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Irreducible Tensors of the Point Groups with Fivefold Rotational Axes

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In order to interprete vibrational spectra of crystals (IR-absorption, IR-reflection, Raman- and Hyper-Raman-scattering, stimulated Raman scattering, and CARS) irreducible tensors of rank 1 to 3 are needed for the 32 classical crystallographic point groups. The detection of quasi-crystals suggested it as useful to calculate these irreducible tensors also for the point groups with fivefold rotational axes. The form of irreducible tensors of rank 1 to 4 without intrinsic symmetries are given in tables for all irreducible representations of pentagonal point groups 5, $\overline{5}$, $\overline{10}$, $\overline{10m2}$, 52, 5m, $\overline{52m}$ and for two icosahedron point groups 235 and (2/m) $\overline{35}$.

The notation of property tensors is in accordance with Birss^t. In detailed tables the components of property tensors which have to vanish because of symmetry reasons are marked by small dots. On the other hand, components which — due to symmetry — may not vanish are symbolized by free black circles. When two or more components are equal, they are connected with a line. When two or more components have different signs but the same modulus they are also connected with a line but one or more circles are not filled. When two components are equal in one representation, they must differ in sign in another representation. For the sake of clarity, letters instead of circles are used for the non-vanishing components of property tensors which are more complicated. When dealing with one-dimensional representations, the same letter refers to the same value only within this representation. In the case of representations which are degenerate to each other the same letter always refers to the same value. Degenerate representations are marked by a long straight horizontal line in the first line of the detailed tables of property tensors.

1. THE PROPERTY TENSORS

Most physical properties of crystals are described by tensors. From the mathematical point of view, a tensor is primarily characterized by its rank. Furthermore, it can be polar or axial, a characteristic which, taking into account the rank, describes the parity behaviour. With regard to time reversal, this can be invariant (i-tensor) or changed (c-tensor). Finally, the mathematical relations defining a particular effect or, under certain conditions, also

experimental conditions may determine intrinsic symmetries of the tensors 1,2,3,4,5

2. THE NEUMANN-MINNIGERODE-CURIE-PRINCIPLE AND ITS EXTENSION

Already F. E. Neumann (1798—1895) imagined a close inter-relation between the structure of a crystal and its physical properties⁶. Minnigerode⁷ stated as an 'empirical principle': 'The structural group of a crystal is contained in every group of its physical properties'. Nowadays, this would be written shortly

$$G_{object} \subseteq G_{property},$$
 (1)

see Shubnikov and Koptsik⁸. Finally, P. Curie⁹ expressed this principle more precisely, essentially by pointing out the role of dissymmetries, i. e. disturbed symmetry. Later on Birss¹ developed a quantitative formula allowing calculation of the structure of property tensors for every point group, see also Cracknell³. In this context, an interrelation was given between the components of the property tensors $d_{q\sigma\tau\ldots}$ (the number of cartesian coordinates $\varrho, \sigma, \tau, \ldots = x, y, z$ of the index defines the tensor rank) and the symmetry operation R of the crystal point group.

For non-magnetic point groups it holds for polar i- and c-tensors

$$d_{\mathbf{p},\varrho\sigma\tau\dots} = R_{\mathrm{a}\varrho} R_{\mathrm{b}\sigma} R_{\mathrm{c}\tau\dots} d_{\mathrm{p},\mathrm{a}\mathrm{b}\mathrm{c}\dots}$$
(2)

and for axial i- and c-tensors

$$d_{\mathrm{ax},\mathrm{o}\sigma\tau...} = \det R \cdot R_{\mathrm{a}\sigma} R_{\mathrm{b}\sigma} R_{\mathrm{c}\tau...} d_{\mathrm{ax},\mathrm{abc}...}$$
(3)

According to Einstein's convention, summation has to be taken over all indices apprearing multiple. $R_{a\varrho}$ etc. are elements of the matrices describing the generating symmetry operations of different point groups. Their values can be seen directly from Jones' exact representation symbols¹⁰ of crystallographic point groups. Birss¹ has worked out a numerical calculation for the total symmetric irreducible representations of all crystallographic point groups and tensors up to rank 4.

Property tensors of non-total symmetric representations of the point groups, however, are also needed, in particular for the evaluation of crystal vibrational spectra. In the case of linear, non-resonant Raman scattering they are known as 'Raman tensors' and are polar, symmetric i-tensors of rank 2.¹¹ In order to calculate the components of these irreducible tensors, equations (2) and (3) have to be slightly modified. Following a suggestion of Bross¹², we write for polar tensors

$$\Delta_{\rm ii}^{-1} (R) \,{}^{\rm J}d_{\rm p,o\sigma\tau...} = R_{\rm ao} R_{\rm b\sigma} R_{\rm c\tau...} \,{}^{\rm J}d_{\rm p,abc...} \tag{4}$$

and for axial tensors

$$\Delta_{\rm ij}^{-1}(R) \,^{j}d_{\rm ax,o\sigma\tau...} = \,\det R \cdot R_{\rm ao} \,R_{\rm b\sigma} \,R_{\rm c\tau...}^{i}d_{\rm ax,abc...}$$
(5)

 Δ_{ij} are the components of irreducible representation matrices for the generating symmetry operations *R* of a point group. i and j run from 1 up to the dimension of the irreducible representation in question. The description of a physical property requires as many irreducible partial tensors in every representation as is the dimension of this representation. These partial ten-

sors are denoted by ${}^{j}d$ and ${}^{i}d$, respectively. Again, summation has to be taken over twofold indices, in this case also on the left hand side over j.

Brandmüller and Winter¹³ calculated the sets of cartesian irreducible tensors without intrinsic symmetry for the 32 classical crystallographic point groups up to rank 4. These include not only the usual Raman tensors but, since calculated without intrinsic symmetry, also those for the resonance Raman effect and because of the higher ranks the hyper Raman tensors too.

The limitation to the 32 classical crystallographic point groups is caused by the fact that crystals are solids with periodically arrangend units, i.e. with translational symmetry. Conformity of the point symmetry of a crystal with translational symmetry requires the point symmetry operations to fulfil a condition: Only those rotations or rotational inversions around an angle φ are allowed for which holds

$$2 \cos \varphi \in \{-2, -1, 0, 1, 2\}.$$
 (6)

This condition is fulfilled only for angles $\varphi = 0^{\circ}$, 360° , 60° , 90° , 120° , and 180° . If a rotation is n-fold, this implies:

$$\varphi = 2 \pi/n. \tag{7}$$

The compatibility between translational symmetry and the point symmetry of a crystal thus reduces n to the values n = 1, 2, 3, 4, and 6, the consequence being the existence of exactly 32 so called classical crystallographic point groups. This seems to have been obvious first to Hessel¹⁴ in 1830. So far, our discussion has concerned three dimensional crystals. Brown et al.¹⁵ have given the corresponding data for dimensions 1, 2, and 4.

The term 'classical' indicates that there are also modern developments. An example are the 58 magnetic crystallographic point groups.³ In the following text, however, we are referring to another extension of the crystal concept, such as given e.g. by Mackay¹⁶.

3. THE PENTAGONAL POINT GROUPS OF MOLECULES

When regarding the structure of single molecules, the requirement of translational symmetry is omitted and hence the restriction of n to certain values. There are molecules with fivefold rotations or rotational inversions, even if not numerous. Some corresponding molecules are listed in Table I. Examples of the two point groups $\overline{5}$ and $\overline{5}2m$ seem not to have been known hitherto. Character tables of the 7 pentagonal point groups are given in several standard books, such as e.g. Wilson, Decius, and Cross^{24} and Salthouse and Ware²⁵. In molecular vibrational spectroscopy these character tables have been used for a longer time in order to deduce the selection rules for IR-absorption- and Raman-spectroscopy and for normal coordinate analysis. Checking these tables shows that for the abelian pentagonal point groups a quantity $\varepsilon = \exp(2\pi i/5)$ plays an important role and for non-abelian point groups a quantity usually denoted by τ . τ is the well known Fibonacci number

$$\tau = (\sqrt{5} + 1)/2 \tag{8}$$

with

$$\cos\left(2\,\pi/5\right) = (\tau - 1)/2,\tag{9}$$

TABLE	Ι
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Notation of	f point group	Туре	Examples for molecules	References
Schönflies	Hermann- Mauguin			
C ₅	5	abelian	(CH3)5C5, Pentamethyl cyclopentadienyl radical	17
S ₁₀	5	abelian		
C _{5h}	$\frac{5}{m} = \overline{10}$	abelian	(CH ₃) ₅ F ₂ I, Pentamethyldifluoridine	17, 18
D _{5h}	$\frac{52}{mm} = \overline{10}m2$	non-	PaCl5, Protactiniumpentachloride	17, 19
	. 90 . 120	abelian	C_5H_{10} , Cyclopentane (C_5H_5) ₂ Fe, Ferrocene (prismatic form)	20 67
D ₅	52	abelian	(C5H5) ₂ Fe, Bis(cyclopentadienyl)iron (II)	17, 21, 22
C_{5v}	5m	abelian	(B ₁₁ H ₁₃) , Tridecahydroundecaborate	17, 23
D _{5d}	52m	abelian	(C5H5) ₂ Fe, Ferrocene (antiprismatic form)	67

The	7	Pentagonal	Point	Groups	and	Molecular	Examples
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which number is of great importance for the theory of numbers. τ is regarded as the main characterizing quantity of a fivefold symmetry and it appears also in the context of the golden section.

