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The lattice constants of a-quartz

J. C. BRICE
Philips Research Laboratories, Redhill, Surrey, UK

Data relating to the lattice constants of quartz are reviewed and it is shown that hydrogen and most other impurities increase the a lattice constant and decrease the axial ratio c/a. The available data can be described by $c/a = 1.100\,13 - 0.20\ (a - a_0)$ where a_0 is the lattice constant of the pure material. The values of a_0 at 25° C are deduced to be 4.9127 and 4.9134 Å, respectively, for natural and synthetic quartz with uncertainties in the last figure of about 1. This difference cannot be attributed to the large hydrogen content of the synthetic quartz since it is shown that this has a negligible effect on a. Neither is it due to differences of growth mechanism since crystals of synthetic quartz grown on different faces behave identically. Thus the differences between natural and synthetic quartz must be attributed to differences in the growth conditions (temperature, pressure and mineralizer). This attribution can account for the spread of natural quartz data.

Values of the cell parameters are suggested which allow interplanar and Bragg angles to be calculated with uncertainties of between 0.001 and 0.003°. Thus for decreasingly pure grades of quartz, natural quartz has a rising from 4.9129 to 4.9138 Å associated with a fall of c/a from 1.100 12 to 1.100 04. Uncertainties in the a values range from 2×10^{-4} to 5×10^{-4} Å and uncertainties in the c/a ratio range from 4×10^{-5} to 12×10^{-5}.

1. Introduction

The production of piezo-electric devices based on quartz is a major industry using over 500 tonnes of quartz per year to make about 600 million devices – mostly resonating or filtering elements in electronic circuits. The properties of such devices are very sensitive to the angles made by the major faces of the device blank with the principal axes of the crystal lattice [1–3]. For example, angular misalignments of 0.008° can change the temperature coefficient of frequency by about 0.1 ppm $^\circ$ C^{-1} or the optimum operating temperature by up to 5° C. Advances [4–6] in the standard X-ray techniques [7, 8] allow angles relative to the lattice planes (often $(0\,1\,\bar{1}\,1)$ which gives the greatest diffraction intensity) to be measured with reproducibilities of about 0.002°. However, the spread of the published lattice parameters is sufficient to make the angles between reflecting planes and the major axis very uncertain. For example, the published values of the axial ratio c/a suggest uncertainties of about 0.008 in the angle between $(0\,1\,\bar{1}\,1)$ and the c-axis of the lattice. Similarly the Bragg angle for the $0\,1\,\bar{1}\,1$ reflection is uncertain to about 0.005°. Depending on the details of the X-ray techniques used, this uncertainty is irrelevant or can add to or subtract from uncertainty in the angle made by a plane with the crystallographic axes. Other possible reference planes are affected in the same way.

This paper reports the results of a study of the available data, presents some new data and suggests values which might be adopted for various types of quartz. A systematic study of this type is necessary at a time when high-grade clear natural quartz is becoming rare and less pure grades or synthetic crystals must be used. This is particularly relevant because, as will be shown, synthetic quartz differs from natural quartz and impurities have a marked effect on the lattice constants.

The structure of quartz is discussed by Frondel [9], Wyckoff [10] and Evans [11]. The atomic co-ordinates are known from the work of Zachariasen [12], Donnay and Le Page [13], Zachariasen and Plettinger [14] and Le Page and Donnay [15].

2. The data

Tables I to VI give all the accurate published

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data which could be found. The information is presented in the form of the values of the *a* lattice constant and the axial ratio *c*/*a* at 25° C. Values at other temperatures (usually 18° C) have been converted using the relations

$$\frac{\mathrm{d}a}{\mathrm{d}T} = 6.7 \times 10^{-5}\,\text{Å}\,\text{K}^{-1} \qquad (1)$$

$$\frac{\mathrm{d}c}{\mathrm{d}T} = 4.0 \times 10^{-5}\,\text{Å}\,\text{K}^{-1} \qquad (2)$$

and

$$\frac{\mathrm{d}(c/a)}{\mathrm{d}T} = \left(a\frac{\mathrm{d}c}{\mathrm{d}T} - c\frac{\mathrm{d}a}{\mathrm{d}T}\right)\Big/a^2. \qquad (3)$$

The expansion coefficient data used to derive these relations is taken from Kirby *et al.* [16] and very similar values are given by Jay [17] and Ackermann and Sorrell [18].

