

would tend to be spread over a wider range of layer lines, but the major error might still remain for the layer line h' .) It is not difficult to show that the condition that $(\sigma_1 - \sigma)$ be greater than $(\sigma_2 - \sigma)$, where σ is the standard deviation resulting only from random errors (and assumed to be the same in the two methods), is

$$A > Bh'^2. \quad (4)$$

In our case for an oxygen atom and the limited data with unit weights we have $A^{\frac{1}{2}} = 9.7 \cdot 10^{-5}$ and $B^{\frac{1}{2}} = 3.1 \cdot 10^{-6}$. Hence, any such error for $h' < 31$ (and hence any such error in our data) will cause a relatively greater increase in the least-squares estimate of the standard deviation of an oxygen parameter than in the estimate from Cruickshank's method.

Another type of systematic error might be described by

$$F_o = F_o^0 + Ch, \quad (5)$$

where F_o^0 is the structure amplitude that would be observed if there were no systematic errors. Equation (5) idealizes a common type of systematic error, namely one which increases (or decreases) with scattering angle. In this case $(\sigma_1 - \sigma)$ will be greater than $(\sigma_2 - \sigma)$ if

$$A \sum_j h^2 > B \sum_j h^4. \quad (6)$$

Our calculations indicate that the inequality (equation

(6)) holds here for the entire data as well as for the limited data.

Without direct evidence concerning the types and magnitudes of systematic errors in our data we cannot, of course, make any calculations of the order of magnitude of the discrepancy to be expected in the standard deviations. On the other hand, the rather qualitative and idealized calculations presented here make it reasonable to suppose that at least part of the discrepancy found between the least-squares and Cruickshank's estimates of standard deviations is due to systematic errors in the data. Clearly this example points once again to the often repeated but often forgotten fact that standard deviations obtained in crystal structure analyses are merely rough estimates, subject to many uncertainties, and are perhaps reasonable only when no systematic errors are to be found in the data. By placing an undue amount of faith in such estimates one may obtain a false impression of the accuracy of the structure determination.

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A Single Crystal Neutron Diffraction Study of Diaspore, $\text{AlO}(\text{OH})$

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A single crystal neutron diffraction study of diaspore has been made in which the intensities of ninety reflections of the $hk0$ and $0kl$ zones were measured. Unit-cell dimensions and their standard errors as redetermined by the X-ray powder method are $a = 4.401 \pm 0.001$, $b = 9.421 \pm 0.004$, and $c = 2.845 \pm 0.001$ Å.

The structure was refined by the method of least squares using an anisotropic temperature factor for each atom. The Al and O position parameters obtained in this way are in good agreement with the X-ray results reported by Hoppe. The hydrogen bonding postulated by Ewing (1935) was confirmed. The H atom is located 0.990 Å from O_{II} , but is not on the line of centers between O_{I} and O_{II} . Instead the $\text{O}_{\text{II}}\text{-H}$ bond makes an angle of 12.1° with the $\text{O}_{\text{II}}\text{-O}_{\text{I}}$ vector.

Introduction

The mineral diaspore, $\text{AlO}(\text{OH})$, has been the subject of several X-ray investigations (de Jong, 1930; DeFlandre, 1932; Takané, 1933). Its structure was cor-

rectly deduced by Ewing (1935) who based his conclusions partly on X-ray data and partly on considerations of ionic size and coordination numbers. A more complete X-ray determination was subsequently made by Hoppe (1941; 1942) who refined the aluminum and oxygen positions by Fourier methods. The present neutron diffraction investiga-

* Operated for the U.S. Atomic Energy Commission by Union Carbide Corporation.

tion was undertaken primarily for the purpose of locating the hydrogen atoms, and it has also resulted in an improvement of all the position parameters together with a complete description of the mean thermal displacements of the nuclei.

