The Degeneracy, Selection Rules, and Other Properties of the Normal Vibrations of Certain Polyatomic Molecules

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The Degeneracy, Selection Rules, and Other Properties of the Normal Vibrations of Certain Polyatomic Molecules

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The number, degeneracies, and symmetries of the normal modes of vibration are given for molecules in which several atoms are bonded to a central atom. Ninety-nine symmetries, including all possible structures with three to seven atoms and the more important structures of eight and nine atoms are listed in tables. The selection rules for the Raman and infrared spectra are included as well as the polarization properties of the Raman lines and the rotational structure of the vibrational bands. In a number of more important cases figures are given showing the normal modes of vibration. Many examples of molecules which are believed to possess certain of the structures are included in the tables, together with references to experimental papers dealing with them.

IN drawing structural conclusions from observed Raman and infrared spectra, it is necessary to know the number of normal frequencies of vibration and the selection rules which characterize the various possible configurations of atoms. The theory of the number and degeneracy of the normal vibrations of symmetric molecules, first developed by Brester,[1] was very concisely expressed by Wigner,[2] using group theory, while the selection rules for the Raman and infrared have been discussed by Placzek,[3] Tisza[4] and others.

In order to provide a tabular presentation of the important results of these theories for a special class of molecules, so arranged that they may be used without any knowledge of group theory, the degeneracies, number of permitted Raman and infrared fundamentals, and the polarization properties of the Raman lines have been calculated for molecules in which two or more atoms (which may be identical or different) are attached to a single central atom. The treatment is intended to be complete up to six attached atoms; that is, every possible symmetry for such molecules is listed, even those which are not very reasonable physically. For molecules with seven and eight outer atoms, only a few of the more reasonable structures are given, since there are very few molecules of these classes known and a very large number of possible symmetries.

The group-theoretical method used to find the number and degeneracies of the normal vibrations was described in a previous paper,[5] where it was used to obtain the normal coordinates and frequency formulas for benzene. The selection rules have also been obtained by the application of group theory[4] and the results checked wherever possible with the table given by Placzek.[3] (The following divergences from his results were found: p. 81 of the English translation,[6] point group S_{pu}, line labelled B_1, fifth column, read "all zero but C_{xy}"; line labelled B_2, fifth column, "all zero but $C_{xx} = -C_{yy}$"; line labelled C, fifth column, "$C_{xy} = C_{ii} = 0$"; line labelled D, sixth column, "$C_{xx} = -C_{yy}$, $C_{ii} = 0$.")

In using these results in connection with experimentally observed spectra, it is necessary to take certain precautions. Thus the number of Raman lines found may not coincide with that theoretically required for two reasons: first, lines which are not forbidden by symmetry restrictions may still be so weak that they do not appear under ordinary conditions, and second, overtones and combinations may occur in special cases. The latter difficulty is one which is rather frequently observed in spite of the fact that overtones and combinations should be much less important in Raman spectra than in infrared spectra. Another phenomenon which sometimes

[1] C. J. Brester, Kristallsymmetrie und Reststrahlen, Utrecht, 1923; Zeits. f. Physik **24**, 324 (1924).

[2] E. Wigner, Gott. Nach. 133 (1930).

[3] G. Placzek, *Leipziger Vorträge*, p. 71, 1931; Zeits. f. Physik **70**, 84 (1931). G. Placzek and E. Teller, Zeits. f. Physik **81**, 209 (1933).

[4] L. Tisza, Zeits. f. Physik **82**, 48 (1933).

[5] E. Bright Wilson, Jr., Phys. Rev. **45**, 706 (1934).

[6] P. Debye, *The Structure of Molecules*, Blackie and Sons, Ltd., London, 1932.

occurs, for example in CO_2 and CCl_4, and which causes deviations from the simple selection rules, is quantum-mechanical resonance between certain of the energy states of the molecule due to accidental coincidence or approximate coincidence of the levels corresponding to different types of vibration. This effect usually allows otherwise forbidden lines to appear in the spectrum, but it is probably not very common.