When values of the lattice constants are quoted in kX units it has been assumed that 1 kX = 1.002 076 4 Å except when the conversion could be made on the basis of the quoted wavelength of the X-rays used [21, 22]. In Tables I to VI values originally given in Å at 25° C are marked with an asterisk. All other data have been converted to allow for either the units or another measurement temperature.

TABLE I Lattice parameters at 25° C of natural quartz with unknown impurity concentrations.

Parameters		Reference
a (Å)	*c*/*a*	
4.912 45	1.100 15	[20]
4.913 25	1.099 92	[20]
4.913 57	1.099 92	[20]
4.913 12	1.100 08	[20]
4.913 00	1.100 08	[20]
4.913 43	1.100 06	[20]*
4.912 9	1.100 02	[20]*
4.913 4	1.099 97	[20]
4.912 68	1.100 10	[21]
4.913 24	1.100 06	[21]
4.913 61	1.100 04	[9]*
4.912 996	1.100 10	[9]*
4.913 631	1.100 06	[9]*
4.913 25	1.100 09	[9]*
4.913 144	1.100 10	[9]*
4.913 29	1.100 09	[9]*
4.913 50	1.100 88	[9]*
4.914 5	1.099 91	[23]*
4.914 9	1.099 97	[23]*
4.913 6	1.099 97	[23]*
4.913 6	1.099 97	[23]*
4.913 8	1.099 95	[23]*
4.914 4	1.099 91	[23]*

* Data for 25° C in Å. All other value converted as described in the text.

TABLE II Lattice parameters at 25° C of the synthetic quartz with unknown impurity concentrations

Parameters		Reference and notes
a (Å)	*c*/*a*	
4.913 83	1.100 01	[21]
4.913 45	1.100 04	[21]
4.913 34	1.100 06	[21]
4.913 4	1.100 13	[19] (0 0 0 1) zone
4.914 2	1.099 93	[19] $(1 0 \bar{1} 1)$ zone of same crystal
4.913 8	1.100 01	[19] (0 0 0 1) zone
4.914 0	1.100 01	[19] $(1 0 \bar{1} 1)$ zone of same crystal
4.913 8	1.100 03	[19] (0 0 0 1) zone
4.914 0	1.100 03	[19] (1 0 1 1) zone of same crystal
4.914 5	1.100 04	[19] (1 0 1 1) zone
4.913 6	1.100 10	[19] (0 0 0 1) zone of same crystal
4.913 7	1.100 11	[19] (0 0 0 1) zone
4.913 5	1.100 02	[19] (0 0 0 1) zone
4.914 2	1.099 95	[19] (0 0 0 1) zone
4.913 4	1.100 10	[19] (0 0 0 1) zone
4.913 3	1.100 10	[19] $(1 0 \bar{1} 1)$ zone
4.913 7	1.100 04	[19] (0 0 0 1) zone
4.913 9	1.100 03	[19] (0 0 0 1) zone
4.913 5	1.100 16	[19]
4.914 0	1.100 02	[19]

TABLE III Lattice parameters at 25° C of natural quartz with known impurity concentrations

Parameters		Impurity concentrations (atomic ppm relative to Si)	Reference
a (Å)	*c*/*a*		
4.913 7	1.099 99	> 2000 Al, 100 Cu, 100 Fe, 100 Li	[22]
4.913 4	1.100 06	50 Al	[22]
4.913 7	1.100 05	> 2000 Al, 150 Ca, 100 Fe	[22]
4.914 4	1.099 93	> 2000 Al, 100 Fe, 100 Li	[22]
4.913 4	1.100 14	> 2000 Al, 100 Fe, 100 Li	[22]
4.912 9	1.100 06	13 Al, 2.5 Li	[9]*
4.913 3	1.099 97	115 Al, 66 Li, 30 Na	[9]*
4.914 5	1.099 91	230 Al, 1250 Li	[9]*
4.913 50	1.100 045	500 Li, 400 Na, 200 K, 800 Al, 100 Ti	[9]*
4.912 89	1.100 049	400 Li, 800 Al, 200 Ti, 500 Fe	[9]*
4.913 20	1.100 045	3800 Li, 1100 Na, 100 K, 1500 Ti, 100 Al, 300 Fe	[9]*
4.913 76	1.100 037	200 Al, 2600 Ti	[9]*
4.913 1	1.100 07	200 Fe	[24]
4.914 2	1.099 89	300 Mg, 400 Al, 200 Fe, 100 Cr	[24]
4.913 1	1.100 02	300 Mg, 100 Cr	[24]
4.913 0	1.100 14	300 Mg, 100 Cr	[24]
4.913 4	1.100 01	300 Mg, 500 Al, 100 Cr, 3000 Ca	[24]
4.912 9	1.100 12	20 000 Al, 600 Na	[24]
4.912 7	1.100 06	8000 Al, 6000 Na	[24]
4.912 6	1.100 33	20 000 Mg, 20 000 Al	[24]
4.912 9	1.100 00		[24]
4.912 8	1.099 89		[24]