The symmetry of diaspore is orthorhombic $Pbnm$, with four molecules in a unit cell, and its structure projected along c is shown in Fig. 1. Each cell has

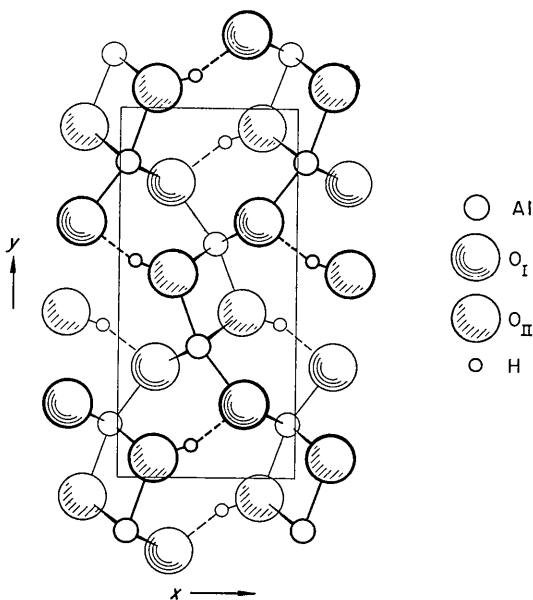


Fig. 1. The crystal structure of diaspore. Atoms drawn with heavy and light lines are located on mirror planes with $z = \frac{1}{4}$ and $z = -\frac{1}{4}$, respectively.

two mirror planes which lie parallel to the page at $z = \pm\frac{1}{4}$ and all of the atoms are situated on these planes, so that for each atom there are only two position parameters, x and y , to be determined. In the figure the atoms in the near plane are drawn more heavily than those in the far one. There are two kinds of oxygen atoms which Ewing designated as O_I and O_{II} , and each aluminum atom has three of each kind of oxygen as neighbors. The resulting octahedra share edges to form what Ewing described as 'double rutile strings' extending in the c -direction, and these double strings are further connected to each other by the sharing of corner oxygens to form a three-dimensional network. Ewing noted that one kind of O_I - O_{II} distance was much shorter than the others and postulated the existence of a hydrogen bond between these atoms. The present neutron diffraction study has verified this conclusion and the hydrogen positions shown in Fig. 1 are those found in this work.

Experimental

Single-crystal neutron diffraction intensities were measured for ninety reflections of the $hk0$ and $0kl$ zones using the method described by Peterson and

Levy (1952). The neutron wavelength was 1.062 Å. Two samples of natural diaspore* were used in the measurements, a 9.30 mg. crystal from Redondo, Uruguay, for the $hk0$ zone, and a 5.57 mg. specimen from Chester, Pennsylvania, for the $0kl$ zone. A preliminary intensity calibration was obtained by comparison with the 400 reflection from a standard NaCl crystal. The crystals were measured and the absorption correction factor for each reflection was calculated with the aid of the high speed computer, the Oracle, using a method which has been described previously (Busing & Levy, 1957a). The experimentally determined value of the linear absorption coefficient was 1.49 cm^{-1} . Because of the good agreement between intensity measurements from the two different sized crystals and also between the observed and calculated structure factors, extinction was judged to be unimportant. The samples were opaque and presumably imperfect enough to eliminate this problem.

Refinement of the structure

The measured intensities were reduced to structure factors in the usual way, and these were compared with values calculated for structures with the hydrogen atom in the postulated hydrogen bond on the line of centers between the two oxygen atoms. Two hydrogen positions were tried, one nearer to O_I and the other nearer to O_{II} , and the latter model was found to give the best agreement. Using signs of the structure factors based on this model, $hk0$ Fourier projections were made to obtain a preliminary refinement of the position parameters. Even at this stage it was apparent that the true hydrogen position was somewhat off the line of oxygen centers. These projections also appeared to rule out any possibility that the hydrogen atom could be statistically distributed between positions adjacent to O_I and to O_{II} .

The refinement of the structure was made by the method of least-squares with the aid of the high speed computer, the Oracle. For this purpose each atom was described by two position parameters, x and y , and the four temperature factor coefficients B_{xx} , B_{yy} , B_{zz} , and B_{xy} . The form chosen for the temperature factor of an atom at $\pm(x, y, \frac{1}{4})$ was

$$\exp [-(B_{xx}h^2 + B_{yy}k^2 + B_{zz}l^2 + 2B_{xy}hk)]$$

and for atoms at $\pm(\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{4})$ this factor was modified by changing the sign of the cross term. (The terms with B_{zz} and B_{yz} vanish because of the symmetry.) An overall scale factor multiplying the calculated structure factors was included for each of the two zones making a total of twenty-six parameters. The scattering amplitudes for Al, O, and H were assumed to be 0.35, 0.58, and -0.378 ($\text{cm} \times 10^{-12}$), respectively (Hughes & Harvey, 1955). The least-

* These samples were kindly supplied by Dr Robert C. Plumb of the Aluminum Company of America.

