TABLE I. Position and width of α and β bands, and intensity ratio between β and F bands at their peaks.

	α Position		Width	β Position		Width	
	$m\mu$	ev	ev	$m\mu$	ev	ev	β max./F max.
NaF	131.5	9.43	0.4	127.0	9.75	0.36	0.9
NaCl	173.0	7.16	0.3	168.0	7.38	0.31	0.90
KCl	178.5	6.95	0.2	169.5	7.31	0.18	0.85

KCl no definite structure was found either, but the accuracy of measurement was not as good as with NaCl because of impurity band. According to the model used by Fuchs, one expects to find in β band of NaCl and KCl a doublet structure with a separation of 0.10 ev,[3] which however was not detected. The reason for the failure to uncover this fine structure may have been that the width of component bands in NaCl is fairly

[3] R. Fuchs, Phys. Rev. 111, 387 (1958).

wide. KCl will be better suited for the examination of the fine structure because of its narrower band width.

LiF was also investigated. Under x-ray irradiation either at room temperature or at liquid nitrogen temperature, a new absorption band of the width of about 0.6 ev was found at 111.5 mμ (11.1 ev). This new band can be bleached by light from a low-pressure mercury lamp, but its origin has not been ascertained.

Note added in proof.—Dr. K. Kobayashi of Tohoku University suggested to the authors that the 167-mμ band in KCl might be due to bromine impurity. He kindly sent the authors his specially made KCl crystal in which the bromine content was reduced to 9×10^{-6} in mole fraction. There was only slight absorption at 167 mμ by this crystal, far feebler than by Harshaw crystal used in the present study. The position of β band was found in the crystal at 168.5 mμ (7.35 ev). The doublet structure of the β band remained still unresolved at liquid nitrogen temperature.

Center Law of the Lattice Vibration Spectra*

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The lattice vibration spectra of a solid, as a whole, can be characterized by one single frequency, defined as the frequency of "the center of gravity" of the infrared spectrum, simply called "center frequency." The data of this frequency have been determined for many nonconducting solids (compounds) from the experimental spectra of lattice vibrations in reflectance as well as in absorption. A striking experimental phenomenon is discovered: The center frequency, whether determined from the reflectance or from the absorption type spectrum, is found to be equivalent and identical with Debye's characteristic frequency. This phenomenon is exhibited for a large variety of nonconducting compounds covering almost the entire range of the vibrational spectra of solids. Moreover, the center frequency remains constant with varying temperature. The equality of the center frequency of the infrared spectrum and the characteristic frequency from specific heat constitutes the "center law of the lattice vibration spectra."

I. INTRODUCTION

THE vibrational (infrared) spectrum of a substance is related to the forces that hold matter together in the solid state. The higher the region of resonance frequencies in the vibrational spectrum, the greater the cohesive forces. The full experimental spectra of lattice vibrations of various solids (commonly shown either in reflectance, or in transmittance, or again as the Raman type, but rarely in absorption), as a function of frequency, differ in range, in number of resonance frequencies, in intensities, and in line widths.[1]

* The gist of this paper was presented by the author at the Gordon Research Conference on Chemistry and Physics of Solids (Lattice Dynamics), August 18, 1959, at Meriden, New Hampshire. In its early stage, it was presented at the International Meeting of European Spectroscopists, Freiburg/Br., Germany, July 12, 1957 (unpublished).
[1] See, for example, R. B. Barnes *et al., Infrared Spectroscopy: Industrial Applications and Bibliography* (Reinhold Publishing Corporation, New York, 1944).

II. CENTER OF GRAVITY OF THE VIBRATIONAL SPECTRUM

In certain cases it is useful to characterize the experimental spectrum of lattice vibrations by one single frequency, such as the frequency of maximum absorption (ν_0) (which is very close to the minimum of transmittance), or of maximum reflectance (ν_r), or the reststrahlen frequency (ν_{rest}).[2] However, for a number of substances, such as LiF, SiO$_2$, diamond (I), etc., these frequencies are ambiguous. Thus in order to characterize the vibrational spectrum unambiguously and as a whole, we introduce the frequency of the "center of gravity"

[2] The reststrahlen frequency is the frequency selected from the infrared spectrum by multiple reflections on a number of polished plates of a crystal substance. In case of a symmetrical reflection curve, ν_{rest} is equal to the frequency of maximum reflectance (ν_r). In case of an unsymmetrical reflection curve, however, ν_{rest} may differ somewhat from ν_r, since the reststrahlen give an average frequency of any continuous spectral area of strong reflectance.