In Tables III to VI the amounts of impurity are quoted in atomic parts per million relative to silicon. Only the major impurities present are given. Impurities at levels below several tens of ppm are likely to have a negligible effect on the lattice constant [19].

Fig. 1 gives the *a* lattice constant measured* in various positions in two crystals as a function of the infra-red absorption. The upper scale on this figure gives the hydrogen content calculated using the factor given by Lias *et al.* [26]. The samples contained no impurities other than hydrogen at a significant level. This figure allows us to deduce the effect of hydrogen on the lattice constant. (One ppm hydrogen changes *a* by 9×10^{-8} Å.)

TABLE IV Lattice parameters at 25° C for natural quartz before and after electrolysis† [25]

Lattice parameters		Impurity concentrations (atomic ppm relative to Si)					
a (Å)	*c*/*a*						
4.913 0	1.099 93	> 4000 Al,	300 Ca,	> 1000 Mg,	200 Fe,	500 Na,	5000 Li
4.912 6	1.100 00	> 4000 Al,	300 Ca,	> 1000 Mg,	70 Fe,	300 Na,	1500 Li
4.912 9	1.099 92	2000 Al,	300 Ca,	300 Mg,	200 Fe,	1200 Na,	< 860 Li
4.912 8	1.099 92	2000 Al,	100 Ca,	< 150 Mg,	< 25 Fe,	700 Na,	< 860 Li
4.913 0	1.099 93	> 4000 Al,	250 Ca,	2000 Mg,	200 Fe,	2600 Na,	4500 Li
4.912 6	1.099 97	> 4000 Al,	250 Ca,	200 Mg,	100 Fe,	< 260 Na,	< 860 Li
4.913 0	1.100 02	> 4000 Al,	600 Ca,	500 Mg,	200 Fe,	1800 Na,	8600 Li
4.912 8	1.100 00	> 4000 Al,	550 Ca,	150 Mg,	100 Fe,	440 Na,	860 Li
4.913 0	1.099 96	> 4000 Al,	450 Ca,	750 Mg,	700 Fe,	3000 Na,	4300 Li
4.912 4	1.100 05	> 4000 Al,	450 Ca,	400 Mg,	30 Fe,		860 Li
4.913 0	1.099 98	> 4000 Al,	< 450 Ca,	< 250 Mg,	200 Fe		
4.912 7	1.100 01	> 4000 Al,	< 450 Ca,	< 250 Mg,	30 Fe		

† The upper value in each pair corresponds to the sample prior to electrolysis. All values were measured at 18° C and have been converted using Equations 1 and 3.

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* Measurements done by Mr B. A. Bellamy, AERE, Harwell, Didcot, Oxfordshire using an Apex Spectrometer.

TABLE V Lattice parameters at 25° C of synthetic quartz with known impurity concentrations [19]

Lattice parameters		Impurities (atomic ppm)			
a (Å)	*c*/*a*	Al	Fe, Mg, Ca	Na	Ge
4.9141	1.09988	940	30	130	
4.9137	1.10003	360	50	50	
4.9137	1.10005	120	120	140	
4.9134	1.10016	210	70	70	
4.9136	1.10009	180	80	20	
4.9136	1.10018	740	3	64	1620
4.9141	1.10006	980	30	42	
4.9138	1.10007	620	60	780	1820
4.9134	1.10014	60	20	250	
4.9142	1.09989	980	30	1100	
4.9134	1.10014	40	10	50	
4.9138	1.09997	22	10	10	
4.9143	1.09984	500	30	420	4970
4.9137	1.09999	190	40	1300	5540
4.9139	1.10003	580	40	580	4110
4.9138	1.10015	580	30	800	4010
4.9135	1.10012	40	30	40	
4.9137	1.10007	340	30	640	