Table 1. *Least-squares parameters of diaspore and their standard deviations*

The position parameters obtained by Hoppe (1942) are given in parentheses

	Al	O _I	O _{II}	H
<i>x</i>	0.0451 ± 0.0008 (0.048)	0.7120 ± 0.0005 (0.713)	0.1970 ± 0.0005 (0.198)	0.4095 ± 0.0009 —
<i>y</i>	-0.1446 ± 0.0003 (-0.146)	0.1989 ± 0.0002 (0.199)	0.0532 ± 0.0002 (0.056)	0.0876 ± 0.0004 —
4 <i>a</i> ² <i>B</i> _{xx}	0.34 ± 0.10	0.31 ± 0.07	0.28 ± 0.07	0.86 ± 0.12
4 <i>b</i> ² <i>B</i> _{yy}	0.15 ± 0.08	0.37 ± 0.05	0.25 ± 0.05	1.68 ± 0.12
4 <i>c</i> ² <i>B</i> _{zz}	0.31 ± 0.23	0.11 ± 0.11	0.56 ± 0.13	1.63 ± 0.33
4 <i>abB</i> _{xy}	0.06 ± 0.09	-0.10 ± 0.02	0.05 ± 0.06	-0.03 ± 0.12
	<i>hk0</i> zone	<i>0kl</i> zone		
Scale factor	0.988 ± 0.001	1.009 ± 0.001		

squares weight, *w*, of each structure factor was taken as the reciprocal of its estimated variance, and determined as described in a previous paper (Busing & Levy, 1957*b*). Off-diagonal terms of the normal equations were included in solving for the corrections to parameters, and the treatment was repeated until the parameters had converged. The matrix of the normal equations was then inverted to determine the standard deviations of the final parameters. (See, for example, Arley & Buch, 1950).

Table 2. *Observed and calculated structure factors for diaspore*

The former have been divided by the appropriate scale factor from the least-squares refinement

<i>h</i>	<i>k</i>	<i>l</i>	<i>F</i> _o	<i>F</i> _c	<i>h</i>	<i>k</i>	<i>l</i>	<i>F</i> _o	<i>F</i> _c
0	2	0	1.02	-1.05	4	5	0	0.52	0.50
0	4	0	0.83	0.78	4	6	0	0.29	-0.19
0	6	0	2.00	2.02	4	7	0	3.20	3.17
0	8	0	2.76	-2.72	4	8	0	1.33	-1.27
0	10	0	1.87	-1.97	4	9	0	0.39	0.40
0	12	0	3.74	-3.71	4	10	0	0.54	0.55
1	1	0	2.37	2.43	5	1	0	0.65	0.57
1	2	0	1.12	1.07	5	2	0	2.14	2.05
1	3	0	0.45	-0.46	5	3	0	2.61	2.64
1	4	0	3.76	-3.81	5	4	0	0.84	-0.86
1	5	0	1.89	-1.86	5	5	0	1.35	-1.27
1	6	0	0.25	-0.29	5	6	0	0	-0.02
1	7	0	0.40	0.44	5	7	0	0.75	0.85
1	8	0	2.33	-2.33	5	8	0	0.42	0.44
1	9	0	1.04	-1.02	6	0	0	1.37	1.39
1	10	0	0	0.04	6	1	0	1.40	-1.42
1	11	0	1.40	-1.20	6	2	0	1.37	1.39
1	12	0	2.50	2.54	6	3	0	0.28	0.30
1	13	0	1.37	1.43	6	4	0	0.39	-0.32
2	0	0	3.28	-3.27	6	5	0	2.78	-2.81
2	1	0	1.59	-1.55					
2	2	0	0.34	-0.34					
2	3	0	1.55	-1.56					
2	4	0	1.70	-1.67					
2	5	0	2.56	-2.49					
2	6	0	1.39	1.35					
2	7	0	0.76	-0.90					
2	8	0	3.82	3.90					
2	9	0	2.29	2.29					
2	10	0	1.51	-1.50					
2	11	0	0.42	-0.43					
2	12	0	1.91	1.97					
2	13	0	0.63	0.66					
3	1	0	0.90	-0.92					
3	2	0	1.94	1.92					
3	3	0	2.96	-3.01					
3	4	0	3.39	3.29					
3	5	0	1.65	1.60					
3	6	0	1.36	-1.38					
3	7	0	1.08	1.17					
3	8	0	1.24	1.27					
3	9	0	1.76	1.76					
3	10	0	0.42	-0.49					
3	11	0	1.20	1.23					
3	12	0	2.44	-2.51					
4	0	0	3.14	3.14					
4	1	0	2.76	2.81					
4	2	0	0.37	-0.38					
4	3	0	0.40	0.34					
4	4	0	0.51	-0.46					