(designated as ν_{ctr}) and define it by

$$\nu_{\mathrm{ctr}} = \frac{\int_0^\infty \nu f(\nu) d\nu}{\int^\infty f(\nu) d\nu}, \tag{1}$$

where ν = frequency, $f(\nu)$ = reflectance R or absorption coefficient K, $f(\nu)d\nu$ = a small area of the spectrum of reflectance or absorption.

In order to determine ν_{ctr} correctly by Eq. (1), we need to know experimentally the entire spectrum of lattice vibrations of a solid either in reflectance or in absorption.[3] The absorption spectrum can be derived either from transmittance spectra at various layer thicknesses,[4] or from reflectance spectra at various angles of incidence.[5] Such data, however, are available only for a very few solids. Hence, in this study, we generally equate $f(\nu) = R$, and, according to availability, also $f(\nu) = K$. In this case, we denote R = reflectance in percent, and define K by the formula

$$J = J_0 e^{-4\pi K(d/\lambda)},$$

which represents the radiation intensity J of wavelength λ after traversing a layer of the thickness d. The limiting frequencies of the spectrum are conveniently defined as those frequencies at which $f(\nu)$ becomes very small and remains so beyond them.

Obviously, the resonance lines occur at both sides of ν_{ctr}, and the latter does not need to coincide with any one of the strong lattice resonance vibrations of the spectrum. In other words, there may or may not be a resonance line at ν_{ctr} itself in the experimental spectrum, whether observed in reflectance, or in absorption, or as Raman type.

As an example, Fig. 1 shows the determination of ν_{ctr} from the reflectance spectrum of crystalline quartz (SiO_2).[6] The easiest way to determine ν_{ctr} [according to
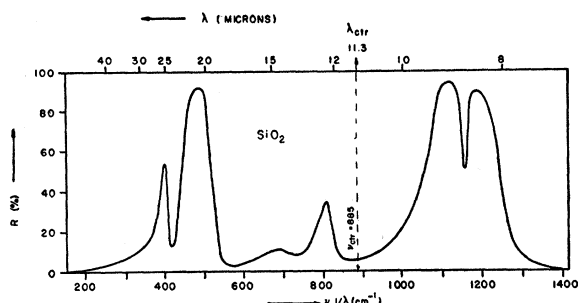

FIG. 1. Determination of ν_{ctr} from the lattice vibration spectrum of crystalline quartz. This spectrum is shown in reflectance (R) as a function of frequency $(\nu = 1/\lambda)$. For the respective references see footnote 6. By cutting the area under the curve of the spectrum from cardboard and determining the point of equilibrium on the abscissa (as mentioned in the text) we obtain

$$\nu_{\mathrm{ctr}} = 885 \text{ cm}^{-1} \quad \text{or} \quad \lambda_{\mathrm{ctr}} = 11.3 \text{ microns}.$$

Eq. (1)] is to cut the area under the curve of the spectrum from cardboard and to determine the point of equilibrium by balancing it on a needle through a hole close to the abscissa. Trying at different points along the abscissa, we succeed at

$$\nu_{\mathrm{ctr}} = 885 \text{ cm}^{-1} \quad \text{or} \quad \lambda_{\mathrm{ctr}} = 11.3 \text{ microns}.$$

As the case of SiO_2 shows, there is no resonance vibration at ν_{ctr} itself.