Explanation of Tables

The results are given in separate tables, arranged according to the number of atoms in the molecule. Thus Table I lists triatomic molecules of the type AB_2 and ABB', Table II includes AB_3, AB_2B', and $ABB'B''$, etc. A is not equivalent by symmetry to any of the B's (although it may be an atom of the same element, as for example in N−N−O).

The numbering, given in the first column of the tables, is designed to indicate the number and character of the attached atoms. The figure in front of the dot gives the total number of attached atoms while the figures following the dot indicate the numbers of symmetrically related atoms. Thus 6.6 means that the molecule is AB_6 in which all six B atoms are equivalent from a symmetry standpoint. 6.42 refers to AB_4B_2', etc. When there are several molecules of the same type but of different symmetries, they are distinguished by using a, b, c, etc. The name, given in the second column, is meant to be descriptive enough to characterize the structure if possible, but in addition the coordinates of the atoms are given under the discussion of each type. The notation R and L following the name of a structure indicates that right and left-handed forms are possible.

The column labelled I gives the point-group symmetry of the structure, the symbols being those of Schönflies,[7] which represent the axes, planes and other elements of symmetry possessed by the molecule. The column headed II tells whether the molecule is a linear rotator L, a spherical top Sp (which has three equal moments of inertia), a symmetric top S (with one distinct and two equal moments of inertia), or an asymmetric top A (which has three unequal moments of inertia).

The columns labelled ν_1, ν_2, ν_3 contain the number of singly, doubly, and triply degenerate normal frequencies of vibration. Only molecules with cubic point-group symmetries can have triply degenerate frequencies. Under R is listed the number of fundamental frequencies of vibration which are allowed to appear in the Raman spectrum, although a line so permitted may be of very small intensity. Following this number, in parentheses, is the number of these Raman fundamentals which have the special depolarization $\rho=\frac{3}{4}$, when plane polarized incident light is used. ρ is the ratio of the intensities of the perpendicular and parallel components of the scattered light. For unpolarized incident light this becomes $\rho=6/7$.

Under I.R. is given the number of fundamental frequencies which are active in the infrared absorption spectra, the figures in parentheses being the number of these bands which are of the || type[8] if the molecule is a symmetric top. Finally, the last column tabulates the symmetries of the possible normal vibrations, the degrees of the factors into which the secular equation for the normal coordinate problem may be factored by the use of the symmetry of the molecule, the degeneracies of these vibrations, and the ones which are active in the Raman and infrared spectra. To illustrate: 2^{R}, 0, 2^{RI}, 1^{R}, $2_2{}^{RI}$ after 4.4d means that there are two frequencies with the symmetry of Γ_1 or A_1, the first irreducible representation of the point-group V_d, none with symmetry Γ_2 or A_2, two with Γ_3 or B_2, one with Γ_4 or B_1, and two doubly degenerate frequencies with symmetry Γ_5 or E_1, the degeneracy being indicated by the subscript. The meaning of the term "irreducible representation" is explained in the paper on benzene already referred to.[5] The order Γ_1, Γ_2, etc. is that used by Wigner[2] in his tabulation of the irreducible representations of the crystallographic point groups. Several point groups which do not occur in crystallography were used: namely $D_{\infty h}$, $C_{\infty v}$, D_{5h}, C_{5v}, C_{7h}, C_{7v}, C_{8h}, C_{8v} and D_{4d}, the characters for their irreducible representations being taken from the general tables given by Tisza.[4]

[7] H. Hilton, *Mathematical Crystallography*, Chapters V, VI. Oxford, 1903.

[8] D. M. Dennison, Rev. Mod. Phys. **3**, 314 (1931).

The numbers with superscript R indicate the frequencies which are active in the Raman spectrum while a superscript I on a number means that this frequency is infrared active. The numbers themselves, besides the significance given to them above, also represent the degrees of the factors of the factored secular equation. For the linear molecules, to which Wigner's tables do not apply, the notation of Tisza[4] is used for the irreducible representations.