4. THE ICOSAHEDRON POINT GROUPS AND MOLECULAR EXAMPLES

Also for the icosahedron point groups which contain fivefold rotational axes τ appears as the character of irreducible representations.^{24,25} Still, in 1961 Matossi²⁶ stated that no molecules exist for the icosahedron groups and in 1962 Hamermesh²⁷ wrote in his standard work on group theory: 'The icosahedron group... has no physical interest, since in crystals fivefold axes cannot occur, and no examples of molecules with this symmetry are known'. Nevertheless, the character tables also for the icosahedron groups have been given in books on molecular spectroscopy for some time. Accidentally, however, an error appears in this context. For the five dimensional irreducible representation H the character in the class of 15 twofold rotational axes does not vanish^{24,25} but is 1. Cohan²⁸ has pointed this out already in 1958. It is easy to verify it by means of the orthogonality relations for the characters^{10,p.21}. Cotton²⁹ (1963) and Harris and Bertolucci³⁰ (1978) pointed out the B₁₂H₁₂----anion as an example of a molecule with a regular icosahedron structure. In 1981, E. v. Cointet³¹ calculated the summetry coordinates for a dodecaedral molecule which was still hypothetical at the time but Ternansky, Balogh and Paquette³² discovered the dodecahedran $C_{20}H_{20}$ as 'the molecule of the year 1982'. It shows the structure of a regular pentagondodecahedron. Furthermore, Kroto, et al.³³ in 1985. found a cluster C₆₀, the Buckminsterfullerene,

showing the structure of a truncated icosahedron with 32 surfaces, 12 of which are pentagonal and 20 hexagonal and with 60 vertices. This is a so called semiregular, or archimedian body.

5. SOLIDS WITH LOCAL ICOSAHEDRAL SYMMETRY

In the meantime icosahedral units have been found with this local symmetry also in solids. In a series of papers concerning clathrasiles, Gies and Gerke³⁴ describe pentagondodecahedral cages in synthetic dodecasile, which they could identify by structure refinement. Wells³⁵ reports that the three boronstructures $\alpha - B_{12}$, $\beta - B_{105}$ and tetragonal B_{50} contain icosahedral units. In $\alpha - B_{12}$ e.g. the icosahedron groups are located in all points of a rhombohedral lattice. There also exist icosahedral coordination groups in complex σ -phase which are formed by a number of transition metals. The 12-icosahedron coordination appears in Mn with Fe, Co, or Ni, not, however, in Mn with V, Cr, and Mo. A case of particular interest is the structure of Mg₃₂ (Al, Zn)₄₉. One atom is surrounded by a icosahedron formed by 12 others. Further, 20 atoms are arranged at the corners of a pentagondodecahedron. Another 12 atoms are located over its 12 surfaces and they, in turn, form another larger icosahedron.

6. CONSIDERATIONS CONCERNING NON-CRYSTALLOGRAPHIC LONG RANGE STRUCTURES

The experimental results reported so far pointed to the existence of icosahedral and dodecahedral units as local symmetries in solids. The existence of a corresponding long range symmetry seemed impossible because of equ. (6) There have been, however, speculations since some time ago whether so called non-crystallographic long range arrangements might exist in solids. In 1962, Mackay³⁶ considered whether a non-crystallographic close packing of identical spheres with icosahedral symmetry might exist. Mackay and Finney³⁷ published some very general considerations concerning structurization in 1973. Their aim was to present the statistics of regular (crystal-) structures and the regularities of statistical structures (liquids and gases) from a unifying point of view. In a particular work, 'The generalized inverse and inverse structure'38 (1977), Mackay also discussed the icosahedron. Referring to a work of Kepler³⁹ from 1611, Mackay⁴⁰ (1981) considered 'de nive quinquangula' and showed that also infinite non-periodic patterns are possible with partial structures exhibiting a fivefold rotational axis. He primarily focused his attention on the two-dimensional Penrose-patterns^{41,42} and made, in this work, the first attempts to generalize the Penrose-pattern to three dimensions, an idea which became concrete⁴³ in 1982. Work by de Bruijn⁴⁴, Kramer⁴⁵ and Neri⁴⁶ is dedicated to the same subject.

7. ALLOYS WITH LONG RANGE ICOSAHEDRON SYMMETRY

All the relevant publications cited so far were purely theoretical until in 1984 the definite experimental verification was published by Shechtman, Blech, Gratias, and Cahn.⁴⁷ If a melt of Al with 10—14 atom $^{0}/_{0}$ Mn, Fe, or Cr is cooled quickly, a metallic metastable alloy of corn, up to 2 μ size, is formed by a phase transition of the first order. Electron diffraction studies on the corn showed the icosahedral point group (2/m) $\overline{35}$ not only locally but also for the complete corn, so that a long range orientational order must exist. The diffraction spots are as sharp as those of crystals but cannot be indicated by any Bravais lattice. Twin structures incidentally showing also icosahedral symmetry could be excluded. The icosahedral phase is remarkably resistant to crystallization. Heating the sample up to 300 °C for 6 hours or to 350 °C for one hour does not induce any crystallization. Only one hour heating to 400 °C causes a conversion to the stable Al₆Mn-phase. The symmetry of the icosahedral phase is some where between that of a crystal (one of the 32 crystallographic point groups) and that of an isotropic liquid (three-dimensional rotation group).

Some time later another important theoretical work was published by Levine and Steinhardt⁴⁸ the title of which »Quasi-crystals: a new class of ordered structures« became of great interest to many solid-state physicists. The idea of a crystal with periodical translational order is systematically extended to the 'quasi-crystal' with 'quasi-periodic' order by replacing the translation by a long-range-bond orientational order (BOO). This is considered a new phase of matter. The electron diffraction diagrams recorded by Shechtman et al.⁴⁷ were simulated by Levine and Steinhardt on a computer and the structure thus identified as a 'quasi-crystal'. The authors show the interrelation with the Fibonacci-number of the golden section and point out also that the icosahedral structure will cause new structural and electronic properties of solids. In the meantime, a further number of papers on this subject have been published, e. g.49-53. Bak54 in particular studied the symmetry, stability and elastic properties. He mentions that the critical parameter for the phase transition from the isotropic to the icosahedral phase (also known as T-phase) is contained in the irreducible representation $\Gamma_5 = H$ of the icosahedron group. Urban, Moser, and Kronmüller^{55,56} showed that the transition from the quasi-crystalline phase to the amorphous state can be activated by irradiation of 1 MeV-electrons at 130 K. Bancel and Heiny⁵⁷ were able to find further Aluminium transition element alloys with a quasi--crystalline phase. Biham, Mukamel and Shtrikman⁵⁸ concluded from general considerations that icosahedral and pentagonal structures may exist as thermodynamically stable phases and they state that their analysis can be extended also to other plane quasi-crystals with rotational axes more than 6-fold. However, there is no lack of critical voices regarding long-range icosahedral symmetry either⁵⁹. In a recent work by Pauling⁶⁰ with the title »So-called icosahedral and decagonal quasicrystals are twins of an 820-atom cubic crystal« he writs: 'The icosahedral nature of the clusters in the cubic crystal explains the appearance of the Fibonacci numbers and the golden ration. I conclude that the evidence in support of the proposal that the so-called icosahedral and decahedral quasicrystals are icosatwins and decatwins of cubic crystals is now convincingly strong. I point out that there is no reason to expect these alloys to have unusual physical properties'.

IRREDUCIBLE TENSORS

8. THE IRREDUCIBLE TENSORS OF THE GROUPS WITH FIVEFOLD ROTATION AXES⁶¹

In order to calculate the components of these tensors, equations (4) and (5) were used. The generating symmetry operations for the different point groups and their irreducible representation matrices are listed in Table II. The corresponding matrices for the pentagonal point groups were listed in analogy to the values for the crystallographic point groups¹⁰. The matrices for the icosahedron group 235 originate from Matossi's book.²⁶ In this context we have to note that on p. 153 an error appears in the last line. The equation should be read correctly $\cos 2\psi = (\sqrt{5} - 1)/(5 - \sqrt{5}) = 1/\sqrt{5}$. In the present work we denote Matossi's angle ψ by ϑ and his φ by α . We, furthermore, note that the matrices are given for the so-called 'passive symmetry operations' by Matossi¹⁰.