Other examples for the determination of ν_{ctr} are shown in Fig. 2 for NaCl, in Fig. 3 for LiF, and in Fig. 4 for MgO. These substances belong to the few solids where the spectrum of absorption is fully available, as is the spectrum of reflectance.[6] Both types of spectra are shown in Figs. 2, 3, and 4. In determining ν_{ctr} in the manner mentioned above, and for each type of spectrum separately, we obtain

for NaCl: $\nu_{\mathrm{ctr}} = 188 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 53$ microns for the absorption type, and

$\nu_{\mathrm{ctr}} = 185 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 54$ microns for the reflectance type;

for LiF: $\nu_{\mathrm{ctr}} = 410 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 24.4$ microns for the absorption type, and

$\nu_{\mathrm{ctr}} = 415 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 24.1$ microns for the reflectance type;

for MgO: $\nu_{\mathrm{ctr}} = 525 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 19.1$ microns for the absorption type,

$\nu_{\mathrm{ctr}} = 515 \text{ cm}^{-1}$ or

$\lambda_{\mathrm{ctr}} = 19.4$ microns for the reflectance type.

[3] For detailed representation of the experimental data of the lattice vibrations for a great number of solids, also comprehensive bibliography of pertinent literature, see H. H. Landolt-R. Boernstein, *Zahlenwerte und Funktionen aus Physik Chemie Astronomie Geophysik und Technik* (Springer-Verlag, Berlin, 1955), Vol. 4, Part 5, p. 546–666.

[4] See, for example, R. W. Wood, *Physical Optics* (Macmillan Company, New York, 1952), p. 102.

[5] J. Simon, J. Opt. Soc. Am. 41, 336 (1951); also N. Neuroth, Z. Physik 144, 85 (1956).

[6] (1) In the case of SiO_2, the data of reflectance (R) as a function of the frequency are taken from measurements by J. D. Hardy and S. Silverman, Phys. Rev. 37, 179 (1931); K. Korth, Z. Physik 84, 684 (1933); and W. Stein, Ann. Phys. 36, 470 (1939). (2) In the case of NaCl, the data of reflectance (R) as a function of the frequency are taken from measurements by L. Kellner, Z. Physik 56, 215 (1929); M. Czerny, Z. Physik 65, 600 (1930); R. B. Barnes and M. Czerny, Z. Physik 72, 447 (1931); C. H. Cartwright and M. Czerny, Z. Physik 85, 269 (1933); and A. Mitsuishi, H. Yoshinaga, and S. Fujita, J. Phys. Soc. Japan 14, 310 (1959); the data of the absorption coefficient K as a function of the frequency are evaluated from transmittance data at variable layer thicknesses taken from measurements of the above authors. (3) In the case of LiF, the data of reflectance (R) as a function of the fre-

quency are taken from measurements by K. Korth, Nachr Ges. Wiss. Göttingen Jahresber. Geschäftsjahr Math.-Physik Kl. 5, 576 (1932); H. W. Hohls, Ann. Phys. 29, 433 (1937); M. Klier, Z. Physik 150, 50 (1958); G. Heilmann, Z. Physik 152, 368 (1958); the data of the absorption coefficient K as a function of the frequency are taken from R. B. Barnes, Z. Physik 75, 723 (1932); G. Heilman, Z. Physik 152, 368 (1958). (4) In the case of MgO, the data of reflectance and absorption as a function of the frequency are taken from measurements by J. C. Willmott, Proc. Phys. Soc. (London) A63, 389 (1950).
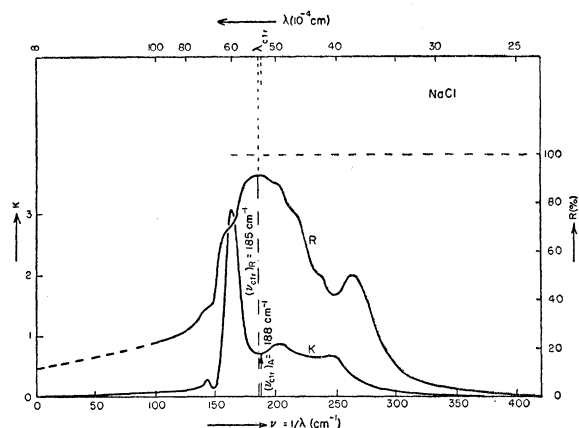
FIG. 2. Determination of ν_{ctr} from the lattice vibration spectrum of NaCl. Two types of this spectrum are shown: the absorption K (as an envelope) and the reflectance R, as a function of frequency ($\nu = 1/\lambda$). The data of the absorption coefficient K are evaluated by the author from transmittance data at various layer thicknesses. For the respective references see footnote 6. By cutting the area under the curve of either type of the spectra from cardboard and determining the point of equilibrium on the abscissa (as mentioned in the text) we obtain

$\nu_{ctr} = 188$ cm^{-1} or $\lambda_{ctr} = 53$ microns for the absorption spectrum,

and

$\nu_{ctr} = 185$ cm^{-1} or $\lambda_{ctr} = 54$ microns for the reflectance spectrum.