Discussion of Results

In the discussion of individual cases which is given below, the number and name of the structure is followed by the Cartesian coordinates of the different atoms, with A always at the origin. u, v, w represent parameters which are not fixed by the symmetry, while the letter o has been printed instead of zero. These were mostly taken from a tabulation by Nowacki[9] of the equivalent positions for the point-groups. (Two slight misprints were found in this paper; namely, in Table III, p. 28, after $D_{2d} \equiv V$ (4) the second line should read $|xxz|\bar{x}x\bar{z}|\bar{x}\bar{x}z|x\bar{x}\bar{z}|$ (C_s). After D_{3d} (6) (b) the second line should read $|\bar{x}0x\bar{z}|x\bar{x}0\bar{z}|0x\bar{x}\bar{z}|$ (C_s).) Wherever possible examples are given of molecules which have been found or which might be supposed to belong to the given type. In a number of examples which seem likely to be of importance and which, so far as I know, have not been previously treated, figures are given showing the normal vibrations, derived from the symmetry restrictions yielded by the group theory. The order used in the diagrams is the same as that in the last column of the tables. Only one representative of a set of degenerate vibrations is shown. An example is Fig. 2 which shows the normal vibrations for 5.32a, the trigonal bipyramid model of AB_3B_2'. The last column of Table IV reads: 2^R, 0, $3_2{}^{RI}$; 0, 2^I, $1_2{}^R$. Therefore the first two motions of Fig. 2, labelled ν_1 and ν_2, belong to Γ_1 or A_1', the first irreducible representation of Wigner's table for D_{3h}, and since 2^R has the superscript R, they are Raman active. The next three motions, ν_3', ν_4', ν_5' belong to Γ_3 or E_1'. They are active in both the Raman and infrared spectra and are doubly degenerate; i.e., for each of them there exists another similar motion with the same frequency, differing only in spatial orientation of the directions of motion. The primes on the ν's indicate that to obtain the three true normal vibrations these three motions enclosed in the square brackets must be compounded with proportions determined by the force constants.

Many of the simpler structures listed in Tables I–VII have been previously studied, and although it is impracticable to give all the references it is hoped that those listed will enable the others to be found.

I am very much indebted to Professor Linus Pauling for many valuable suggestions in connection with this paper.

Table I. *Molecules with three atoms.*

No.	Name	I	II	ν_1	ν_2	R	I.R.	Irreducible representations
2.2a	Symmetrical collinear	$D_{\infty h}$	L	2	1	1(0)	2	$A_{1g}{}^R$, $A_{2u}{}^I$, $E_{1u}{}^I$(2).
2.2b	Symmetrical bent	C_{2v}	A	3		3(1)	3	2^{RI}, 0, 0, 1^{RI}.
2.11a	Unsymmetrical collinear	$C_{\infty v}$	L	2	1	3(1)	3	$2A_1{}^{RI}$, $E_1{}^{RI}$(2).
2.11b	Unsymmetrical bent	C_s	A	3		3(0)	3	3^{RI}, 0.

Molecules with Three Atoms

2.2a. Symmetrical collinear. B : oow, oo$\bar{w}$. CO_2,[10, 11] CS_2.[10, 12] Normal coordinates.[10]

2.2b. Symmetrical bent. B : uow, $\bar{u}$ow. H_2O,[10] SO_2,[10] H_2S.[10] Normal coordinates.[10]

2.11a. Unsymmetrical collinear. B : oow. B′ : oow′. N_2O,[10, 13] COS.[14] Normal coordinates.[10]

2.11b. Unsymmetrical bent. B : uow. B′ : u′ow′. H^1H^2O,[15] H^1H^2S. Normal coordinates.[10, 16]

[9] W. Nowacki, Zeits. f. Kristallographie (A) **86**, 19 (1933).

[10] K. W. F. Kohlrausch, *Der Smekal-Raman-Effekt*, Springer, Berlin, 1931, pp. 169–186.

[11] A. Adel and D. M. Dennison, Phys. Rev. **44**, 99 (1933).

[12] G. Placzek, reference 6, p. 88.

[13] E. K. Plyler and E. F. Barker, Phys. Rev. **38**, 1827 (1931).

[14] C. R. Bailey and A. B. D. Cassie, Proc. Roy. Soc. **A135**, 375 (1932).