Table III gives a survey of the abelian point groups $5 (= C_5)$ and $5 (= S_{10})$. The form of the corresponding irreducible tensors has been abbreviated by capital letters for the different irreducible representations in analogy to and as an extension of the nomenclature used by Birss.¹ Table IV summarizes these forms for tensors of ranks 0 (scalar), 1 (vector), 2 and 3. All components which have to vanish by symmetry arguments are denoted by small dots. The components of a vector in cartesian coordinates are written by a columm-

TABLE II

The Generating Symmetry Operations and Their Irreducible Representations for the 7 Pentagonal and the 2 Icosahedral Point Groups

5 = C ₅	$C_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	
A	$\Delta = 1$	-
$E_{\gamma} (\gamma = 1, 2)$	$\Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix}$	- Industria de la pré Propose de la président
$\overline{10} = C_{Sh}$	$C_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$\sigma_{Z} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
A'	$\Delta = 1$	$\Delta = 1$
A"	$\Delta = 1$	$\Delta = -1$
E_{γ} ' ($\gamma = 1,2$)	$\Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
$E_{\gamma}'' (\gamma = 1,2)$	$\Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$

 $\alpha = \frac{2\pi}{5}$

Table II continued

design of the second seco		
$\overline{10}$ m 2 = D _{5h}	$S_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \end{pmatrix}$	$C_{2x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
A ₁	$\begin{pmatrix} 0 & 0 & -1 \end{pmatrix}$ $\Delta = 1$ $\Delta = 1$	$\begin{pmatrix} 0 & 0 & -1 \end{pmatrix}$ $\Delta = 1$ $\Delta = -1$
A [*] ₁ A [*] ₂	$\Delta = -1$ $\Delta = -1$	$\Delta = 1$ $\Delta = -1$
E_{γ} ' ($\gamma = 1,2$)	$\Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
E_{γ} " ($\gamma = 1,2$)	$\Delta = \begin{pmatrix} -\cos\gamma\alpha & \sin\gamma\alpha \\ -\sin\gamma\alpha & -\cos\gamma\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$
52 = D ₅	$C_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$C_{2x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$5 \mathrm{m} = \mathrm{C}_{5\mathrm{v}}$	$C_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$\sigma_{y} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
A ₁ A ₂	$\begin{array}{l} \Delta = 1 \\ \Delta = 1 \end{array}$	$\begin{array}{rcl} \Delta = & 1 \\ \Delta = & -1 \end{array}$
E ₁	$\Delta = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
E ₂	$\Delta = \begin{pmatrix} \cos 2\alpha & -\sin 2\alpha \\ \sin 2\alpha & \cos 2\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
	$\overline{10} \text{ m } 2 = D_{5h}$ $A_{1}^{'} A_{2}^{'}$ $A_{1}^{'} A_{2}^{''}$ $E_{1}^{''} (\gamma = 1, 2)$ $E_{1}^{'''} (\gamma = 1, 2)$ $5 2 = D_{5}$ $5 \text{ m} = C_{5v}$ A_{1} A_{2} E_{1} E_{2}	$ \begin{array}{c} \overline{10} \ \mathbf{m2} = \mathbf{D_{5h}} \mathbf{S_{5z}^{+}} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & -1 \end{pmatrix} \\ \begin{array}{c} \mathbf{A_{1}^{\prime}} \qquad \Delta = & 1\\ \mathbf{A_{2}^{\prime}} \qquad \Delta = & 1\\ \mathbf{A_{2}^{\prime\prime}} \qquad \Delta = & -1\\ \hline \mathbf{E_{1}^{\prime\prime}} \left(\gamma = 1, 2 \right) \qquad \Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix} \\ \hline \mathbf{E_{1}^{\prime\prime}} \left(\gamma = 1, 2 \right) \qquad \Delta = \begin{pmatrix} \cos\gamma\alpha & -\sin\gamma\alpha \\ \sin\gamma\alpha & \cos\gamma\alpha \end{pmatrix} \\ \hline \\ \overline{52} = \mathbf{D_{5}} \qquad \mathbf{C_{5z}^{+}} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix} \\ \hline \\ \overline{\mathbf{5m}} = \mathbf{C_{5v}} \qquad \mathbf{C_{5z}^{+}} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix} \\ \hline \\ \mathbf{A_{1}} \qquad \Delta = & 1\\ \mathbf{A_{2}} \qquad \Delta = & 1\\ \mathbf{A_{2}} \qquad \Delta = & 1\\ \mathbf{E_{1}} \qquad \Delta = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \\ \sin\alpha & \cos\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \\ \hline \\ \mathbf{E_{2}} \qquad \Delta = \begin{pmatrix} \cos2\alpha & -\sin\alpha \\ \sin2\alpha & \cos2\alpha \end{pmatrix} \\ \hline \end{array} $

Table II to be continued

vector. The form N_1 (i) implies that only the z-component of a vector does not vanish by symmetry arguments in the total symmetric representation. For such non-vanishing components we use either a black full circle or, if clearer or more convenient, small Latin letters. Full circles connected with a straight line, as e. g. in the form N_2 , indicate that the two components have to be identical for symmetry reasons, i. e. $d_{xx} = d_{yy}$. Identical small Latin letters for different components of a tensor in one irreducible representation or degenerate tensors such as for $Q_2^{"}$ do also mean that the corresponding components must be identical by symmetry arguments holds e. g. ${}^1d_{xz} = -{}^2d_{yz}$.or $Q_2^{"}$. A tensor component symbolized by an open circle connected with another full circle means that e. g. $d_{yz} = -d_{xy}$ holds (as for N₂). Special symmetry conditions such as e. g. $d_{xxx} + d_{yyy} + d_{yyx}$ for $Q_3^{"}$ are abbreviated by A = a + b + c. Index numbers on the right hand side outside the brackets denote the number of independent components which do not vanish for symmetry reasons.

Tal	bl	e	II	co	n	tiı	nı	ıe	d

235 = I	$C_{5z}^{+} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$C_{2yz}^{icos} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -\cos 2\vartheta & -\sin 2\vartheta \\ 0 & -\sin 2\vartheta & \cos 2\vartheta \end{pmatrix}$
A	$\Delta = 1$	$\Delta = 1$
F ₁	$\Delta = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$\Delta = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -\cos 2\vartheta & -\sin 2\vartheta \\ 0 & -\sin 2\vartheta & \cos 2\vartheta \end{pmatrix}$
.F ₂	$\Delta = \begin{pmatrix} \cos 2\alpha & -\sin 2\alpha & 0\\ \sin 2\alpha & \cos 2\alpha & 0\\ 0 & 0 & 1 \end{pmatrix}$	$\Delta = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -\cos 2\vartheta' & -\sin 2\vartheta' \\ 0 & -\sin 2\vartheta' & \cos 2\vartheta' \end{pmatrix}$
G	$\Delta = \begin{pmatrix} \cos\alpha & 0 & 0 & -\sin\alpha \\ 0 & \cos2\alpha & -\sin2\alpha & 0 \\ 0 & \sin2\alpha & \cos2\alpha & 0 \\ \sin\alpha & 0 & 0 & \cos\alpha \end{pmatrix}$	$\Delta = \begin{pmatrix} \sin 2\vartheta' & \cos 2\vartheta' & 0 & 0 \\ \cos 2\vartheta' & -\sin 2\vartheta' & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
H	$ \left(\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{pmatrix} -\frac{1}{5} & 0 & 0 & -\frac{\sqrt{12}}{5} & -\frac{\sqrt{12}}{5} \\ 0 & -\frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} & 0 & 0 \\ 0 & -\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} & 0 & 0 \\ -\frac{\sqrt{12}}{5} & 0 & 0 & \frac{3}{5} & -\frac{2}{5} \\ -\frac{\sqrt{12}}{5} & 0 & 0 & -\frac{2}{5} & \frac{3}{5} \end{pmatrix}$
$\alpha = \frac{2\pi}{5}$ $= 72^{0}$	$\cos\alpha = \frac{1}{4}(\sqrt{5} - 1) = \frac{1}{2}(\tau - 1)$ $\sin\alpha = \frac{1}{2}\sqrt{\tau + 2}$ $\cos 2\alpha = -\frac{1}{4}(\sqrt{5} + 1) = -\frac{\tau}{2}$ $\sin 2\alpha = \frac{1}{2}\sqrt{3 - \tau}$	$\cos 2\vartheta = \frac{\cos \alpha}{1 - \cos \alpha} = \frac{1}{\sqrt{5}} = \frac{1}{2\tau - 1}$ $\sin 2\vartheta = \frac{2}{\sqrt{5}} = \frac{2}{2\tau - 1}$ $\cos 2\vartheta' = \frac{\cos 2\alpha}{1 - \cos 2\alpha} = -\frac{1}{\sqrt{5}} = \frac{1}{1 - 2\tau}$ $\sin 2\vartheta' = \frac{2}{\sqrt{5}} = \frac{2}{2\tau - 1}$

Table V correspondingly shows the forms of 4th rank irreducible tensors. Table VI summarizes the abelian point group $\overline{10}$ (= c_{5h}). Table VII presents the tensor forms of rank 0 to 3 and Tab. VIII those of rank 4. In Tables IX to XIV the forms of the irreducible tensors are given for the

The irreducible tensor forms for the two icosahedron point groups are listed in Table XV to XVII. For the 4-fold and 5-fold degenerated irreducible representations, respectively, fairly complicated interrelations exist between degenerated tensors.

non-abelian pentagonal point groups.