Although the two types of spectra are very different from each other, they show identical values of ν_{ctr} (considering the experimental inaccuracies of about ±3%). Also shown are the frequencies of maximum reflectance ν_r and of maximum absorption ν_0.

Although the two types of spectra, reflectance and absorption, are very different from each other for each one of these solids (as is characteristic for the alkali halides), ν_{ctr} remains equivalent for both types, considering the over-all inaccuracy averaging ±3%. According to expectation, however, ν_{ctr} is entirely different for the Raman type of spectrum (not shown here).

In regard to the reflectance spectra, the center frequency in many cases is close to the frequency of maximum reflectance (ν_r) as Figs. 2 and 4 show. This agreement, however, by no means applies to SiO$_2$ nor to LiF, as Figs. 1 and 3 show. On the other hand, in regard to the absorption spectra, ν_{ctr} is close to a minimum in all four cases (Figs. 1 to 4); i.e., ν_{ctr} does not coincide with any resonance line there.

Investigating the temperature dependence of ν_{ctr}, we determine (1) from the absorption spectra of LiF at various temperatures[6]:

at 293°K $\nu_{ctr} = 410$ cm^{-1},

at 593°K $\nu_{ctr} = 400$ cm^{-1},

at 893°K $\nu_{ctr} = 415$ cm^{-1};

(2) from the reflectance spectra at 293°K: $\nu_{ctr} = 415$ cm^{-1} with no change indicated at 87°K.[6]

In the case of LiF, this comparison shows that ν_{ctr} remains constant with varying temperatures, from the vicinity of liquid air temperature to somewhat below the melting point, considering the over-all inaccuracy of

data determination (about ±3%, averaging $\nu_{ctr} = 410$ cm^{-1}).

Thus, as far as the available data allow, we establish the following unique fact concerning the center frequency:

The "center of gravity" of the lattice vibration spectrum remains the same, whether determined from the reflectance or from the absorption type of spectrum. It also remains constant for varying temperatures [within a range in reduced temperatures (see below) from T/θ = 0.14 to 1.45 in the case of LiF, which is the only one examined so far].

III. CENTER OF GRAVITY OF THE VIBRATIONAL SPECTRUM AND THE CHARACTERISTIC TEMPERATURE

Another frequency also peculiar for each substance, according to Debye, is defined by the characteristic temperature θ as

$$\nu_\theta = k/h\theta, \qquad (2)$$

where k = Boltzmann's constant, and h = Planck's constant. The characteristic temperature can be determined from various data such as specific heat, or elasticity, compressibility, melting point, and electrical resistance.[7] But we restrict the term θ to the representation of specific heat data only.
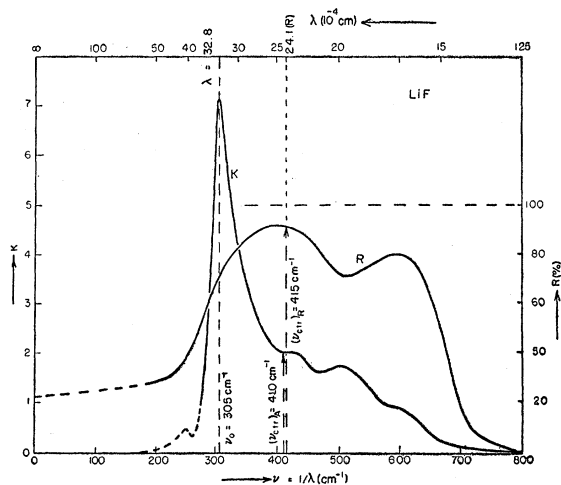

FIG. 3. Determination of ν_{ctr} from the lattice vibration spectrum of LiF. Proceeding in the same manner as mentioned in Fig. 2, we obtain

$\nu_{ctr} = 410$ cm^{-1} or $\lambda_{ctr} = 24.4$ microns for the absorption spectrum,

and

$\nu_{ctr} = 415$ cm^{-1} or $\lambda_{ctr} = 24.1$ microns for the reflectance spectrum,

i.e., both quantities of ν_{ctr} are identical to each other, considering the experimental inaccuracies of about ±3%. For the respective references see footnote 6.