[15] R. W. Wood, Nature **132**, 970 (1933).

[16] P. C. Cross and J. H. Van Vleck, J. Chem. Phys. **1**, 350 (1933).

TABLE II. *Molecules with four atoms.*

No.	Name	I	II	ν_1	ν_2	R	I.R.	Irreducible representations
3.3a	Plane equilateral triangle	D_{3h}	S	2	2	3(2)	3(1)	1^R, 0, $2_2{}^{RI}$; 0, 1^I, 0.
3.3b	Regular pyramid	C_{3v}	S	2	2	4(2)	4(2)	2^{RI}, 0, $2_2{}^{RI}$.
3.21a	Plane isosceles triangle	C_{2v}	A	6		6(3)	6	3^{RI}, 1^{RI}, 0, 2^{RI}.
3.21b	Pyramid	C_s	A	6		6(2)	6	4^{RI}, 2^{RI}.
3.111a	Linear	$C_{\infty v}$	L	3	2	5(2)	5	$3A_1{}^{RI}$, $2E_1{}^{RI}(2)$.
3.111b	Plane scalene triangle	C_s	A	6		6(1)	6	5^{RI}, 1^{RI}.
3.111c	Pyramid (R+L)	C_1	A	6		6(0)	6	6^{RI}.

MOLECULES WITH FOUR ATOMS

3.3a. Plane equilateral triangle. B : (ovo)$(\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{o})(-\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{o})$. $CO_3{}^{--}$,[17] $NO_3{}^-$.[17] Normal coordinates.[17, 18]

3.3b. Regular pyramid. B : (o, v, w)$(\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{w})(-\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{w})$. NH_3,[19] $AsCl_3$,[17, 20] PCl_3,[17, 20] AsF_3,[20] etc.[21] Normal coordinates.[17]

3.21a. Plane isosceles triangle. B : uvo, ūvo. B′ : ov′o. H_2CO.[22] Approximate normal coordinates.[22, 23]

3.21b. Pyramid with isosceles base. B : uvw, ūvw. B′ : ov′w′. PCl_2Br,[24] $PClBr_2$,[24] NH_2Cl.

3.111a. Linear. B : oow. B′ : oow′. B″ : oow″.

3.111b. Plane scalene triangle. B : uvo. B′ : u′v′o. B″ : u″v″o. H^1H^2CO.

3.111c. Pyramid with scalene base. B : uvw. B′ : u′v′w′. B″ : u″v″w″.

TABLE III. *Molecules with five atoms.*

No.	Name		I	II	ν_1	ν_2	ν_3	R	I.R.	Irreducible representations
4.4a	Regular tetrahedron		T_d	Sp	1	1	2	4(3)	2	1^R, 0, $1_2{}^R$, $2_3{}^{RI}$, 0.
4.4b	Plane square		D_{4h}	S	5	2		3(2)	3(1)	1^R, 0, 1^R, 1^R, 0; 0, 1^I, 0, 1, $2_2{}^I$.
4.4c	Square pyramid		C_{4v}	S	5	2		7(5)	4(2)	2^{RI}, 0, 2^R, 1^R, $2_2{}^{RI}$.
4.4d	Tetragonal sphenoid		V_d	S	5	2		7(5)	4(2)	2^R, 0, 2^{RI}, 1^R, $2_2{}^{RI}$.
4.4e	Plane rectangle		V_h	A	9			3(1)	5	2^R, 0, 1^R, 0; 1, 2^I, 1^I, 2^I.
4.4f	Orthorhombic sphenoid	(R+L)	V	A	9			9(6)	6	3^R, 2^{RI}, 2^{RI}, 2^{RI}.
4.4g	Rectangular pyramid		C_{2v}	A	9			9(6)	7	3^{RI}, 2^{RI}, 2^R, 2^{RI}.
4.31a	Trigonal pyramid		C_{3v}	S	3	3		6(3)	6(3)	3^{RI}, 0, $3_2{}^{RI}$.
4.22a	Linear		$D_{\infty h}$	L	4	3		3(1)	4	$2A_{1g}{}^R$, $2A_{2u}{}^I$, $E_{1g}{}^R(2)$, $2E_{1u}{}^I(2)$.
4.22b	Plane rhombus		V_h	A	9			3(1)	6	2^R, 0, 1^R, 0; 0, 2^I, 2^I, 2^I.
4.22c	Plane trapezoid		C_{2v}	A	9			9(5)	8	4^{RI}, 1^{RI}, 1^R, 3^{RI}.
4.22d	Rhombic pyramid		C_{2v}	A	9			9(5)	8	4^{RI}, 2^{RI}, 1^R, 2^{RI}.
4.22e	Plane parallelogram		C_{2h}	A	9			3(0)	6	3^R, 0, 2^I, 4^I.
4.22f	Trapezoidal pyramid		C_s	A	9			9(4)	9	5^{RI}, 4^{RI}.
4.22g	Monoclinic sphenoid	(R+L)	C_2	A	9			9(4)	9	5^{RI}, 4^{RI}.
4.211a	Plane		C_{2v}	A	9			9(5)	9	4^{RI}, 2^{RI}, 0, 3^{RI}.
4.211b	Monoclinic sphenoid		C_s	A	9			9(3)	9	6^{RI}, 3^{RI}.
4.1111a	Linear		$C_{\infty v}$	L	4	3		7(3)	7	$4A_1{}^{RI}$, $3E_1{}^{RI}(2)$.
4.1111b	Plane		C_s	A	9			9(2)	9	7^{RI}, 2^{RI}.
4.1111c	General	(R+L)	C_1	A	9			9(0)	9	9^{RI}.