The results are listed in Table 1 which includes for comparison the position parameters determined by Hoppe (1942). It will be seen that there are no major discrepancies with these older values, the largest change being that of *y*(O_{II}) for which the difference is equivalent to 0.03 Å. In this table the temperature factor coefficients have been scaled as indicated to correspond to the usual Debye-Waller *B*. It is apparent that these coefficients are not nearly as well determined as are the position parameters. This is especially true for the *B*_{zz} which depend entirely on the measurements of twenty *0kl* reflections from the smaller sample.

Listed in Table 2 are the observed structure factors together with those calculated from the final parameters. The observed values for the *hk0* and *0kl* zones have been divided by 0.988 and 1.009, respectively, the scale factors resulting from the least-squares treatment. The conventional discrepancy factor, $\sum |F_o| - |F_c| / \sum |F_o|$, is 3.9% and the weighted root-mean-square discrepancy factor, $[\sum w(F_o - F_c)^2 / \sum w F_o^2]^{1/2}$, is 3.5%. The standard deviation of an observation of unit weight given by the expression $[\sum w(F_o - F_c)^2 / (m - n)]^{1/2}$ (where *m* is the number of observations and *n* is the number of parameters determined) is 2.0. Since the expectation value of this quantity is unity, the fit is not so good as one would predict from the estimated accuracy of the data. Either this accuracy was overestimated, or there is a deficiency in the expression from which the structure factors were calculated. The latter could arise, for example, from a failure to describe the thermal motion correctly.

Unit-cell dimensions

There is some discrepancy between the unit-cell dimensions reported by Ewing (1935) and by Hoppe (1941)

Table 3. *Unit-cell dimensions in diaspore*

	Ewing (1935)*	Hoppe (1941)*	Present work (Å)
<i>a</i>	4.40	4.42	4.401 ± 0.001
<i>b</i>	9.39	9.44	9.421 ± 0.004
<i>c</i>	2.84	2.84	2.845 ± 0.001

* Probably kX units.

(see Table 3), and it was apparent that these uncertainties would limit the accuracy of the calculated bond distances and angles unless the cell dimensions were redetermined. Debye-Scherrer powder photographs were therefore made with Cu $K\alpha$ radiation using Straumanis' scheme of film arrangement and measurement to eliminate radius and shrinkage errors. (See, for example, Buerger, 1942, chapter 20.) Two anomalous lines appeared on these photographs, one of which was apparently the forbidden (100) reflection, the presence of which has been explained by Garrido (1945) as the result of double internal reflection. The other, found at a position corresponding to a 3.29 Å spacing, is assumed to be due to an unidentified impurity. As an aid to indexing the pattern the X-ray intensities were calculated using the neutron diffraction parameters, and in this way forty well resolved reflections, eight of them with $\theta > 50^\circ$, were unequivocally identified.

The parameters a , b , and c were then adjusted by the method of least-squares to minimize $\sum w(\theta_o - \theta_c)^2$ where θ_o and θ_c are the observed and calculated Bragg angles and w is the weight assigned to an observation. With the aid of the Oracle the least-squares procedure was repeated until the parameters no longer changed, and the standard deviations were obtained from the inverse matrix of the normal equations. The wavelengths were taken as 1.54057 Å and 1.54439 Å for the Cu $K\alpha_1$ and Cu $K\alpha_2$ lines, respectively. For reflections with $\theta < 50^\circ$, however, the doublet was not resolved, and these data were treated as though the wavelength was a 2:1 weighted average of the above. Reflections in this category were given less weight than the others, but, except for this, all observed Bragg angles were considered to be equally accurate. The resulting unit-cell dimensions and their standard deviations are listed in Table 3 together with the older values for comparison.