[7] For detailed representation of the specific heat of solids, tables of θ values and their discussion, also bibliography of pertinent literature, see the comprehensive articles by M. Blackman and G. Leibfried in *Handbuch der Physik* (Springer-Verlag, Berlin, 1955), Vol. VII/1, pp. 325–382 and 104–324, respectively.

In reality, the Debye theory is not in perfect agreement with experiment.[7] Hence θ, instead of being a constant, is a function of T. Within the practical range of temperatures, however, the deviation of θ from the respective constant is but a few percent for many solids, although it may extend to a higher percentage for some solids. Nevertheless, it is customary to consider θ as a constant. In this case θ refers, in general, to the middle portion of the c_v curve (see Fig. 5), except for the very high θ values (as for the diamond) where the lower portion prevails (since T/θ is very small at room temperature).

The characteristic frequency (ν_θ) was assumed by Debye as a maximum and cutoff frequency, in such a manner that above ν_θ no vibrations should exist, and below ν_θ a continuous frequency distribution represented by a parabola $[f(\nu) \propto \nu^2]$ should occur. The known experimental spectra of lattice vibrations of many solids reveal, however, that a considerable number of distinct resonance vibrations exist, without any preference for ν_θ, and that they are located at both sides of ν_θ. Hence the latter does not show up directly in the experimental spectrum; and this is the very same property which ν_{ctr} exhibits.

A striking experimental phenomenon is discovered when we compare the characteristic frequency ν_θ with the frequency ν_{ctr} for as many solid compounds as we have data on hand. It appears that both wavelengths λ_θ and λ_{ctr} are equal throughout the entire range of vibrational spectra of solids.[8]

FIG. 5. Atomic heat capacity of simple solids (according to Debye).

The equality of center frequency with characteristic frequency is shown in Table I for eighteen nonconducting solids (compounds) for which complete data on both the lattice vibrations and the characteristic temperatures are available.[9] The substances of Table I belong to six different lattice structures and cover the range from $\lambda_{ctr} = 120$ microns, as for CsBr, to $\lambda_{ctr} = 5.9$ microns, as for the diamond (I).[10] This is almost the entire range of the vibrational spectra of solids (measured in center frequencies).

In detail: Table I includes thirteen solids (Numbers 1, 5, 8 to 12, and 14 to 18) for which sufficient experimental data are available to determine λ_{ctr} correctly (besides λ_θ).[11] In comparing the λ_{rest} of these solids with λ_{ctr}, it appears that ten of them show almost the same quantity for both λ_{rest} and λ_{ctr}, whereas the remaining three (Numbers 14, 15, and 18) have double values of λ_{rest} which are far apart from each other (in the frequency scale).[12] In the latter case, λ_{rest} remains ambiguous. Hence we conclude that both λ_{rest} and λ_{ctr} are very close to each other, provided that λ_{rest} has one value only. We now make use of this fact for another variety of solids (Numbers 2 to 4, 7, and 13) for which λ_{rest} is known (single values of course), but not the complete infrared spectrum, in order to determine λ_{ctr} correctly. Thus, in approximating λ_{ctr} by λ_{rest}, we in-
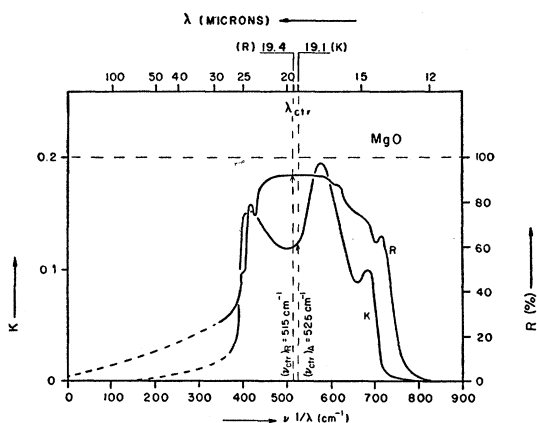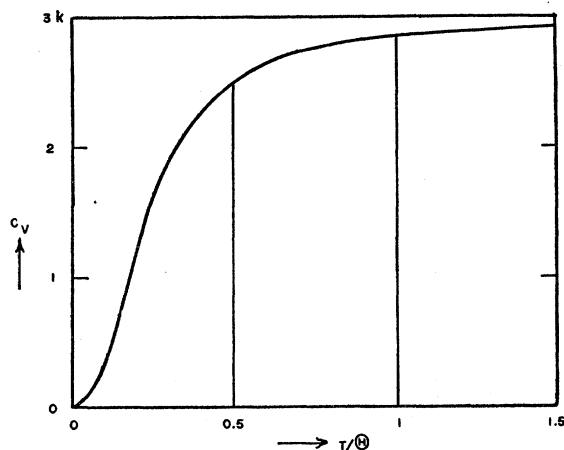