MOLECULES WITH FIVE ATOMS

4.4a. Regular tetrahedron. B : www, w̄ww̄, w̄w̄w, ww̄w̄. CCl_4,[25] CBr_4,[25] $SiCl_4$,[25] etc. Normal coordinates.[25, 26]

4.4b. Plane square. B : woo, owo, w̄oo, ow̄o. $PtCl_4{}^{--}$, $PdCl_4{}^{--}$.

4.4c. Pyramid with square base. B : wov, owv, w̄ov, ow̄v. SCl_4, $TeCl_4$. Normal coordinates.[27]

4.4d. Tetragonal sphenoid. B : wwv, w̄wv̄, w̄w̄v, ww̄v̄.

4.4e. Plane rectangle. B : uvo, ūv̄o, ūvo, uv̄o.

4.4f. Orthorhombic sphenoid. B : uvw, uv̄w̄, ūvw̄, ūv̄w.

4.4g. Pyramid with rectangular base. B : uvw, ūv̄w, ūvw, uv̄w.

4.31. Trigonal pyramid. B : (o, v, w)$(\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{w})(-\frac{1}{2}\sqrt{3}\text{v}, -\frac{1}{2}\text{v}, \text{w})$. B′ : oow″. CH_3Cl,[28] CH_3Br,[28] etc.

[17] Kohlrausch, reference 10, pp. 195–205.

[18] H. H. Nielsen, Phys. Rev. **32**, 773 (1928).

[19] C. M. Lewis and W. V. Houston, Phys. Rev. **44**, 903 (1933).

[20] D. M. Yost and J. E. Sherborne, J. Chem. Phys. **2**, 125 (1934).

[21] J. H. Hibben, Chem. Rev. **13**, 345 (1933).

[22] Kohlrausch, reference 10, pp. 211–212.

[23] F. Matossi and H. Aderhold, Zeits. f. Physik **68**, 683 (1931).

[24] B. Trumpy, Zeits. f. Physik **68**, 675 (1931).

[25] Kohlrausch, reference 10, pp. 212–218.

[26] D. M. Yost, C. C. Steffens and S. T. Gross, J. Chem. Phys. **2**, 311 (1934).

[27] V. Guillemin, Ann. d. Physik **81**, 173 (1926).

[28] Kohlrausch, reference 10, p. 208.

4.22a. Linear. B : oow, oo$\bar{w}$. B′ : oow′, oo$\bar{w}$′. C_3O_2.[29]

4.22b. Plane rhombus. B : uoo, ūoo. B′ : ov′o, o$\bar{v}$′o.