An attempt was made to compensate for absorption errors by using only high angle reflections and adding

Table 4. Bond angles and interatomic distances in diaspore

The unprimed symbols represent atoms on a given mirror plane (e.g. $z = +\frac{1}{2}$) while primed symbols designate those on a plane adjacent to this one (e.g. $z = -\frac{1}{2}$). No corrections for thermal motion have been applied to these values.

Angles about Al (degrees)	Angles about O _I (degrees)
O _I -Al-O _I ' 97.6 ± 0.1	Al-O _I -Al' 124.8 ± 0.1
O _I '-Al-O _I ' 100.4 ± 0.2	Al'-O _I -Al' 100.4 ± 0.2
O _I -Al-O _{II} 91.0 ± 0.1	Al-O _I -H 90.7 ± 0.2
O _I '-Al-O _{II} 93.7 ± 0.1	Al'-O _I -H 106.4 ± 0.1
O _I '-Al-O _{II} ' 83.0 ± 0.1	
O _{II} -Al-O _{II} ' 76.8 ± 0.1	Nearest neighbor distances (Å)
O _{II} '-Al-O _{II} 92.2 ± 0.2	Al-O _I 1.858 ± 0.004
Angles about O _{II} (degrees)	Al-O _I ' 1.851 ± 0.002
Al-O _{II} -Al' 103.2 ± 0.1	Al-O _{II} 1.980 ± 0.003
Al'-O _{II} -Al' 92.2 ± 0.2	Al-O _{II} ' 1.975 ± 0.003
Al-O _{II} -H 128.8 ± 0.3	O _I -O _{II} 2.650 ± 0.003
Al'-O _{II} -H 111.5 ± 0.2	O _I -H 1.694 ± 0.005
O _I -O _{II} -H 12.1 ± 0.3	O _{II} -H 0.990 ± 0.004

Table 5. Thermal motion of the atoms in diaspore

The vectors μ describe the root-mean-square displacements along the principal axes of the ellipsoidal distribution, with μ_1 and μ_2 parallel to the x , y plane and μ_3 perpendicular to it. The angle α specifies the direction of μ_1 with respect to the x -axis

	μ_1 (Å)	μ_2 (Å)	μ_3 (Å)	α (degrees)
Al	0.067 ± 0.009	0.040 ± 0.013	0.063 ± 0.023	17 ± 21
O _I	0.075 ± 0.006	0.054 ± 0.008	0.037 ± 0.019	128 ± 12
O _{II}	0.063 ± 0.008	0.052 ± 0.008	0.084 ± 0.010	145 ± 26
H	0.146 ± 0.005	0.104 ± 0.007	0.144 ± 0.014	88 ± 8

to θ_c a correction term, $D \cos^2 \theta_c$, where D was used as a fourth parameter in the least-squares treatment. It was found, however, that the correction did not substantially improve the agreement, and it was concluded that the data were not sufficiently accurate to warrant this procedure. The cell dimensions obtained in this way differed from those reported here by only a little more than one standard deviation.

Further calculations

The results of the two least-squares treatments were used to calculate bond angles and interatomic distances, and the principal axes of thermal motion for each atom were found in the way described by Waser (1955). The calculations were made with the aid of the Oracle using a program which evaluates any function of the parameters together with its standard deviation. The latter is determined from the variance-covariance matrix which results from the least-squares calculation. The derived quantities with their standard deviations are listed in Tables 4 and 5, and some of them are represented graphically in Figs. 2 and 3.