FIG. 4. Determination of ν_{ctr} from the lattice vibration spectrum of MgO. Proceeding in the same manner as mentioned in Fig. 2, we obtain

$\nu_{ctr} = 525 \text{ cm}^{-1}$ or $\lambda_{ctr} = 19.1$ microns for the absorption spectrum,

and

$\nu_{ctr} = 515 \text{ cm}^{-1}$ or $\lambda_{ctr} = 19.4$ microns for the reflectance spectrum,

i.e., both quantities of ν_{ctr} are identical to each other, considering the experimental inaccuracies of about $\pm 3\%$. For the respective references see footnote 6.

[8] The wavelength scale is chosen instead of frequencies because the original data in pertinent literature are mainly presented in wavelengths.

[9] Considering the over-all inaccuracy of data determination which averages $\pm 3\%$ for ν_{ctr}, but varies from ± 2 to $\pm 10\%$ for θ.

[10] $\lambda_{ctr} = 5.9$ microns applies to the ordinary diamond of type (I).

[11] Most data of the characteristic temperatures are taken from the comprehensive articles by G. Leibfried and M. Blackman in *Handbuch der Physik* (see reference 7), pp. 104–382; also from K. Lonsdale, Acta Cryst. 1, 142–149 (1948). The data of the reststrahlen wavelengths are taken mainly from C. Schaefer and F. Matossi, *Das Ultrarote Spektrum* (Springer-Verlag, Berlin, 1930). The values of λ_{ctr} are determined mainly from data on lattice vibrations compiled in H. H. Landolt-R. Boernstein, *Zahlenwerte und Funktionen aus Physik Chemie Astronomie Geophysik und Technik* (see reference 3). See also the comprehensive bibliography there, pp. 663–666.

[12] Double values of λ_{rest} indicated by double maxima of reflectance apply to LiF, SiO_2, double maxima of absorption to the diamond (I). The double maxima of each one of these solids are equally strong and may or may not be symmetrical to ν_{ctr}.

TABLE I. Comparison of the characteristic frequency with the frequency of the center of gravity.

No.	Substance	Structure	θ °K	λ_θ microns	λ_{ctr} microns	λ_{rest} microns
1	CsBr	(cesium chloride)	120	120	120	125
2	RbI	(rocksalt)	115	125	...	117
3	AgBr	(rocksalt)	130	111	...	113
4	RbBr	(rocksalt)	130	111	...	105
5	KI	(rocksalt)	155	93	98	94
6	KBr	(rocksalt)	170	85	85	82.5
7	AgCl	(rocksalt)	180	80	...	81.5
8	KCl	(rocksalt)	225	64	65	63.5
9	NaCl	(rocksalt)	275	53	53(A) 54(R)	52
10	NaF	(rocksalt)	440	33	34	35
11	ZnS	(zinc blende)	450	32	32	31
12	CaF$_2$	(fluorite)	470	31	31	31.5
13	CaO	(rocksalt)	510	28	...	27.5
14	LiF	(rocksalt)	620	23.5	24.4(A) 24(R)	17 and 26
15	MgO	(rocksalt)	740	19.5	19.1(A) 19.4(R)	20
16	SiC	(zinc blende)	1200	12	12	12
17	SiO$_2$	(quartz)	~1300	~11	11.3	8.8 and 21
18	C—C(I)	(diamond I)	2340	6.1	5.9	4.5 and 8.0