TABLE III

system	quasi- Laue		point group		genera- ting	reps	tense	or of rank	tens	or of rank
	class	Hermann- Mauguin	Schön- flies	abstract	elements		polar g	axial u	polar u	axial g
pentagonal	-5	5	C5	G5 ¹	C _{5z} +	A	N _m	Nm	N _n	Nn
						i) E ₁	Q _m "	Q _m "	Q _n "	Q _n "
						i) E ₂	R _m "	R _m "	R _n "	R _n "
	(184	5	S ₁₀	G ₁₀ ¹	S _{10z} +	Ag	N _m		-	Nn
		= 5 x Ī			oder	A _u	-	N _m	N _n	-
					C _{5z} +, I	i) E _{1g}	Q _m "	ς.	-	Q'n
						i) E _{1u}		Q _m ".	Q _n ".	÷
						i) E_{2g}	R _m "		÷	R _n '
						i) E ₂₁₁	- ⁰	R _m "	R _n "	-

Survey of the Abelian Point Groups 5 and $\overline{5}$

TABLE IV

The Irreducible Tensor Forms of Rank 0 to 3 for the Point Groups 5 and $\overline{5}$



TABLE V

auasi-							Γ	1)		are)		2)			[(1	1)		,	1(2)
Laue	N_4	(A	f	• •)	(~	G`	Q4	"(a	~	H)	3-)	κ	i	R_4	A	I	-k
class		e	a	•	1	L	P	S				p		F	α	k		J	$\frac{B}{1}$	i
Ē		·	•	1		C	1	·		D	-c				1	ι		19	1	u
5		-						8			_	-		1	Va	10		-	T_	-
		a	D	÷		2	ሯ	I		12	\sim	0			$\sqrt{\mathbf{p}}$	-i			$\binom{c}{r}$	1 1
			ь	m		e	La			-h	h	4 •		1	6	u		1	5	_t
	- 01					1	Ľ	_	1.0		\Ľ	-		L		_		Ľ		_
	-			n		Е	m	1		F	Vi					v		lla		w
	-2		•	0	1	1	g	н.		-h	$\int \mathbf{k}$				×0	w			5	-v
	A. 3	g	h	a •		·	1.	z'		· /	1.	z"		x	y	·		у	-x	•
	_					+	+			14	+					-		∥⊢	-	-
		-B	с	·		6	م	q		16	A	-n		θ	$-\gamma$	k		L	-D	i
		b	-d	•		p	9	0		1	\sim	r		β	η	-i		-C	K	k
		·	•	-m		d	b	·	1	-a	e				9	u		17	1	-t
			•	-				_			_	-			T,			-	f_{τ}	_
	141.01	a f	-e			2	< C	р ц			\sim	's _G	100	$\left \frac{-\alpha}{\kappa} \right $	15	-1 -k	0.041			k i
				1		C	D			f	- <u>-</u> C	-0		0	8	-t			6	-u
				_		18	_									_			_	
				-0		k	h			-g	1			La	D	w		L		-v
				n		i	F			m	-E			Q	SQ.	-v			Ş	-w
		-h	g	•		·	·	z"		· ·	•	-z'		у	-x	•		-x	-у	•
						-				-				-				-		
		•	•	•1		0	ρ	·		P	-ν	•		5	~	σ		3	~	τ
		•	•	-		π	λ			-μ	ξ	•			P	τ			7	-σ
		1	1	1.1				ε			•	5		Ψ	X			X	-φ	
		1	F			2		_		1	_				2	-			_	_
		./	1.	2		S	μ P			-^	π 			2	\leq	-σ		>	5	-0 -7
	-	6	1	÷.		·		۲.				-ε'		χ	-φ	•		-φ		
		_	_				_	-		-		_		_			÷.	_		
		•						Y				δ'		ψ	ω			ω	ψ	
		0	5					δ'			•	-γ'		ω	-ψ	·		-ψ	-ω	÷
		(.		• ,	19	(α'	β'	• ,	34	(β'	-α	•)	$(\cdot$	•	•)	28	(•	•	• ,
		A = a	a + b	+ c		C	= a +	- b +	с											

The Irreducible Tensor Forms of Rank 4 for the Point Groups 5 and $\overline{5}$

 $A=a+b+c \qquad C=a+b+c$ $B=d+e+f \qquad D=d+e+f$ E=g+h+i F=k+1+m G=n+o+p H=q+r+s $O=\lambda+\mu+\nu$ $P=\xi+\pi+\rho$

$$\begin{split} A &= \frac{1}{2}(\zeta + \eta + \vartheta + \kappa) \qquad I = \frac{1}{2}(\alpha + \beta - \gamma + \varepsilon) \\ B &= \frac{1}{2}(-\zeta + \eta + \vartheta - \kappa) \qquad J = \frac{1}{2}(\alpha - \beta + \gamma + \varepsilon) \\ C &= \frac{1}{2}(\zeta - \eta + \vartheta - \kappa) \qquad K = \frac{1}{2}(-\alpha + \beta + \gamma + \varepsilon) \\ D &= \frac{1}{2}(-\zeta - \eta + \vartheta + \kappa) \qquad L = \frac{1}{2}(-\alpha - \beta - \gamma + \varepsilon) \end{split}$$

TABLE VI

Survey of the Abelian Group $\overline{10}$

system	quasi- Laue		point group		genera-	reps	tens	sor of	tensor of		
	class	Hermann- Mauguin	Schön- flies	abstract	elements		polar	axial u	polar u	axial	
pentagonal		10	Cgh	G10 ¹	S _{5z} +	A'	Nm	-		Nn	
		= 5 😡 m			oder	Α"	1	Nm	Nn	-	
					C_{5z}^+, σ_z	i) E ₁ '	R _m "'	Q _m '	Q _n '	R _n "'	
						i) E_1 "	Q _m '	R _m "'	R _n "'	Q _n '	
						i) E ₁ '	R _m ⁽⁴⁾	0 _m "'	0 _n '''	R _n (4)	
						i) E2"	0 _m "'	R _m ⁽⁴⁾	R _n ⁽⁴⁾	0 _n "'	

TABLE VII

The Irreducible Tensor Forms of Rank 0 to 3 for the Point Group $\overline{10}$ $\overline{10} = C_{5b}$

N ₀ (•) ₁	(·) ₀	(2) R ₀ ''' (·)	$(\cdot)_0 \qquad Q_0'$	(2)	$(\cdot)_0 = R_0^{(4)}$	(2) (·)	$(\cdot)_0 O_0'''$	(2) (·)
$N_1 \begin{pmatrix} \cdot \\ \cdot \\ \bullet \end{pmatrix}_1$	$\left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}\right)_0$	R_1 ()	$\begin{pmatrix} a \\ b \\ \cdot \end{pmatrix}_2$ Q_1'	$\begin{pmatrix} b\\ -a\\ \cdot \end{pmatrix}$	$ \begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}_0 \qquad \qquad$	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}_0$ O_1	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$
$\overset{N_2}{} \left({}{}{}{}{}{}{}$	$\begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}_0$	$\begin{array}{ccc} R_2^{m} & \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} \end{array}$	$ \begin{pmatrix} \cdot & \cdot & e \\ \cdot & \cdot & f \\ g & h & \cdot \end{pmatrix}_4 Q_2'$	$\begin{pmatrix} \cdot & \cdot & f \\ \cdot & \cdot & -e \\ h & -g & \cdot \end{pmatrix}$	$ \begin{pmatrix} c & d & \cdot \\ d & -c & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}_2 R_2^{(4)} $	$\begin{pmatrix} d & -c \\ -c & -d \\ \cdot & \cdot \end{pmatrix}$	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot &$	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}^{-1}$
		R ₃ " (· · · · · · · · · · · · · · · · · ·	$ \begin{pmatrix} A & f & \cdot \\ e & a & \cdot \\ \cdot & \cdot & 1 \\ d & b & \cdot \\ c & B & \cdot \\ \cdot & \cdot & m \\ \hline & & - & m \\ \hline & & - & - \\ \cdot & \cdot & p \\ \cdot & \cdot & q \\ \end{pmatrix} $	$ \begin{pmatrix} B & -c & \cdot \\ -b & d & \cdot \\ \cdot & \cdot & m \\ \hline -a & e & \cdot \\ f & -A & \cdot \\ \cdot & \cdot & -l \\ \hline - & - & -p \\ \cdot & \cdot & -p \end{pmatrix} $	$ \begin{pmatrix} \cdot & \cdot & g \\ \cdot & \cdot & h \\ i & k & \cdot \\ \hline & - & - \\ \hline & - & - \\ h \\ \cdot & \cdot & - g \\ k & -i & \cdot \\ \hline & - & - \\ n & 0 & - \\ 0 & -n & \cdot \\ \end{pmatrix} \ \ \ \ \ \ \ \ \ \ \ \ \$	$ \begin{pmatrix} \cdot & \cdot & h \\ \cdot & \cdot & -g \\ k & -i & \cdot \\ - & - & -g \\ \cdot & \cdot & -h \\ -i & -k & \cdot \\ -i & -k & -h \\ -i & -h & -h \\ -i & -n & -h \\ -n & -n & -h $		
()	()	(· · ·)	$(r s \cdot)_{12}$ A = a + b + c	$(s - r \cdot)$ B = d + e + f	()6	()	(· · · ·) ₂	()

9. DISCUSSION OF THE FORMS OF IRREDUCIBLE TENSORS AND THEIR INFLUENCE ON THE PHYSICAL PROPERTIES

More than 50 years ago Hermann⁶² deduced the influence of crystal symmetry on those material constants which can be described by tensors. In analogy to but also in extension of his considerations, the following discussion will be given. There are no peculiarities with fivefold rotations and point groups in contrast to space groups. We are first going to discuss the totally symmetric irreducible representations.