TABLE VI Lattice parameters at 25° C of synthetic quartz with known impurity concentrations [22]

Parameters		Impurity concentrations (atomic ppm relative to Si)
a (Å)	*c*/*a*	
4.9137	1.10003	60 Al, 30 Fe
4.9139	1.10009	60 Al, 100 Ge
4.9135	1.10011	200 Al, 100 Cu
4.9138	1.10014	200 Al, 500 Rb
4.9142	1.09997	600 Al, 100 Fe, 1000 Ge, 800 Li

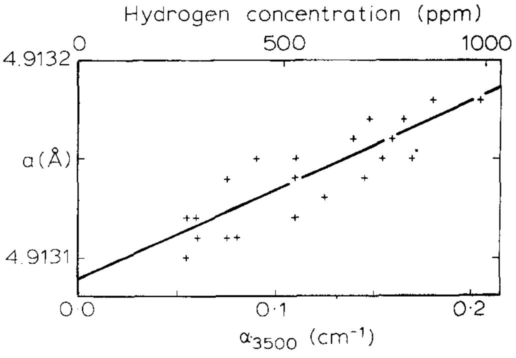

Figure 1 The variation of the *a* lattice parameter of quartz measured on a $(10\bar{1}0)$ face using the $60\bar{6}0$ reflection as a function of infra-red extinction coefficient (lower axis) or hydrogen concentration (upper axis). Note that while the precision of the Apex measurements is good (≈ 1 ppm) the absolute accuracy is probably only a few parts in 10^5.

3. Discussion

Figs. 2 and 3 give plots of *c*/*a* as a function of *a* for natural and synthetic quartz, respectively. The full lines on these figures are the best fit to the data. Both lines have slopes of $(0.20 \pm 0.03)\,\text{Å}^{-1}$. The broken lines in each case are the full line from the other figure. Clearly the data on the two figures come from different populations and there is much greater spread in the data for natural quartz. In terms of *c*/*a* the standard deviation of points from the synthetic quartz line is 5×10^{-5} which would be expected if the individual lattice constants had uncertainties of 0.000 17 Å which is larger than the precision quoted by some of the authors but which seems a realistic average value of relative accuracy. (Relative in the sense that different workers had different apparatus, techniques and standards.) The points for natural quartz have a standard deviation about their line of about 9×10^{-5}. If it is assumed that the relative accuracy is the same as for the synthetic quartz, the natural quartz data has an intrinsic spread of about 7×10^{-5} (i.e. the square root of the difference of the variances).

A number of hypotheses could be advanced to explain this intrinsic variability and the apparently genuine differences in *a*, which are discussed later.

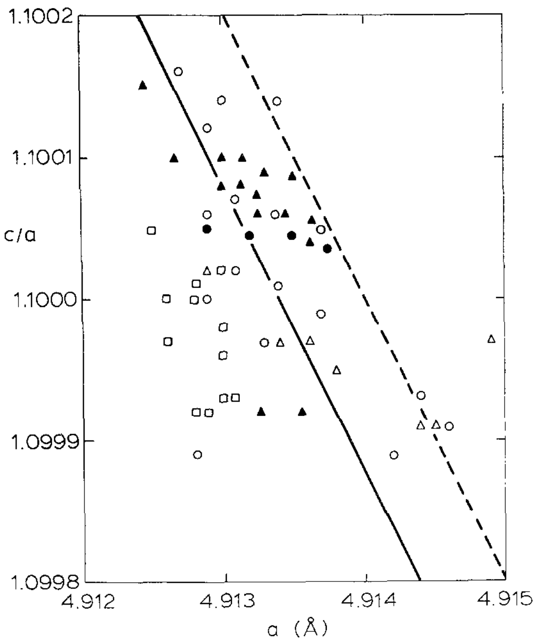

Figure 2 *c*/*a* as a function of *a* for natural quartz at 25° C. Triangles, circles and squares are for data from Tables I, III and IV, respectively. Filled symbols imply a particularly accurate determination.