4.22c. Plane regular trapezoid. B : uvo, ūvo. B′ : u′v′o, ū′v′o.

4.22d. Rhombic pyramid. B : uow, ūow. B′ : ov′w′, o$\bar{v}$′w′. If the two B′ atoms are placed above A with 2B below, this structure is a distorted tetrahedron. CH_2Cl_2,[30] CF_2Cl_2.[31]

4.22e. Plane parallelogram. B : uvo, ū$\bar{v}$o. B′ : u′v′o, ū′$\bar{v}$′o.

4.22f. Pyramid with trapezoidal base. B : uvw, ūvw. B′ : u′v′w′, ū′v′w′.

4.22g. Monoclinic sphenoid. B : uvw, ū$\bar{v}$w. B′ : u′v′w′, ū′$\bar{v}$′w′. If B and B′ are on same side of A this is a pyramid with a parallelogram for a base.

4.211a. Plane. B : uow, ūow. B′ : oow′. B″ : oow″. CH_2CO.

4.211b. Monoclinic sphenoid. B : uvw, uv$\bar{w}$. B′ : u′v′o. B″ : u″v″o. $CHFCl_2$.[31]

4.1111a. Linear. B : oow. B′ : oow′. B″ : oow″. B‴oow‴.

4.1111b. Plane. B : uvo. B′ : u′v′o. B″ : u″v″o. B‴ : u‴v‴o.

4.1111c. General. No symmetry.

TABLE IV. *Molecules with six atoms.*

No.	Name	I	II	ν_1	ν_2	R	I.R.	Irreducible representations
5.5a	Plane pentagon	D_{5h}	S	2	5	3(2)	3(1)	1^R, 0, 2_2^I, 2_2^R; 1^I, 0, 0, 1_2.
5.5b	Pentagonal pyramid	C_{5v}	S	2	5	7(5)	4(2)	2^{RI}, 0, 2_2^{RI}, 3_2^R.
5.41a	Square pyramid	C_{4v}	S	6	3	9(6)	6(3)	3^{RI}, 0, 2^R, 1^R, 3_2^{RI}.
5.41b	Rectangular pyramid	C_{2v}	A	12		12(8)	10	4^{RI}, 3^{RI}, 2^R, 3^{RI}.
5.32a	Trigonal bipyramid	D_{3h}	S	4	4	6(4)	5(2)	2^R, 0, 3_2^{RI}; 0, 2^I, 1_2^R.
5.311a	Polar trigonal bipyramid	C_{3v}	S	4	4	8(4)	8(4)	4^{RI}, 0, 4_2^{RI}.
5.221a	Plane	C_{2v}	A	12		12(7)	11	5^{RI}, 4^{RI}, 1^R, 2^{RI}.
5.221b	Triangular bipyramid	C_{2v}	A	12		12(7)	11	5^{RI}, 3^{RI}, 1^R, 3^{RI}.
5.221c	Trapezoidal pyramid	C_s	A	12		12(5)	12	7^{RI}, 5^{RI}.
5.221d	(R+L)	C_2	A	12		12(6)	12	6^{RI}, 6^{RI}.
5.2111a	Triangular bipyramid	C_s	A	12		12(4)	12	8^{RI}, 4^{RI}.
5.11111a	Linear	$C_{\infty v}$	L	5	4	9(4)	9	$5A_1^{RI}$, $4E_1^{RI}(2)$.
5.11111b	Plane	C_s	A	12		12(3)	12	9^{RI}, 3^{RI}.
5.11111c	General (R+L)	C_1	A	12		12(0)	12	12^{RI}.

MOLECULES WITH SIX ATOMS

5.5a. Plane pentagon. B : (o, v, o)(av, bv, o)(cv, −dv, o)(−cv, −dv, o)(−av, bv, o). Here a=sin 72°, b=cos 72°, c=sin 36°, d=cos 36°.

5.5b. Pentagonal pyramid. B : (o, v, w)(av, bv, w)(cv, −dv, w)(−cv, −dv, w)(−av, bv, w). a, b, c, d as in 5.5a.