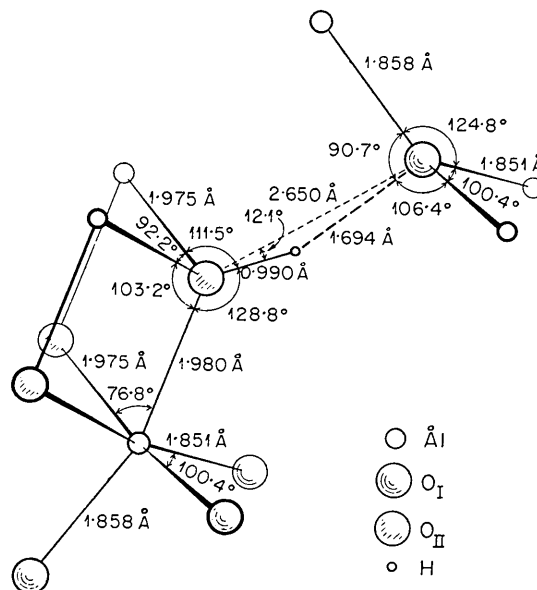


Fig. 2. Some bond angles and interatomic distances in diaspore. The atoms drawn with lightest, intermediate, and heaviest lines are located on mirror planes with $z = -\frac{1}{2}$, $z = \frac{1}{2}$, and $z = \frac{3}{2}$, respectively. No corrections for thermal motion have been applied to these values.

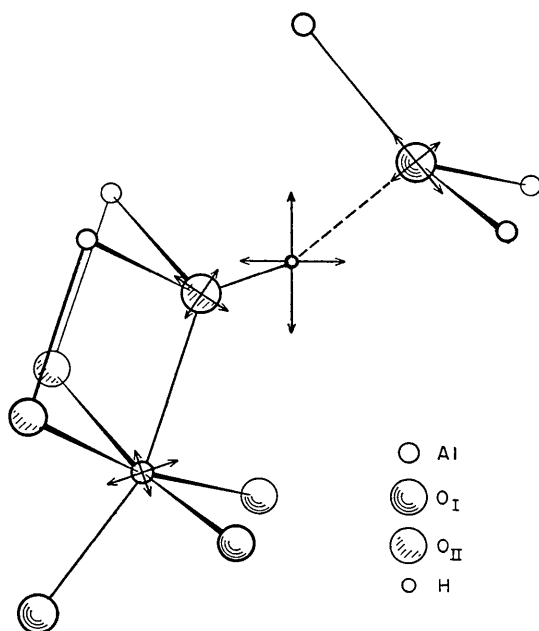


Fig. 3. The thermal motion in diaspore. The vectors show the directions of the principal axes of the thermal motion ellipsoids in the x, y plane and are drawn with lengths equal to the root-mean-square displacements on a scale five times that of the interatomic distances. The third axis is in the z -direction and is not shown.

Discussion

Ewing favored a structure in which the hydrogen was shared more or less equally between the two kinds of oxygen atoms, but it now seems likely that a symmetric O-H-O bond requires a much shorter O-O distance than that in diaspore (see, for example, Lippincott & Schroeder, 1955), and the present results indicate clearly that the hydrogen atom belongs to O_{II} . The association of hydrogen with O_{II} rather than with O_I is compatible with the fact that the Al- O_{II} distances (1.980 Å and 1.975 Å) are longer than the Al- O_I distances (1.858 Å and 1.851 Å) since an OH⁻ ion would be less strongly attracted to Al⁺³ than would an O⁼ ion. The difference in Al-O distances may be due to other causes, however, as these differences are also found in corundum, Al₂O₃, (Pauling & Hendricks, 1925) in which all the oxygens are equivalent. The location of hydrogen is also consistent with the fact that the O_{II} atom forms a pyramid with the three aluminum atoms adjacent to it while O_I is more nearly coplanar with its three aluminum neighbors. The hydrogen atom in a position near O_{II} is therefore farther from positive aluminum ions than it would be if it were associated with O_I .

The hydrogen atom is not on the line of centers between the two oxygen atoms, but instead the O-H bond makes an angle of $12.1 \pm 0.3^\circ$ with this line. This fact can be interpreted as the result of repulsion of the hydrogen by Al⁺³ ions. The Al- O_{II} -H angles

are 128.8° and 111.5° so that the arrangement of atoms about O_{II} is roughly tetrahedral, but if the hydrogen were on the line of oxygen centers these angles would be 141° and 104° , respectively.