TABLE VIII

The Irreducible Tensor Forms of Rank 4 for the Point Group $\overline{10}$

 $\overline{10} = C_{5h}$



Table VIII to be continued

J. BRANDMÜLLER AND R. CLAUS

Table VIII continued



system	quasi- Laue		point group			reps	tens	or of rank	tensor of odd rank	
	class	Hermann- Mauguin	Schön- flies	abstract	elements		polar g	axial u	polar u	axial g
pentagonal		10m2	D _{5h}	G ₂₀	S _{5z} +, C _{2x}	A1'	Pm	-	· ·	Pn
		= 52 🗙 m				A1"		Pm	Pn	-
		= 10 (\$)2				A2'	Qm	-		Q _n
						A2"		Qm	Qn	-
						E ₁ '	U_m**	T _m '	T _n '	U,*''
						E1"	"Tm	U _m (4)	Un ⁽⁴⁾	T _n "
						E2'	U _m (5)	S _m "	S _n "	U _n (5
						E2"	S _m "	U _m (6)	U _n (6)	S _n "

 TABLE IX

 Survey of the Non-Abelian Point Group 10m2

TABLE X

The Irreducible Tensor Forms of Rank 0 to 3 for the Point Group $\overline{10}m2$ TABLE Xa



a) Abelian Point Groups with Pure Rotations Only

Point group $5 (= C_5)$ is cyclic and thus an abelian point group with fivefold rotation (n = 5) as the generating element, see Table II and III. This group has 5 irreducible representations in all, two pairs of which,

TA	BL	E	x	Ь
				-

10 m	$2 = D_{5h}$				U _ν ''' a	and $U_{v}^{(4)} =$	0 for v = 0, 1, 2, 3			
10 10 m										
$\begin{array}{c} \hline (1) \\ (\cdot)_0 \\ \end{array} \\ T_0' \\ \end{array}$	(2) (·)	(1) (·) ₀	T0"	(·)	(1) (·) ₀	U ₀ ⁽⁵⁾	(·)	(1) (·) ₀	U ₀ ⁽⁶⁾	(2)
$ \begin{pmatrix} a \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}_{12} \qquad T_1'$	$\begin{pmatrix} \cdot \\ -a \\ \cdot \end{pmatrix}$	$\begin{pmatrix} \cdot \\ b \\ \cdot \end{pmatrix}_{1\cdot 2}$	T1"	$\begin{pmatrix} b \\ \cdot \\ \cdot \end{pmatrix}$	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}_0$	U ₁ ⁽⁵⁾	$\begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$	$\left(\begin{array}{c} \cdot \\ \cdot \end{array} \right)_0$	U ₁ ⁽⁶⁾	
$ \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & f \\ \cdot & h & \cdot \end{pmatrix}_{22} T_2'$	$\begin{pmatrix} \cdot & \cdot & f \\ \cdot & \cdot & \cdot \\ h & \cdot & \cdot \end{pmatrix}$	$\begin{pmatrix} \cdot & \cdot & e \\ \cdot & \cdot & \cdot \\ g & \cdot & \cdot \end{pmatrix}_2.$	T2"	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & -e \\ \cdot & -g & \cdot \end{pmatrix}$	$\begin{pmatrix} c & \cdot & \cdot \\ \cdot & -c & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}_1$	U ₂ ⁽⁵⁾	$\begin{pmatrix} \cdot & -\mathbf{c} & \cdot \\ -\mathbf{c} & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	$ \begin{pmatrix} \cdot & d & \cdot \\ d & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}_{1\cdot 2}$	U ₂ ⁽⁶⁾	$\begin{pmatrix} d & \cdot & \cdot \\ \cdot & -d & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$
$ \begin{pmatrix} A & \cdot & \cdot \\ \cdot & a & r \\ \cdot & b & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot$	$ \begin{pmatrix} \cdot & -c & \cdot \\ -b' & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ -a & \cdot & \cdot \\ \cdot & -A & \cdot \\ \cdot & -A & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -p \\ \cdot & \cdot & -p \\ \cdot & -r & \cdot \end{pmatrix} $	$\left(\begin{array}{ccc} \cdot & f & \cdot \\ e & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \hline d & \cdot & \cdot \\ \cdot & B & \cdot \\ \cdot & \cdot & m \\ \hline \hline \cdot & \cdot & r \\ \cdot & \cdot & q \\ \cdot & s & \cdot \end{array}\right)$) T ₃ "	$ \begin{pmatrix} B & \cdot & \cdot \\ \cdot & d & \cdot \\ \cdot & \cdot & m \\ \hline & & e & \cdot \\ f & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \hline & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ s & \cdot & \cdot \end{pmatrix} $	$\left(\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & h \\ \cdot & k & \cdot \\ \hline \cdot & \cdot & h \\ \cdot & \cdot & \cdot \\ k & \cdot & \cdot \\ k & \cdot & \cdot \\ \hline \cdot & 0 & \cdot \\ 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{array}\right)$	U ₃ ⁽⁵⁾	$\begin{array}{cccc} \cdot & \cdot & h \\ \cdot & \cdot & \cdot \\ k & \cdot & \cdot \\ \hline & & \cdot & \cdot \\ \cdot & \cdot & -h \\ \cdot & -k & \cdot \\ \hline & & -k & \cdot \\ \hline & & -k & \cdot \\ \cdot & -0 & \cdot \\ \cdot & -k & \cdot \\ \end{array}$	$ \begin{pmatrix} \cdot & \cdot & g \\ \cdot & \cdot & \cdot \\ i & \cdot & \cdot \\ \hline & - & - & - \\ \cdot & \cdot & - g \\ \cdot & -i & \cdot \\ \hline & -i & \cdot \\ \hline & n & - & \cdot \\ \cdot & -n & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} $	U ₃ ⁽⁶⁾	$ \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & -g \\ \cdot & -i & \cdot \\ - & - & -g \\ \cdot & \cdot & \cdot \\ -i & \cdot & \cdot \\ -i & \cdot & \cdot \\ -n & \cdot \\ -n & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} $

respectively, show complex conjugate characters i.e. 'irreducible representations of the third kind' (ref. 10, p. 20) denoted by 'i'. Group 5 appears in the sequence of abelian pure rotation groups 1, 2, 3, 4, 5, 6, ..., ∞ . Any distinction between polar and axial tensors is superfluous since it always holds that R = +1, i.e. tensors with even (g-) and odd (u-) parity exhibt the same form. The results of extensive calculations in⁶¹ allow a comparison of the tensor forms of different rank ν in the total symmetric representations of point groups 1, 2, 3, ..., ∞ . We find the following characteristics: Up to rank $\nu = n - 1$, the tensor forms are identical to those with n = infinity. From rank $\nu = n$ on, the number of independent tensor components is larger than for $n = \infty$. Additional components which don't have to vanish by symmetry arguments thus appear for $n = \infty$.

b) Abelian Point Groups with Rotational Inversions

Point groups 5 and 10 show identical forms to those of 5. Only all odd tensors of the totally symmetric representations A_g and A' vanish for parity reasons.

c) The Non-Abelian Point Group $10 m^2$ (= D_{5h})

The results fit the sequence D_{nh} without any problems. Again we find that up to rank $\nu = n - 1$ the irreducible tensor forms are identical to those for the continuous point group $D_{\infty h}$.⁶¹ Now, because of the rotational inversion, however, even and odd tensors differ: all odd tensors vanish in the total symmetric irreducible representation A_1 ' for parity reasons.

TABLE XI

The Irreducible Tensor Forms of Rank 4 for the Point Group $\overline{10}m2$ TABLE XIa

 $\overline{10}$ m 2 = D_{5h}



A = a + b + c B = d + e + f

TABLE XIb

for $\overline{10}\ m\ 2=D_{5h}$ and not bound to such that the second straight statement of

(1) (2)	(1) (2)	(1) (2)
$(\cdot \cdot \cdot \cdot) T_4'(\cdot \cdot H)$	$(\cdot \cdot G) T_4''(\cdot \cdot \cdot)$	$(\mathbf{\cdot} \cdot \cdot) \mathbf{U}_{4}^{\prime\prime\prime}(\cdot \cdot \cdot)$
· · s · · · ·	· · · · · -p	· 0 ·
• f • D • •	C · · · · · -c ·	· · · · · · · · · · · · · · · · · · ·
<u></u>	. 8	
· · r · · ·	· · · · · · -0	
q	· · n . · ·	0
e · · · d ·	· a · -b · ·	
· m · F · ·	E. · · · · · · ·	
1 · · · k ·	• g • -h • •	$ \cdot \langle \cdot \cdot \rangle \cdot \cdot \cdot $
· · · Z"	· · z' · · ·	
· • q • • •	· · · · · - n	
· · · · r	· · o · · ·	10 · · 01 ·
d·· · e·	• b • -a • •	
s	p	la · · · p ·
• • H • • •	· · · · · -G	· • ·
• D • f • •	c · · · -C ·	· · · · · · · · · · · · · · · · · · ·
k · · · 1 ·	• h • -g • •	
• F • m • •	i · · · -E ·	
••• z" •••	. · · · · · · -z'	· · · · · · ·
· p · P · ·	0 · · · -v ·	
π · · · ξ ·	· λ · -μ · ·	
· · · · · ζ'	••• ε' ••••	
ξ··π·	$ \cdot \mu \cdot -\lambda \cdot \cdot $	
· P · ρ · ·	v · · · -0 ·	
· · ζ' · · ·	· · · -ε'	
· · · · · · · · · · · · · · · · · · ·	$ \cdot \cdot \gamma' $ $ \cdot \cdot \cdot $	
· · δ' · · · ·	· · · ·	
$(\cdot \beta' \cdot)_{16\cdot 2} (\beta' \cdot \cdot)$	$(\alpha' \cdot \cdot)_{16\cdot 2} (\cdot -\alpha' \cdot)$	$(\cdot \cdot \cdot \cdot)_{1\cdot 2} (\cdot \cdot \cdot \cdot)$
$\mathbf{C} = \mathbf{a} + \mathbf{b} + \mathbf{c}$	G = n + o + p	
$\mathbf{D} = \mathbf{d} + \mathbf{e} + \mathbf{f}$	H = q + r + s	
E = g + h + i	$O = \lambda + \mu + \nu$	
F = k + l + m	$P = \xi + \pi + \rho$	