crease the number of comparable solids in Table I from thirteen to eighteen. In this manner, we assemble a large variety of nonconducting solids for which we definitely possess the data required for checking the results.

For more than 30 years, as a matter of fact, it has been known that the quantities of λ_θ and λ_{rest} are almost equal for a few solid compounds, such as NaCl, KCl, and CaF$_2$. More recently, the θ values of a few additional
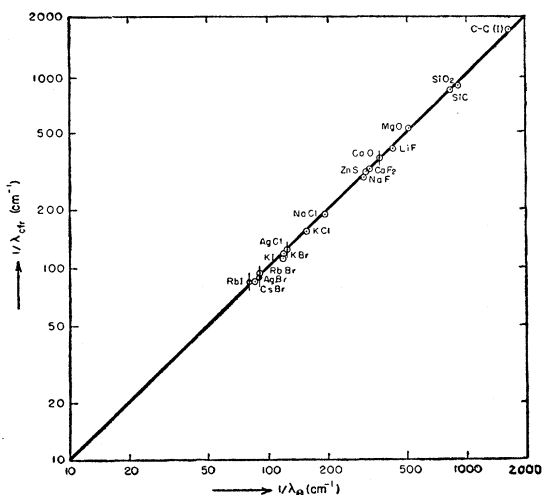

FIG. 6. Identity of the characteristic frequency with the center frequency (applying the data of Table I). Both frequencies $1/\lambda_\theta$ and $1/\lambda_{ctr}$ are plotted against one another and in logarithmic scales. They cover almost the entire range of the vibrational spectra (also of the characteristic temperatures) of solids. The deviation from the bisector (small as it is) stands for the deviation from the identity of both frequencies. The data are mean values, and their average inaccuracy is indicated by the size of the circles, the radius of which corresponds to about ±3% (this radius being a constant in the logarithmic scales). Small vertical lines through some of the circles indicate solids where the center frequencies are determined by reststrahlen data.

ionic crystals were estimated by reststrahlen data. It was considered remarkable, however, that in these cases only the θ values determined by the reststrahlen frequency agree quite well with the average θ values from specific heat, whereas neither the "natural frequency," corresponding to the main resonance of absorption, nor any one of the strong secondary resonance frequencies seems to have any direct relation to θ. This was the more remarkable as the reststrahlen frequency was considered obsolete. Consequently, the good agreement of the average θ values from specific heat with the θ values from reststrahlen data was regarded as due to "a combination of favorable circumstances" only, but not based on direct relation between the two quantities.[13] This conclusion, moreover, was emphasized by the lack of agreement observed in LiF, SiO$_2$, and the diamond (I).[12] However, if we introduce the center frequency instead of the reststrahlen frequency we observe identity between both λ_{ctr} and λ_θ, throughout all the solids listed in Table I. Thus it is ν_{ctr} that should be deemed the true "natural frequency" of the vibrational spectrum.

The tight equality between the two frequencies, ν_{ctr} and ν_θ, can best be seen in Fig. 6 where $1/\lambda_{ctr}$ is plotted against $1/\lambda_\theta$ (both in wave numbers) for all substances of Table I. The deviation from the bisector, which stands for the deviation from equality of both frequencies, is very small indeed and remains within the over-all inaccuracy of data determination.[9] As Table I and Fig. 6 equally indicate, we attain the following unambiguous and obvious relation:

The characteristic frequency (defined by the characteristic temperature) and the center frequency (defined by the "center of gravity" of the lattice vibration spectrum) of nonconducting solids are identical with one another.

