_1]$$

where θ_1 determines the distance Si-O along the line of intersection of the planes (001) and (110).

For the (222) reflection, the structure amplitude is zero. This is

¹ The parameters are expressed as angular differences of phase, the dimensions of the axes representing 360° in their respective directions.

again opposed to observation, for the (222) reflection is 36.3 per cent. of that of NaCl (400 reflection).

(2) Two O-atoms could be associated with a Si-atom and two with a Zr-atom, the O-atoms being situated in the same c -plane as the atom to which they are attached, and on reflection planes at equal distances on each side of the Si- or Zr-atom in consideration. It is justifiable to assume that the distances Si-O and Zr-O are different.

Two arrangements might be considered. If, on the one hand, the O-atoms are distributed so as to lie wholly in the planes (110) or in the perpendicular set, the crystal will not be tetragonal. Moreover, between a Si-atom and a neighbouring Zr-atom would be fixed two oxygen atoms. The distance Si-Zr deduced from cell dimensions is 3.30 Å. It is impossible to pack two O-atoms side by side between the silicon and the zirconium atoms, and we must reject this distribution. On the other hand, the oxygens belonging to the Si-atoms might be situated on the (110) reflection planes, those related to the Zr-atoms being placed on the perpendicular set of planes ($1\bar{1}0$). The oxygen atoms themselves would then satisfy symmetry requirements, but if considered in conjunction with the Si-atom or the Zr-atom the arrangement would not be tetragonal. With such an arrangement, it is found that the (222) reflection has no finite value, which is contrary to observed facts.

This spectrum would have a finite value if the oxygen atoms were not in the same horizontal planes as the Si- and Zr-atoms. If we displace the two atoms belonging to a silicon, symmetry demands that we move the other set of O-atoms attached to the Zr-atom on the same axis vertically so that the two sets of oxygens lie at equal distances, say θ_2 , on each side of the Si-atom, where θ_2 is the c -co-ordinate of the atoms lying in the planes (110) and ($1\bar{1}0$). The four atoms would have to be equidistant from the diagonal axis passing through the Si-atom, and a single parameter θ_1 fixes the positions of the O-atoms in their respective c -planes, θ_1 being the distance along the lines of intersection of the plane (001) with the planes (110) and ($1\bar{1}0$).

Briefly, each Si-atom is surrounded by four O-atoms placed at the corners of a tetrahedron, the centre of which is occupied by the silicon. The evaluation of the two parameters θ_1 and θ_2 suffices to fix the positions of the O-atoms in the structure. In what follows it will be assumed that this tetrahedron is approximately regular, so that the parameter θ_2 is automatically fixed when θ_1 is evaluated. Examination of other silicates has indicated the probability of a regular SiO_4 group of this kind, though it cannot be regarded as definitely established. The

amplitude of the reflected wave due to all the atoms in the unit is given by

$$8 \cos(h+k+l) \frac{\pi}{4} \cdot [\text{Si} + (-1)^l \cdot \text{Zr} + 4\text{O} \cdot \cos h\theta_1 \cdot \cos k\theta_1 \cdot \cos l\theta_2] \\ + 8 \sin(h+k+l) \frac{\pi}{4} \cdot [4\text{O} \cdot \sin h\theta_1 \cdot \sin k\theta_1 \cdot \sin l\theta_2]. \quad (1)$$

Since the factor 8 occurs in all reflections it may be omitted.

IV. *Evaluation of the Parameters.*—An investigation of the absolute values of a few intensities showed that zircon behaved like a mosaic crystal and therefore the intensity was assumed to be proportional to the square of the structure amplitude. The formula used for the integrated reflection ρ was

$$\rho = \frac{N^2 \lambda^3}{4\mu} \cdot \frac{e^4}{m^2 c^4} \cdot \frac{1 + \cos^2 2\theta}{\sin 2\theta} \cdot S^2 (\Sigma F)^2 \cdot e^{-B \sin^2 \theta}, \quad (2)$$

where μ = linear absorption coefficient.

S = structure amplitude.

ΣF = sum of the F factors for the atoms in one molecule, when the atoms are all in phase.

In order to correct for extinction, ρ is assumed to be proportional to $\frac{S^2}{\mu_0 + \epsilon}$, where ϵ is the extinction factor, and μ_0 is the ordinary coefficient of linear absorption. The extinction factor is dependent upon the intensity of reflexion ρ , and can be written¹ $\epsilon = a\rho$.