Table XIb to be continued

IRREDUCIBLE TENSORS

Survey of the Non-Abelian Fonst Groups 52, Inc. and 52m Table XIb continued

Jam also	direct they be	234 - J	T(a)	man. Terrat	
(1)	(4)	(1) (5)	(2)	(1)	(2)
$(\cdot \land \cdot)$	$U_4^{(q)}(\mathbf{Q} \cdot \cdot)$	$\left(-\varepsilon \cdot \cdot \right) U_4^{(3)}$	$\left(\cdot I \cdot \right)$	$\begin{pmatrix} \cdot & \kappa & \cdot \end{pmatrix}$	$U_4^{(0)} (A \cdot \cdot \cdot$
· · · ·	· M.	· α ·	J · ·	ζ	· B ·
9 .	14 Par	A . O .	· · · .	· 8 · 1	·······································
4	· / ·	·β·	K · ·	$\eta \cdot \cdot$	· C ·
. 9.	· · ·	γ	$\cdot L \cdot$	· v ·	$D \cdot \cdot$
	\cdot	· · ·	· · -t	···u	· · · ·
		<u></u>			
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· · ·	· · · 9	· · · · · · · · · · · · · · · · · · ·	· · -v	• • w	• • •
$ \cdot \cdot\cdot $	131 · · b	x · ·	· -x ·	· y ·	у
$ -\!\! -\!\!- $	-+-I			· ·	
4	·	· - γ ·		v · ·	· -D ·
. 9.	· · ·	β··	· K ·	· η ·	-C · · ·
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		· · -t			· · -u
		×	· · -v	· · w	
		· · -v			· · -w
		· -x	-x · ·	y	· _y ·
, im, and	Point Groups 52	to a <u>for the</u>	Aught jo an	Tensor, Tor	Irreducitie
		· · σ			· · τ
			· · -σ	· · τ	
		φ · ·	· - φ ·	· χ ·	χ
		·			
			· · - σ	· · τ	
		· · -σ			· · - τ
		· • ·	-o · ·	x · ·	·
		Ť		~	~ ~
					(a) · · ·
		Ψ	_ψ	I	· - ····
1 CO 10 10 10		-Ψ	ι-Ψ		

 $I = \frac{1}{2}(\alpha + \beta - \gamma + \varepsilon)$ $J = \frac{1}{2}(\alpha - \beta + \gamma + \varepsilon)$ $K = \frac{1}{2}(-\alpha + \beta + \gamma + \varepsilon)$ $L = \frac{1}{2}(-\alpha - \beta - \gamma + \varepsilon)$ $A = \frac{1}{2}(\zeta + \eta + \vartheta + \kappa)$ $B = \frac{1}{2}(-\zeta + \eta + \vartheta - \kappa)$ $C = \frac{1}{2}(\zeta - \eta + \vartheta - \kappa)$ $D = \frac{1}{2}(-\zeta - \eta + \vartheta + \kappa)$

system quasi- Laue			point group	0	genera- ting	reps	tens	sor of 1 rank	tensor of odd rank		
class	Hermann- Mauguin	Schön- flies	abstract	elements	2-1	polar g	axial u	polar u	axial g		
pentagonal	52m	52	D ₅		C _{5z} +, C _{2x}	À1	Pm	Pm	Pn	Pn	
		= 5(3) 2				A_2	Qm	Qm	Qn	Qn	
						E_1	Т _т "	т _m "'	T _n "'	T _n "'	
						E ₂	U _m (7)	U _m (7)	U _n (7)	U _n (7)	
		5m	C _{5v}		C_{5z}^{+}, σ_y	A ₁	Pm	Qm	Qn	Pn	
		= 5 (s) m				A ₂	Qm	Pm	Pn	Qn	
						E ₁	T _m (4)	T _m (5)	T _n (5)	T _n (4)	
				A -		E ₂	U _m (8)	U _m (9)	U _n (9)	U _n (8)	
		52m	D _{5d}		C _{5z} +, C _{2x,} I	A _{1g}	Pm	-		Pn	
		= 52 🛞 Ī				A _{lu}		Pm	Pn		

			TAE	BLE XI	r .				_
Survey	of	the	Non-Abelian	Point	Groups	52,	5m,	and	52m

TABLE XIII

The Irreducible Tensor Forms of Rank 0 to 3 for the Point Groups 52, 5m, and $\overline{52m}$





d) The Non-Abelian Point Groups 52, 5m, and 52m

These groups also fit the sequences D_n , C_{nv} , and D_{nd} . In the pure rotational group 52 there are no differences between polar and axial tensors. Point group 5m also contains rotational inversions, the consequence being that the forms of polar and axial tensors differ. For 52 m, all components of the odd tensors vanish in the total symmetric representation. Again, it holds (which proved to be the rule) that up to rank $\nu = n - 1$ the irreducible tensors in the total symmetric representation already exhibit the same form as for the existence of an infinite-fold rotation axis. From $\nu = n$ on, the point groups discussed so far have more independent components than the corresponding Curie-limiting groups⁶⁴ with infinite-fold rotations.

e) The Two Icosahedral Point Groups

The icosahedron group 235 is located between the crystallographic cubic point group 432 (= O) and the pure three dimensional rotation group 0^+ (3). Comparing the forms of the total symmetric irreducible tensors of these 3 point groups listed in Table XVIa and XVII or in⁶¹, respectively, provides the following result:

(i) Comparison of 235 with 432

Up to rank $\nu = 3$ the tensor formes are identical. The 4th rank tensor shows in the cubic point group 432 an additional independent component relative to the icosahedron group 235. Comparing the two forms, one finds that they are quite similar: only the linear interrelation $d_{xyyx} = d_{xxxx} - d_{xxyy} - d_{xyxy}$ is

TABLE XIV

The Irreducible Tensor Forms of Rank 4 for the Point Groups 52, 5m, and $\overline{52m}$ TABLE XIVa

52 m



Up to rank $(\Psi^{**})^*$ for tensor throws and identical Mhe 40 range leave www.inthe cubic point group 424 as additional independent component (duritica efficient possibedron, group 235. Comparing the five forms, and fixed that they have the quite simular: only the locar index class durit $d_{con} = d_{con} = d_{con}$ is



52 m



dolland i bolgiver C=a+b+c nol contribution E=g+h+i

G=n+o+p

 $O = \lambda + \mu + \nu$

components for a othic strike

D=d+e+fF=k+1+m H=q+r+s P=\xi+\pi+\rho





lost in the cubic point group 432. We have abbreviated it in Table XVIIa $I_{4^{A}}$ by $d_{xyyx} = a - b - c$. This difference might be of importance for an experimental check of Pauling's⁶⁰ opinion which refers to a cubic fundamental structure with regard to the 'so-called quasicrystals'. Measuring the elastic constants should provide 3 independent components for a cubic structure, but 2 for an icosahedral structure. These constants are described by a 4th rank tensor with the intrinsic symmetry

ρστυ

system	quasi- Laue	-	point group)	genera- ting	reps	ter	nsor of en rank	ten	sor of I rank
	class	Hermann- Mauguin	Schön- flies	abstract	elements		polar g	axial u	polar u	axial g
icosahedral		235	I	A ₅	C _{5z} +, C ₂	А	I _m A	I _m A	I _n A	I _n A
						F_1	$I_m^{F_1}$	$I_m^{F_1}$	$I_n^{\ F_1}$	$I_n^{F_1} \\$
					F_2	$I_m^{F_2}$	ImF2	$I_n^{F_2}$	$I_n^{F_2}$	
						G	$\mathbf{I}_{\mathbf{m}}^{\mathbf{G}}$	I_m^G	I_n^G	$\mathbf{I}_{\mathbf{n}}^{\mathbf{G}}$
						Н	\mathbf{I}_{m}^{H}	$\mathrm{I}_{m}{}^{\mathrm{H}}$	$\mathbf{I_n^H}$	$\mathbf{I}_{n}^{\mathbf{H}}$
		$\frac{2}{m}$ 3 5	I _h		C _{5z} +, C ₂ , I	Ag	I _m A		•	InA
		= 235 🐼 Ī				A _u	÷ .	$\mathbf{I}_{\mathbf{m}}^{\mathbf{A}}$	I_n^A	-
						F _{1g}	$\mathbf{I}_m^{F_1}$	C	-	I _n F1
						F_{1u}	$2^{(1)}$	$\mathbf{I_m^{F_1}}$	$\mathrm{I}_n^{F_1}$	-
						F _{2g}	$\mathbf{I}_m^{F_2}$	-	-	I _n F2
						F _{2u}	120-	$I_m^{\rm F2}$	$I_{\eta}F_{2}$	-
						•				

TABLE XV

Survey of the Icosahedron Point Groups 235 and (2/m) $\overline{35}$ and (3/m)

TABLE XVI

The Irreducible Tensor Forms of Rank 0 to 3 for the Point Groups 235 and (2/m) 35