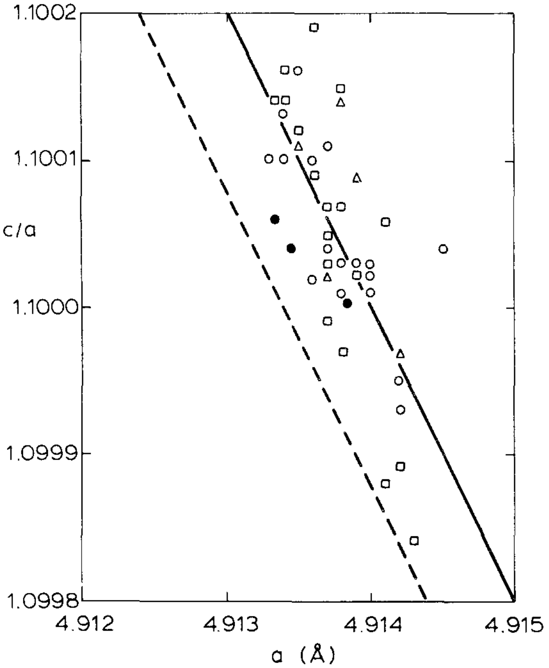

Figure 3 c/a as a function of a for synthetic quartz at 25° C. Circles, squares and triangles are for data from Tables II, V and VI, respectively.

Fig. 1 discounts the theory that the cause is related directly to the greater hydrogen content of synthetic quartz: the variation of a with hydrogen content is negligible (about 9×10^{-8} Å per ppm). It could be suggested that natural quartz only grows on the natural (singular) faces of the crystal while synthetic quartz grows largely on unnatural (rough) faces. See Brice [27] for a discussion of growth mechanisms. However Frank-Kamenetskii and Kamentsov [19] measured samples from zones grown on singular and rough faces and their data (Tables II and V) form a single population. Thus we are forced to conclude that the effects seen are caused by differences in the growth conditions (temperature, pressure and mineralizer). If each set of conditions gives a different relation between c/a and a then natural quartz grew under much more widely varying conditions than synthetic material.

TABLE VII Values of b in the relation $a = a_0 + \Sigma\, b_i C_i$

Element	b_i (μÅ per atomic ppm)
Fe	1
Cr	1
Ca	0.3
Mg*	0.2
Al*	0.2
Na	0.2
Ge	0.1
H	0.09
Ti	0.05
Li	0.01

*Values only applicable to 2000 ppm. At higher concentrations these elements appear to have small or even negative effects. Cohen and Sumner [22] discuss this and conclude that at high concentrations some impurities sit on interstitial sites.

Some authors give impurity concentrations (Tables III to VI) and it has been suggested [19, 22] that a relation of the form

$$a = a_0 + \Sigma\, b_i C_i \qquad (4)$$

may be used to represent the lattice constants as a function of the concentration C_i of the ith impurity. Here b_i is a constant at least for small values of C_i. From the available data (Figs. 2 and 3) bearing in mind the experimental uncertainties it is possible to predict that a_0 for natural quartz should be slightly less than 4.9127 Å and for synthetic quartz a_0 should be slightly less than 4.9135 Å. From the data in Tables III to VI, values of b_i can be estimated. One possible set of b_i values is given in Table VII. Applying Equation 4 with these values to the available data gives the results shown in Table VIII. However, the values of b_i in Table VII are not unique and other sets can be chosen in which the individual values of b_i are changed by factors of about 2. However, the values of a_0 are relatively insensitive to these changes. Value changes of more than 1×10^{-4} Å are associated with large increases in the standard deviations. Thus the values of b_i given can be regarded as reasonable estimates and they appear to be reasonable in the light of other information. For example replacing all the silicon by germanium increases a by 0.06 Å [20], giving $b_{\mathrm{Ge}} = 0.06\,\mu$Å ppm^{-1}. Similarly calculations based on the data given by Shannon and Prewitt [29] suggest that

TABLE VIII The values of a_0

	Natural quartz	Synthetic quartz
a_0(Å)	4.912 69	4.913 46* 4.913 37†
Standard deviation of sample	0.000 64	0.000 33
Standard deviation of mean	0.000 12	0.000 07

* Before allowing for hydrogen content.
† After allowing for hydrogen content.