The value of μ_0 for zircon, calculated from Wingårdh's mass absorption coefficients² for Mo-radiation is 52.7. In Table I are given the F -values adopted in this paper.

Table I.

Sin θ .	Zr ⁺ .	Si ⁺ .	O ⁻ .
0.00	36.0	10.0	10.0
0.05	35.3	9.9	9.4
0.10	33.7	9.7	6.8
0.15	31.3	9.5	4.6
0.20	28.9	9.1	3.5
0.25	26.5	8.5	2.6
0.30	24.6	7.9	1.9
0.35	23.1	7.3	1.3
0.40	22.1	6.5	0.8
0.45	21.2	5.9	0.4
0.50	20.1	5.1	0.2
0.55	18.8	4.5	0.1
0.60	17.4	3.9	—
0.65	15.8	3.3	—
0.70	14.0	2.9	—

¹ W. L. Bragg, *Phil. Mag.*, 1925, ser. 6, vol. 50, p. 306.

² K. A. Wingårdh, *Zeits. Physik*, 1922, vol. 8, p. 375.

The F -curves for silicon and zirconium are those obtained from Hartree.¹ The oxygen-scattering power curve, however, was rejected because of the increasing values beyond a certain value of the glancing angle. James and Wood² found that this curve did not fall away sufficiently rapidly. The same observation was made by Dr. A. Claassen in a determination of F -curves from the magnetite structure. As this work has not yet been published, the author is much indebted to Dr. Claassen for the use of the F -values for oxygen. In a later part of the present paper (Table III), intensities are calculated for lines of the powder spectrum, which was obtained by means of copper K_{α} -radiation. To obtain the corresponding F -curves, the values in Table I can be used if the glancing angle is multiplied by a factor 2.17, which is the ratio of the wave-length of Cu- K_{α} -radiation to that of Mo- K_{α} -radiation.

A theoretical normal reflection curve for various values of $\sin \theta$ was obtained from the formula

$$\rho_n = \frac{\Lambda^2 \lambda^3}{4 \mu_0} \cdot \frac{e^4}{m^2 c^4} \cdot \frac{1 + \cos^2 2\theta}{\sin 2\theta} \cdot (\Sigma F)^2. \quad (3)$$

By comparing equations (2) and (3) we see that, neglecting the temperature factor throughout,

$$\frac{\mu \rho}{S^2} = \mu_0 \rho_n, \quad \text{or} \quad \rho_n = \frac{\rho}{S^2} \cdot \frac{\mu_0 + \alpha \rho}{\mu_0}. \quad (4)$$

Thus the calculated values of ρ_n obtained from equation (3) should be comparable with the observed values of ρ_n obtained from equation (4). These appear in Table II.

The parametral values chosen are $\theta_1 = 38^\circ$ and $\theta_2 = 60^\circ$, as compared with Vegard's value³ $\theta_1 = 34^\circ$, and $\theta_2 = 70^\circ$. In consequence, the structure factors are different in the two cases. For the former parametral values, α is estimated to be 4.41×10^5 , whereas for the latter set α is 5.27×10^5 .

¹ D. R. Hartree, *Phil. Mag.*, 1925, ser. 6, vol. 50, p. 289.

² R. W. James and W. A. Wood, *Proc. Roy. Soc. London, Ser. A*, 1925, vol. 109, p. 588.

³ L. Vegard (*loc. cit.*). The parameters α and γ used in Vegard's paper represent the displacements of O-atoms from Zr-atoms, and not, as in the present paper, displacements from Si-atoms. Consequently

$$\theta_1 = \frac{\pi}{2} - \alpha, \quad \text{and} \quad \theta_2 = \frac{\pi}{2} - \gamma.$$

Table II.

(hkl)*	sin θ .	$\rho \times 10^6$ observed.	With parametral values $\theta_1 = 38^\circ, \theta_2 = 60^\circ$.			$\rho_n \times 10^6$.	With Vegard's values $\theta_1 = 34^\circ, \theta_2 = 70^\circ$.		
			$\frac{\rho_0 + \rho_p}{\rho_0} \cdot \rho$.	S^2 .	$\frac{\rho}{\rho_0} \cdot \frac{\rho}{S^2}$.		$\frac{\rho_0 + \rho_p}{\rho_0} \cdot \rho$.	S^2 .	$\frac{\rho}{\rho_0} \cdot \frac{\rho}{S^2}$.
(111)	0.0805	80.0	133.6	0.0566	2360	2360	144.0	0.0610	2360
(222)	0.1610	35.1	45.4	0.0605	750	680	47.5	0.0272	1746
(333)	0.2415	20.8	24.4	0.0930	262	274	25.2	0.130	194
(444)	0.3220	48.0	67.3	0.581	116	130	71.7	0.719	99.7
(555)	0.4025	5.2	5.4	0.961	56.5	66.7	5.5	0.0773	71.2
(666)	0.4830	?	?	0	?	36.5	?	0.000029	?