TABLE XVIa

$\frac{2}{m}\overline{3}\overline{5}$					
	(1)] (2)	(3)	(1) (2)	(3)
$I_0^{r_*}(\bullet)_1$	(·) ₀	$I_0^{i_1}$ (·)	(\cdot)	$(\cdot)_0 \qquad \mathbf{I}_0^{F_2} \qquad (\cdot)$	(•)
$I_1^A \left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array} \right)_0$	$\begin{pmatrix} a \\ \cdot \\ \cdot \end{pmatrix}_{1\cdot 3}$	$\begin{bmatrix} I_1^{F_4} & & \\ & & \\ & & & \\ & & & \\ \end{bmatrix} \begin{pmatrix} \cdot \\ a \\ \cdot \end{pmatrix}$		$\left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{array} \right)_{0}^{*} \begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{array} \begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \end{array} \right)_{0}^{*} \begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \end{array} \left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \end{array} \right)$	с с (с) с с (с)
$I_2^A \left(\underbrace{\cdot \cdot \cdot}_{\cdot, \cdot} \right)_1$	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & -b \\ \cdot & b & \cdot \end{pmatrix}_{1}$	$\begin{array}{ccc} I_2^{F_1} & \begin{pmatrix} \cdot & \cdot & -b \\ \cdot & \cdot & \cdot \\ b & \cdot & \cdot \\ b & \cdot & \cdot \end{array} \end{array}$	$= \begin{pmatrix} \cdot & b & \cdot \\ -b & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}_{L}$	$\begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}_0 \qquad \qquad I_2^{F_2} \qquad \qquad (\cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	
	(a · · · · · · · · · · · · · · · · · ·	$ \begin{array}{c} I_{3,1}^{F_1}, & -a+b+c \\ -a+b+$	$ \begin{array}{c} & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & $	$\begin{pmatrix} d & \cdot & \cdot \\ & d & d \\ & d & \cdot \\ & - & - \\ & d & d \\ & 1 & \cdot & \cdot \\ & 1 & \cdot & \cdot \\ & - & - & - \\ & - & - & - \\ & - & - &$	$ \begin{array}{c} \mathbf{d} \\ \cdot \\ $

Table XVI to be continued

Table XVI continued has this apports resold according to be presented.

		(1) (·) ₀	(·)	(3) I ^G ₀ (·)	(4) (·)	
		$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}_0$	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix}$	$I_1^G \left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array} \right)$		
		$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}_0$	$\begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix}$	$ I_2^G \begin{pmatrix} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} $		
		$ \begin{pmatrix} \cdot & e & \cdot \\ e & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \hline e & \cdot & \cdot \\ e & \cdot & \cdot \\ \cdot & 3e & \cdot \\ \cdot & -4e \\ \hline - & - & - \\ \cdot & \cdot & -4e \\ \cdot & -4e & \cdot \\ \cdot & -4e & \cdot \\ \end{pmatrix}_{1:4} $	$ \begin{pmatrix} \cdot & 3e & 2e \\ 3e & \cdot & \cdot \\ 2e & \cdot & \cdot \\ \hline & - & - \\ 3e & \cdot & \cdot \\ \cdot & -3e & -2e \\ \cdot & -2e & \cdot \\ \hline & - & - \\ 2e & \cdot & \cdot \\ \cdot & -2e & \cdot \\ \cdot & \cdot & \cdot \end{pmatrix} $	$I_{3}^{G} \begin{pmatrix} -3e & \cdot & \cdot \\ \cdot & 3e & -2e \\ \cdot & -2e & \cdot \\ -2e & \cdot & -2e \\ \cdot & 3e & -2e \\ 3e & \cdot & \cdot \\ -2e & \cdot & -2e \\ \cdot & -2e & \cdot \\ -2e & \cdot & -2e \\ \cdot & \cdot & \cdot \end{pmatrix}$	$ \begin{pmatrix} 3e & \cdot & \cdot \\ \cdot & e & \cdot \\ \cdot & \cdot & -4e \\ \hline - & - & - \\ \cdot & e & \cdot \\ e & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ - & - & - \\ \cdot & \cdot & -4e \\ \cdot & \cdot & \cdot \\ -4e & \cdot & \cdot \end{pmatrix} $	
8 (m/C) 5				, 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		
(·) ₀		(•)	I ^H ₀ (·)	1	(4) (·)	(5)
$\left(\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}\right)_{0}$		(\cdot)	I_1^H (·)		(\cdot)	(\cdot)
~ ~ 0		(.)	· (.)		(.)	(.)
$\begin{pmatrix} c & \cdot & \cdot \\ \cdot & c & \cdot \\ \cdot & \cdot & -2c \end{pmatrix}$	1.5	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \sqrt{3}c \end{pmatrix}$	$I_2^{H} \begin{pmatrix} \cdot & - \cdot \\ -\sqrt{3}c \\ \cdot \end{pmatrix}$	$ \begin{bmatrix} \sqrt{3}c \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \qquad \begin{pmatrix} -\sqrt{2} \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} $	$ \begin{bmatrix} \cdot \\ \cdot \end{bmatrix} $	$\begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ -\sqrt{3}c \end{pmatrix}$

TABLE >	VII
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The Irreducible Tensor Forms of Rank 4 for the Point Groups 235 and (2/m) $\overline{35}$ TABLE XVIIa

 $\frac{2}{m}\overline{3}\overline{5}$

55					0)				0	2)			10	
A		. `	\ \	(.		· . ·)	$\mathbf{L}^{\mathbf{F}_1}$	(.		d	`	(.	-d	,
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	,	b			-a		1		·e			97		÷.	
1	10-1	1 Dec		_	1	_					_				_
	c		10-10			b	1	, i	10.0				-D		
a-b-c			-9-12				100		.3		в			-f	
		•	1000	c	•	ł	-	- 20		С					-A
0-5-	1 1	5	012	_	1	11	1.0	*							
	. 8	C			-b	3		1.00	D						
1	. d-	8-0	× .	-c		٠.	× .		ţŢ.	A				Ì.	-C
a-b-c	•						-	10 × 10 × 1			f			-B	
		·	240	1			1.0	÷					-	_	_
	a-b-c	0.0-	-	1.	21	·B				•			f		÷.
c							1.				b		1.	D	7
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	a	•				d							d		ŵ.
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· .	1.1	d-n		A		۰.		- 0		-0					C
1 - L		c	22		D			×.,	-b						
· .	a-b-c	2	5-6			f	3-6						в		
		-		_		_		-	_		_				_
		a-b-c			-B		- 24.4	in di	-f						
				-C						-A					
c	• .	•			1.						-D			-b	
		_				_			_		_		-	_	
				-A						-C					6
		a-b-c	8		-f .	4	8	. 1	-B						
· .	c					-D		- 1					b		
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		a			-d	.)	0		-d		.)				
1.405		. ,	3		-	. '	0.3								

A = b + c - d - e + fB = -a - b + dC = a - c + eD = -d - e + f

Table XVIIa to be continued

where square brackets indicate the exchangeability of indices. A possible influence of the twin-structure, however, has to be considered.

(ii) Comparision of 235 with 0^+ (3)

In this case we find, up to rank $\nu = 5$, for the total symmetric irreducible tensors an equal number of independent components, namely 6, up to rank

Table XVIIa continued

TABLE XVIIa

2 -	-			1743		antron and							
m 3	5	F		10				(2)				(3)	
AAR		I_{4}^{12}	(.	٠	•		(.	-a	-a))	(•	a	•)
			•	b	a	1	a-b	۰	• •		b-a	٠	•
			•	b-a	Ъ	I.	a-b	6	•		•		٠
				Greenad)	-		-	(-	0	
			•	С	a.		atc		•		-a-c		•
			A		•			-B	a			-B	•
			b-a	٠	. •	1	•	b-a	-b		. •	•	-D
		÷		(annexes)					-				
			•	-a-c	c		atc	٠	•				
	0		-a-c	•	•			-a-c	с		a	• •	С
		зà. "	-A		٠			A	•		. •	-b+c	•
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		-		-A	a		-B		•		B	· .	
		(2)	-c	•		. 8		a+c	a			a+c	
			b-a		×.	1		b-a	-b			•	D
			b					a-h	à			a-h	
						0.0		•	•		-2		
				a-b	-b		b-a	•					
				-	_			_					
		°. 1	-2-0	•				-2-0	C .		· · ·		C
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		~ 1	R		.	- ·		R	- 4			÷.	-b-c
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							-						
			-b	•	•	1	1:	b	• •		•	-2a+b	•
			•	b			b	•	• •		2a–b	•	•
		1	• •	•	•)	3.3	(.	٠	•)		(•	•	•)

.