The O_{II} -H interatomic distance calculated from the position parameters is 0.990 Å, but this apparent bond length is probably somewhat foreshortened because of the large thermal motion of the hydrogen. A better measure of the bond length may be the mean interatomic distance which can be estimated if it is assumed that the H atom is attached only to the O_{II} atom and therefore exhibits a thermal motion which includes the O_{II} motion. It can be shown (Busing & Levy, 1958) that under these circumstances the mean distance \bar{R} is given approximately by

$$\bar{R} = R_0 + \left(\frac{1}{2}R_0\right) \sum_{i=1}^3 (\nu_{Hi}^2 - \nu_{O_i}^2),$$

where R_0 is the uncorrected interatomic distance and where the ν_{Hi}^2 and $\nu_{O_i}^2$ are the mean square principal thermal displacements for the H and O_{II} atoms, respectively, projected on a plane perpendicular to the interatomic vector. The O_{II} -H bond distance obtained in this way is 1.005 Å. These distances are of the order to be expected for an $O_{II} \cdots O_I$ distance of 2.650 Å. The corrected and uncorrected bond lengths bracket the theoretical function of Lippincott & Schroeder (1955) which has been given graphically for $g = 1.78$ by Welsh (1957).

It is interesting to note that the temperature factor coefficients for diaspore are only about one-third to one-half as large as those for the corresponding atoms in Ca(OH)₂ (Busing & Levy, 1957b). This is consistent with the great difference in the structure types of these compounds. Diaspore with its higher ionic charges forms a network structure with a hardness of 6.5 to 7, while Ca(OH)₂, in which all the anions are dipolar, crystallizes in a sandwich layer arrangement and has a hardness of only 2.

Table 5 lists the r.m.s. components of the displacement of the atoms along the principal axes of the temperature factor ellipsoids, together with the angles α which describe the orientations of the principal axis vectors μ_1 with respect to the x -axis. Fig. 3 shows the vectors μ_1 and μ_2 drawn to a scale five times that for interatomic distances. The vector μ_3 is not shown since symmetry requires it to be oriented in the z direction. The standard deviations of these quantities are also given in Table 5, and it is clear that the relative errors are much greater than are those of the position parameters.

Comparison of the μ 's for the hydrogen atom shows that its temperature factor ellipsoid is oblate, and this is to be expected since the bending of the O_{II} -H bond should occur more readily than its stretching. However, this simple interpretation fails to explain the fact that μ_2 for hydrogen is not parallel to the O_{II} -H bond but instead makes an angle of 21 ± 8

degrees with it. The temperature factors of the remaining atoms all show some anisotropy, but the orientations of their principal axes do not appear to bear a simple relationship to the structure. Further interpretation seems to require an understanding of the dynamics of the infinite aluminum-oxygen network.

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The Crystal Structures of Some Anthracene Derivatives. II. 9:10-Dibromoanthracene

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The crystal structure of 9:10-dibromoanthracene has been determined from Patterson and Fourier projections along two crystallographic axes, and values of the bond lengths and valency angles in the molecule and intermolecular distances are given.

Introduction

The first molecule which was examined in the present series of investigations of anthracene derivatives (Trotter, 1958) was 9:10-dibromoanthracene. The structure of this molecule has been investigated previously (Kitajgorodskij, 1946a; *Structure Reports*, 1945-46) but as no details of the structure or coordinates of the atoms are given, a full analysis by X-ray diffraction methods has been carried out.

Experimental

Crystals of 9:10-dibromoanthracene were obtained by crystallization from petroleum ether. They are greenish-yellow in colour, and consist of prisms elongated along the *a*-axis with (010) and (001) faces developed. The density was determined using a Berman balance (Berman, 1939) with carbon tetrachloride as displacement liquid. The unit-cell dimen-

sions and space group were determined from rotation and oscillation films about the *a*-axis, *Ok**l* and *1kl* Weissenberg films, and *h*0*l*, *h*1*l*, *hk*0 and *hkl* precession films.

Crystal data

9:10-dibromoanthracene, C₁₄H₈Br₂; *M* = 336.0; m.p. 226 °C. Triclinic,

a = 4.06 ± 0.01, *b* = 8.88 ± 0.02, *c* = 16.15 ± 0.04 Å,
α = 98° 50' ± 10', β = 97° 05' ± 10', γ = 100° 21' ± 10'.

Volume of the unit cell = 559.3 Å³.

Density, calculated (*Z* = 2) = 1.983 g.cm.⁻³,
measured = 1.981 g.cm.⁻³.

Absorption coefficient for X-rays,

λ = 1.542 Å, μ = 92.7 cm.⁻¹;

λ = 0.7107 Å, μ = 78.2 cm.⁻¹.

Total number of electrons per unit cell = *F*(000) = 324.

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