The discrepancy between the calculated and observed values of ρ_n for the (222) reflection appearing in columns 7 and 10 is rather large. The agreement between values in columns 6 and 7 is indeed much better than between those in columns 7 and 10.

A more complete, but less accurate, analysis was then effected by means of the powder photograph. Table III has been drawn up on the lines of that in Vegard's paper, and will enable an easy comparison to be made.

The cell dimensions had been previously determined by the spectrometer method. The values were found to be applicable to photographic measurements, as will be seen on glancing at columns 5 and 6. In the latter column appear the calculated spacings determined from the relation

$$\frac{\lambda}{2 \sin \theta} = \frac{d}{n} = \frac{a}{\sqrt{h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2}}.$$

The theoretical intensity of reflection is given by the relation

$$I = N \cdot (\Sigma F)^2 \cdot \frac{1 + \cos^2 2\theta}{\sin 2\theta} \cdot e^{-B \sin^2 \theta},$$

where N = number of planes corresponding to the form $\{h k l\}$,

ΣF = sum of the F -factors for the atoms in a molecule.

$\frac{1}{\sin 2\theta}$ = correction factor for the increase in diffusion of the reflected beam in passing from the direction of the incident beam to the perpendicular direction.

The structure amplitude for any plane $\{h k l\}$ is given by equation (1), in which is substituted the values $\theta_1 = 38^\circ, \theta_2 = 60^\circ$. The temperature factor $e^{-B \sin^2 \theta}$ is neglected throughout in calculating the intensities of

reflection. The method of evaluating observed intensities is, though not very accurate, yet sufficiently satisfactory to allow comparisons to be made between neighbouring lines on the film, and it furnishes us with an idea of the intensity distribution throughout the spectrum.

Table III.

No. of line.	S_i	θ°	$\sin \theta_c$	$\frac{d}{n}$ (obs.),	$\frac{d}{n}$ (calc.),	(hkl).	Calc. Intensity.	Nature of line. ¹	Estimate of Intensity.
1	1.76	10.05	0.1744	4.413	4.410	(111)	79.4	m. +	40
2	2.37	13.53	0.2338	3.291	3.290	(220)	147.5	v.v.s.	120
3	2.98	17.02	0.2927	2.629	2.636	(311)	23.8	w. -	10
4	3.12	17.82	0.3060	2.515	2.503	(202)	125.0	s.	70
5	3.37	19.23	0.3293	2.336	2.325	(400)	21.1	w.	15
6	3.58	20.43	0.3490	2.205	2.205	(232)	12.1	w. -	10
7	3.83	21.85	0.3721	2.068	2.057	(331)	25.3	m. -	25
8	4.16	23.75	0.4026	1.912	1.897	(118)	18.2	w. +	20
9	4.58	26.12	0.4402	1.748	1.744	(511)	10.7	w. -	10
10	4.69	26.75	0.4500	1.710	1.701	(422)	100	v.s.	100
11	4.89	27.93	0.4683	1.644	1.645	(440)	40.1	m. +	40
11					1.643	(133)			
12	5.22	29.82	0.4973	1.545	1.540	(351)	8.4	w. -	10
12					1.483	(004)			
13	5.52	31.52	0.5227	1.472	1.471	(620)	31.9	m.	30
13					1.470	(333)			
13					1.438	(442)			
14	5.95	33.98	0.5587	1.374	1.374	(602)	27.8	m.	30
15	6.01	34.33	0.5639	1.365	1.354	(224)	21.6	w. +	20
15					1.342	(513)			
15					1.318	(622)			
16	6.43	36.72	0.5978	1.287	1.284	(551)	11.6	w. -	10
16					1.284	(711)			
16					1.252	(404)			
17	6.61	37.75	0.6121	1.257	1.252	(533)	21.6	w. +	20
17					1.243	(533)			
17					1.209	(244)			
17					1.196	(731)			
17					1.196	(731)			
18	7.10	40.55	0.6500	1.184	1.183	(462)	24.7	m. -	25
19	7.24	41.34	0.6604	1.165	1.169	(115)	10.9	w. -	10
19					1.163	(800)			
20	7.74	44.20	0.6972	1.104	1.103	(444)	17.6	w. +	20
20					1.102	(315)			
21	7.80	44.54	0.7013	1.096	1.097	(660)	13.9	w.	15
21					1.096	(553)			
21					1.096	(713)			
21					1.064	(751)			
22	8.20	46.82	0.7292	1.055	1.054	(822)	21.4	m. -	25