A = 2a - b + c

 $\mathbf{B} = \mathbf{a} - \mathbf{b} + \mathbf{c}$ C = 2a - 2b + c operations that for a point D = -2a + b - 2c

a this care we find, up to rank V = 5, for the total symmetric breadening a an equal purcher of independent components, namely 6, up to make

TABLE XVIIb

$\begin{array}{c c c c c c c c c c c c c c c c c c c $		•				1					1			
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$		$\frac{2}{m}\overline{3}$	5 (1)		-	1	(2)			(3)	-		(4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	IG	(.	а	b)	<i>(</i> .	a-2b	3b-2a)	(-a	digite-		(-a		
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-4	a				a-2c				-E	3b-2a		а	-8
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		c		-090	2	3c-2a	ι.	. 1	and she	3c-2a	-Z		-ζ	
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$						1	-				_			
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			-a	d			σ	2a-3b	Δ			a		.'
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		•	b-c+d	02-d	-15	1. 22	2a-3c	τ	3c-2a	6-6-9	68 .×3	-δ	-	
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		· ·	β	•		1	-φ	χ	a			-η		
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		~	•	-b-d		•	ψ		ψ		· · ·			
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		a	•	•		σ				$-\Delta$	3b-2a		а	ε−2t
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		· · ·	-a	γ			ρ	2a-3b	$-\Delta$		1.1	a		
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\cdot \cdot \cdot $b+c-a$ \cdot $-Z-2a$ \cdot $4a-$				4(c-a)			b+c-a		Z+2a	÷	· · ·			
		•		۰.		b+c-a			· •	-Z-2a	m = 10		-	4a-4
4(b-a) · · · · · · · · · · · · · · · · · · ·		(4(b-a))		۰.) _{4·4}	(.		.)	(.		•)	(.	4a-4b	

Table XVIIb to be continued

5 an icosahedral quasicrystal thus behaves as completely isotropic. Ripamonti⁶⁵ supposed this to be only up to rank 5. Group theory allows calculation of the number of independent components for finite as well as for continuous point groups in a fairly easy manner. A 6th rank tensor shows 16 independent components in the icosahedron group whereas there are only 15 in the pure rotation group. From the 6th rank tensor on, an icosahedral quasicrystal thus does not behave as isotropic any longer. Ripamonti⁶⁵ points out that phonon--phason-coupling is described by a 6th rank tensor and the phason-phasoncoupling by a tensor of rank 8.50,54.66

le XVIIb continuel.

Table XVIIb continued

$$\begin{aligned} \alpha &= \frac{1}{4} (8a-3b-4c+d) & A &= \frac{1}{2} (4a-3b+d) \\ \beta &= \frac{1}{4} (-8a+7b+4c+3d) & B &= \frac{1}{2} (4a+b-4c+d) \\ \gamma &= -4a+2b+4c-d & \Gamma &= \frac{1}{2} (2a+b-4c+d) \\ \delta &= -4a+3b+3c-d & \Delta &= \frac{1}{2} (2a-3b+d) \\ \epsilon &= 4a-b-4c & E &= 3a-2b-2c \\ \zeta &= 4a-4b-c & Z &= -4a+2b+2c \\ \eta &= \frac{1}{4} (8a+3b-12c-d) \\ \theta &= \frac{1}{4} (8a+3b-12c-d) \\ \theta &= \frac{1}{4} (8a-13b+4c-d) \\ \iota &= \frac{1}{4} (-20a+13b+16c-3d) \\ \lambda &= 4a-3b-4c+d \\ \mu &= \frac{1}{4} (12a+b-16c+d) \\ \nu &= \frac{1}{4} (12a-15b+d) \\ \rho &= \frac{1}{2} (-6a+3b+4c-d) \\ \sigma &= \frac{1}{2} (-2a+b+d) \\ \tau &= 2(2a-b-c) \\ \varphi &= \frac{1}{4} (16a-9b-12c+3d) \\ \chi &= \frac{1}{2} (-b+4c-d) \\ \psi &= \frac{1}{2} (3b-d) \\ \omega &= \frac{1}{4} (4a-3b-3d) \end{aligned}$$

f) The Non-Total Symmetric Irreducible Representations

There are remarkably larger differences of the tensor forms of non-total symmetric irreducible representations for the classical, and pentagonal and icosahedral point groups, respectively. This originates in particular from the very much differentiated degeneracies. There are 4- and 5-fold degenerated representations in the icosahedron point groups e.g. which do not occur in classical point groups. This has also a severe influence on the number of

TABLE XVIIc

$\frac{2}{m}\overline{3}\overline{5}$	(1)		(2)				(3)		,	
									1Sg	
TH	(α · ·)	$3^{-1/2} x$ (. ε	ζ	$3^{-1/2}$ x	(.	τ	-e)	3. 1	
14	· a ·	1	ε · 3			φ				
	· · d		η .	•		-ε	•			
			<u>.</u>			_		_		
			ε · 3			Y		.		
			·	2c+f		· ~	ψ.	ε		
			· 2b+e			•	ε	-2a+4d		
	(0 = q + h)			_	100			_		
5 A 1818-1	1-1		θ.	•		-e				
			· 2a-4d				ε	-2b-e		
	f · ·			ι		•	-2c-f			
		1 .				· _				
			ε · 3			w.				
	h · · ·		·. –ε	κ			χ	ε		
stanta and a star	1 (.	1771	· 2c+g	· ·		•	3	-2a+4d		
	Carden of Com	1		-		_				
			·ε	λ		• • •	Ø.	ε		
for a second second	· α ·		-e •			τ	:	· ·		
			λ .	•		3				
	$\lambda + 1 = \lambda^{-1}$									
	$\mu=2\pi+2$		• 2c+g			•	з	-2b-e		
	1. 15 e		ĸ	•		ε		•		
	· f ·		• •	•		-2c-f	•	•		
	No. of the state		<u> </u>	_	1.1			_		
	· · σ		μ. •	•		-E	•	.		
			• 2a-4d	•		• •	ε	-2c-g		
	β··		·	ν		•	-κ			
		-		_		-		_		
		1.4	· 2b+e				з	-2c-g		
	g	2	c+f ∙	•		ε	·			
	····		· ·	•	×1	-κ	•	•		
	A	-		_		·		_		
	v · ·			ρ			$-\lambda$			
	· γ .					-λ		•		
	· · 8	(σ.	•)	(•	•	· ·)		
		7.5								
						m 11				
						Table	e X	vile to	be c	ontir

independent tensor components. All physical effects originating from non-total symmetric irreducible representations should, therefore, show characteristic differences in the pentagonal and icosahedral point groups. Phonon induced properties might play a role here. Phonons —when not totally symmetric cause a breakdown of symmetry so that properties may become allowed which do not exist in the 'static' crystal. New developments can be expected with vibrational spectroscopy in this context. The tables presented can be used a basis for further discussion.

Table XVIIc continued

	-)		(4)				(5)		
тH	$3^{-1/2} x$ (ω		. `	3 ^{-1/2}	-ε	•	.)	
14	2 J -		A	$-2a \pm 4d$	1.1.1		-λ	-~	
	2	,	C	20140					
			D			· .	c		
	_	g-f		-6		E			
		-ε	- 1			-2c-g			
		2.19						_	
	1.1.1.1.1.1		-e	-2b-e		•	$-\kappa$		$\alpha = a + b + c$
	1.5.000	-ε				-2c-g	•	·	B = b lo alfir
		-2c-f	•			·	•	•	p = -b + c - c + 1 + g
	1-65					_		-	$\gamma = -a + c + 4d + f + g$
			f-g	-ε		•	ε	-2c-f	$\delta = -2(a+b+2c+f+g)$
	1.00	-B				З	·		$\varepsilon = -c - f - g$
		-ε	•	•		-2b-e	•		$\zeta = a + b + 4c + 4d - e + 3f + 2g$
		-				-	-	-	n = a + 2b + 3c + 4d + e + f + 2e
	Aller Lar	-A	•			ε	•	•	
			-0)	ε		•	-8	-ξ	$\vartheta = 2a + b + 3c - 4d - e + 1 + 2g$
	-3	•0	3	2a-4d	1 1 3	•	-η	•	$\iota = 2a + 2b - 4d + e - f - 2g$
		-							$\kappa = b + c - e + f + g$
		-8	•	•		-2a+4d	•	•	$\lambda = a + c + 4d + f + g$
		-	З	2b+e			$-\vartheta$	•	u = 2a + 2b + 2c - 4d + e + f
		•	2c+f					-1	
			-	_		-		—	v = 2a + b + c - 4d - e - f
		•	-8	-2c-g			-2c-f		$\rho = a + 2b + c + 4d + e - f$
		3-		•		-2b-e			$\sigma = a + b + 2c + 4d - e + f$
		-ĸ	· •				* [•] /		$\tau = -a - b - 3c - 4d + e - 2f - f$
		-	-	-		-			a = -a - 2b - 2c - 4d - e - g
		-8				-2a+4d	·	÷	
	-		3	2c+g			-μ		$\chi = -2a - b - 2c + 4d + e - g$
			к					-v	$\psi = -2a - 2b - c + 4d - e + g$
		_	—	_		-			$\omega = -3a - 3b - 4c - f - g$
		-λ	•	•					A = -a + c + 8d + f + g
			٨	÷				-p	B = -b + c - 2e + f + g
		(.			/	(-0)	2 010 201115

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SAŽETAK

Ireducibilni tenzori točkinih grupa s peterokratnim rotacijskim osima

J. Brandmüller i R. Claus

U svrhu interpretacije vibracijskih spektara kristala (IR-apsorpcija, IR-refleksija, Ramanovo i hiper-Ramanovo raspršenje, stimulirano Ramanovo raspršenje i CARS) potrebni su ireducibilni tenzori ranga 1 do 3 za 32 klasične kristalografske točkine grupe. Otkriće kvazi-kristala navelo je na potrebu proračuna ovakvih ireducibilnih tenzora i za točkine grupe s peterokratnim rotacijskim osima. Oblik ireducibilnih tenzora ranga 1 do 4 bez intrinzičnih simetrija prikazan je tablično za sve ireducibilne reprezentacije pentagonskih točkinih grupa: 5, 5, 10, 10m2, 52 5m, 52m, te za dvije ikozaedarske točkine grupe: 235 i (2/m)35.