[13] See M. Blackman, Handbuch der Physik (see reference 7), pp. 375–376.

Consequently, we conceive the center frequency as the optical (infrared) value of the characteristic frequency.

As we know, the spectrum of lattice vibrations as a whole contributes to the specific heat of a solid. In order to represent the entire spectrum in this case unambiguously and effectively by one single frequency, we may imagine the spectrum to be concentrated in its center of gravity and thus the accordant frequency to be identical with the characteristic frequency from specific heat.

IV. CENTER LAW OF THE LATTICE VIBRATION SPECTRA

As we conclude from Fig. 6, the center frequencies of the lattice vibration spectra of nonconducting solids can be determined simply by their characteristic temperatures. Introducing this fact into Eq. (2), we obtain

$$\nu_{ctr} = k/h\theta. \qquad (3)$$

This relation expresses the equality of the characteristic temperatures with the center of gravity of the lattice vibration spectra in absorption as well as in reflectance. It states:

The higher the characteristic temperature of a solid, the higher also the frequency region of the vibrational spectrum.

Applying Eq. (3), we may now determine the centers of the vibrational spectra in absorption and reflectance for nonconducting solids from characteristic temperature data, or vice versa. The reciprocal case applies to a number of solids whose vibrational spectra we know but incompletely. Among these substances are, e.g., BN,

BeO, Al_2O_3, etc., with structures different in some cases from those of Table I. Other and more important applications of the center law, concerning the study of the solid state in general, will be treated in successive papers.

V. CONCLUSION

The accepted percentage of impurities in the investigated nonconducting solids (averaging close to 1%) may cause small deviations in some of the experimental data. However, no changes, beyond the over-all inaccuracies of the experimental data, are to be expected, either in the center frequency or in the characteristic frequency, provided the small impurities do not influence the electrical conductivity of the materials to any substantial degree.[14]

In the past, for various reasons, many experimental data in the far infrared have not met the standards that would be desirable. Hence comparisons made in our study are hampered in many respects by this fact. It is exactly the purpose of this paper to stimulate extensive and more accurate work within the experimental aspect of this field, in order to provide confirmation or modification of our results.

Optical Mode Scattering Contribution to Electrical Resistivity in Zirconium Hydride*

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(Received March 21, 1960)

Electrical resistivity measurements on fcc $ZrH_{1.54}$ and fct $ZrH_{1.96}$ between 1.2°K and 400°K have revealed a sizeable optical mode scattering contribution. Excellent fits to the data are obtained using a simple additive combination of Grüneisen and Howarth-Sondheimer functions for the respective acoustical and optical mode scattering contributions. The corresponding acoustical and optical mode characteristic temperatures are in good accord with values derived from earlier inelastic neutron scattering experiments.

R ECENT neutron scattering experiments[1-5] have shown that hydrogen atoms occupy tetrahedral lattice sites in fcc and fct zirconium hydride (approxi-

[1] R. E. Rundle, C. G. Shull, and E. O. Woolan, Acta Cryst. 5, 22 (1952).
[2] I. Pelah, C. M. Eisenhauer, D. J. Hughes, and H. Palevsky, Phys. Rev. 108, 1091 (1957).
[3] A. Andresen, A. W. McReynolds, M. Nelkin, M. Rosenbluth, and W. Whittemore, Phys. Rev. 108, 1092 (1957).
[4] W. L. Whittemore and A. W. McReynolds, Phys. Rev. 113, 806 (1959).
[5] S. S. Sidhu, L. Heaton, and M. H. Mueller, J. Appl. Phys. 30, 1323 (1959).

mately $ZrH_{1.5}$ to ZrH_2), and further that these hydrogen atoms behave much like independent simple harmonic or "Einstein" oscillators. A value of 0.133 ev (average of two neutron scattering determinations) was obtained for the level spacing of these Einstein or optical modes, and a value of approximately 0.02 ev was obtained for the high-frequency cutoff of the acoustical modes. These energies correspond to an Einstein characteristic temperature $\theta_E = 1550°K$ for the optical branch and a characteristic temperature of approximately 230°K for the acoustical branch. The purpose of this note is to describe electrical resistivity measurements on zirconium