v.s. = very strong, s. = strong, m. = medium, w. = weak, v.w. = very weak.

Table III (continued) :

No. of line.	λ .	θ° .	$\sin \theta$.	d — n (obs.).	d — n (calc.).	(<i>hkl</i>).	Calc. Intensity.	Nature of line. ¹	Estimate of Intensity.			
23	8.26	47.18	0.7333	1.049	1.045	(624)	22.8	m. —	25			
					1.045	(335)						
24	8.34	47.62	0.7387	1.041	1.040	(480)	12.2	w. —	10			
					1.040	(733)						
					1.029	(662)				0	absent	—
					1.012	(911)				1.8	absent	—
25	8.82	50.37	0.7700	0.999	0.997	(155)	3.9	v.w.	5			
					0.982	(842)				0	absent	—
					0.974	(644)				0	absent	—
26	9.23	52.71	0.7956	0.967	0.969	(206)	14.2	w. —	10			
					0.967	(931)						
27	9.46	54.03	0.8092	0.951	0.953	(355)	6.1	v.w.	5			
					0.949	(753)						
					0.949	(226)						
28	10.03	57.27	0.8411	0.915	0.926	(771)	2.4	absent	—			
					0.916	(804)						
					0.912	(10.2.0)				29.0	w. +	20
					0.912	(913)						
29	10.41	59.44	0.8610	0.894	0.898	(824)	0.2	absent	—			
					0.894	(426)				26.6	w. +	20
					0.893	(951)						
30	10.50	59.96	0.8656	0.889	0.888	(10.0.2)	36.4	m. —	25			
					0.888	(862)						
31	10.64	60.77	0.8726	0.882	0.882	(664)	16.1	w. —	10			
					0.882	(555)						
					0.882	(715)						
					0.879	(933)				3.2	absent	—
32	11.25	64.24	0.9006	0.855	0.872	(10.2.2)	34.9	m. —	25			
					0.852	(844)						
					0.852	(735)				0.3	absent	—
					0.849	(773)				2.2	absent	—
					0.848	(446)						
33	11.80	67.39	0.9230	0.834	0.842	(117)	1.0	absent	—			
					0.834	(606)				21.7	w.	15
					0.834	(11.1.1)						
34	11.90	67.95	0.9267	0.830	0.829	(10.4.2)	35.5	m. —	25			

V. *Atomic distances*.—The distance Si—O is found to be 1.70 Å. Each Zr-atom is surrounded by eight oxygen atoms, four at distances 1.96 Å., and four at distances 2.41 Å., the latter four being situated, two above and two below. The centre distance between the two nearest O-atoms is 2.77 Å.

¹ v.s. = very strong, s. = strong, m. = medium, w. = weak, v.w. = very weak.

Summary.—An examination of the structure of zircon, ZrSiO_4 , has been made by the ionization spectrometer and by a Debye-Scherrer powder photograph. The lattice upon which the structure is based corresponds to the space-group D_{4h}^{19} , possessing the symmetry of the ditetragonal-bipyramidal class. The unit cell, containing eight molecules ZrSiO_4 , has the dimensions $a = 9.30$, $c = 5.93 \text{ \AA}$.

The silicon and zirconium atoms form two interpenetrating face-centred lattices. Eight digonal axes pass vertically through each unit cell and on each axis is situated one silicon and one zirconium lying at a distance $c/2$ apart. Symmetry considerations limit the assembling of oxygen atoms to tetrahedra, each enclosing a silicon atom. All the atoms in the structure are situated on reflection planes.

The structure resembles in some ways that of anhydrite, CaSO_4 , an account of which appears in another paper.¹ The analogous dispositions of atoms in the planes (110) in zircon and in the planes (001) in anhydrite is most interesting. The distribution of atoms about the c -axis in zircon is similar to that about the a -axis in anhydrite.

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