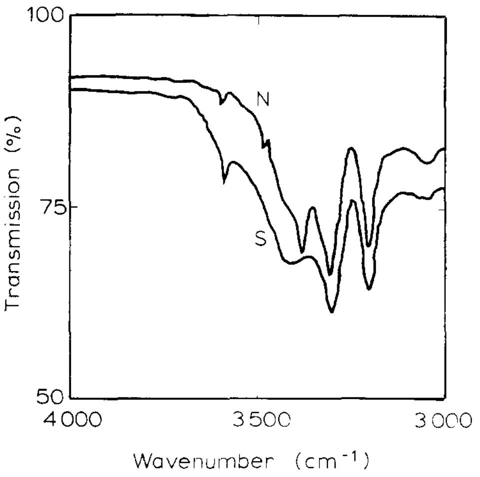

Figure 4 Infra-red transmission spectra of natural (N) and synthetic (S) quartz in the range 3000 to 4000 cm^{-1}.

the values are reasonable, e.g. the length of a Cr–O bond is 20% greater than an Si–O bond giving $b_{\mathrm{Cr}} \simeq 1\,\mu\text{Å}\,\text{ppm}^{-1}$. In other cases, e.g. Ca, the agreement is less good but charge compensation effects would be significant [19]. It seems that there are real differences between synthetic and natural quartz both in terms of a_0 and the variation of c/a with a. One obvious difference is that in general synthetic quartz contains more dislocations but the range found is very large (from $< 10\,\text{cm}^{-2}$ to $> 10^5\,\text{cm}^{-2}$) [28] and even for high densities the change expected is small. Another and perhaps more plausible hypothesis is that in the more rapidly grown synthetic material, there are point defects. These might account for the differences in the infra-red spectra. Natural quartz for example does not show the broad absorption at 3410 cm^{-1} which is associated with both the lattice and with hydrogen [28] (see Fig. 4).

Finally, on the basis of the available data, it is possible to suggest likely values for the cell parameters of various grades of quartz such values are given in Table IV. In drawing up this table it was assumed that premium-grade quartz was only marginally contaminated and that as shown previously [28] even medium-grade synthetic material contained only minor amounts of impurity. Medium-grade natural quartz was assumed to be near to the median values reported and both types of low-grade quartz were assumed to be near the lower quartiles. Since a change in c/a of 4×10^{-5} gives an interplanar angle uncertainty of about 0.001° and a change of a of 0.0004 Å changes Bragg angles by roughly 0.001°, the use of these values should limit angle uncertainties to 0.003° in the worst cases and probably to 0.001° when high-grade quartz is used. In constructing Table IX, it has been assumed that the spread of c/a values increases with a. Figs. 2 and 3 suggest that this is a reasonable assumption.

4. Conclusions

Data relating to the lattice parameters of quartz has been reviewed and the conclusion has been reached that wide variations in a and c/a are found. However, these changes depend systematically on purity so that it is possible to select values appropriate to the grade of the crystal and so eliminate much of the uncertainty. There are clear systematic differences between natural and synthetic quartz. The reasons for these differences are not yet understood.

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Mr W. S. Metcalf, Cathodeon Crystals Ltd, Linton, drew attention to the problem posed by the vari-

TABLE IX Suggested values of parameters at 25° C

Grade of quartz*	Type	a (Å)†	c/a†
Pure	Natural	4.912 7 ± 2	1.100 13 ± 4
	Synthetic	4.913 4 ± 1	1.100 13 ± 2
Premium	Natural	4.912 9 ± 2	1.100 10 ± 6
($Q > 2$ million)	Synthetic	4.913 4 ± 2	1.100 12 ± 4
Medium	Natural	4.913 2 ± 3	1.100 04 ± 9
($Q \approx 1$ million)	Synthetic	4.913 6 ± 3	1.100 08 ± 6
Low	Natural	4.913 8 ± 5	1.099 92 ± 12
($Q \ll 1$ million)	Synthetic	4.913 8 ± 5	1.100 04 ± 10

* Q is the reciprocal of the anelastic losses in the crystal. Q is related usually to hydrogen content [28].

† The uncertainties quoted are in the last figure, e.g. 4.913 8 ± 5 is 4.913 8 ± 0.000 5 and 1.099 92 ± 12 is 1.099 92 ± 0.000 12.

ations in lattice constants. Miss A. M. Cole carried out the infra-red measurements, Dr J. F. Connolly, RMIC, Oak Ridge, provided references to some of the data used and Dr K. L. Bye, Philips, Redhill, gave much time for the discussion of the various problems.

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