5.41a. Square pyramid. B : uuw, uūw, ūūw, ūuw. B′ : oow′. PF_5.[32] Modes of vibration, Fig. 1.

5.41b. Rectangular pyramid. B : uvw, ū$\bar{v}$w, ūvw, u$\bar{v}$w. B′ : oow′.

5.32a. Trigonal bipyramid. B : (o, v, o)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o). B′ : (oow′)(oo$\bar{w}$′). PF_3Cl_2. Modes of vibration, Fig. 2.

5.311a. Polar trigonal bipyramid. B : (o, v, w)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w). B′ : (oow′). B″ : (oow″). PF_3ClI, CH_3CN.

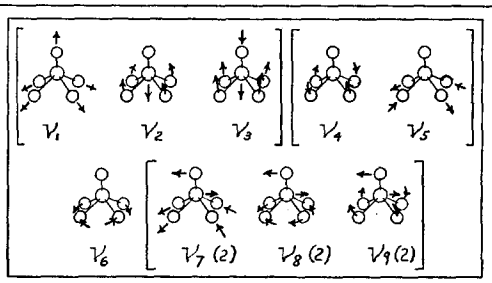

FIG. 1. Modes of vibration of 5.41a, square pyramid. Bracketed motions must be combined to give true modes.

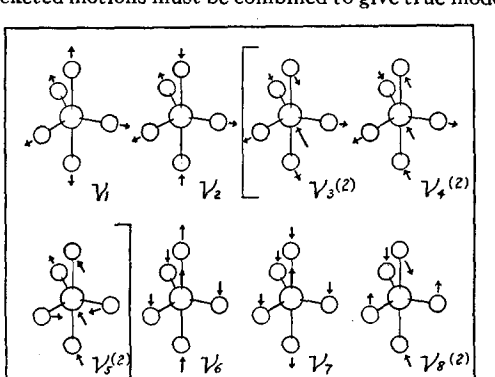

FIG. 2. Modes of vibration of 5.32a, trigonal bipyramid. Bracketed motions must be combined to give true modes.

[29] L. O. Brockway and Linus Pauling, Proc. Nat. Acad. Sci. 19, 860 (1933).

[30] Kohlrausch, reference 10, p. 305.

[31] C. A. Bradley, Jr., Phys. Rev. 40, 908 (1932).

[32] L. O. Brockway. Private communication. Electron diffraction studies give this structure for PF_5.

5.221a. Plane. B : uow, ūow. B′ : u′ow′, ū′ow′. B″ : oow″.

5.221b. Triangular bipyramid. B : uow, ūow. B′ : ov′w′, ov̄′w′. B″ : oow″.

5.221c. Trapezoidal pyramid. B : uvw, uvw̄. B′ : u′v′w′, u′v′w̄′. B″ : u″v″o.

5.221d. B : uvw, ūv̄w. B′ : u′v′w′, ū′v̄′w′. B″ : oow″.

5.2111a. Triangular bipyramid. B : uvw, uvw̄. B′ : u′v′o. B″ : u″v″o. B‴ : u‴v‴o.

5.11111a. Linear. $B^{(i)}$: oow_i.

5.11111b. Plane. $B^{(i)}$: u_iv_io.

5.11111c. General. No symmetry.

TABLE V. *Molecules with seven atoms.*

No.	Name		I	II	ν_1	ν_2	ν_3	R	I.R.	Irreducible representations
6.6a	Regular octahedron		O_h	Sp	1	1	4	3(2)	2	1^R, 0, $1_2{}^R$, $1_3{}^R$, 0; 0, 0, 0, 1_3, $2_3{}^I$.
6.6b	Regular plane hexagon		D_{6h}	S	5	5		3(2)	3(1)	1^R, 0, 0, 1, $2_2{}^R$, 0; 0, 1^I, 1, 1, 1_2, $2_2{}^I$.
6.6c	Hexagonal pyramid		C_{6v}	S	5	5		7(5)	4(2)	2^{RI}, 0, 2, 1, $3_2{}^R$, $2_2{}^{RI}$.
6.6d	Trigonal prism		D_{3h}	S	5	5		7(5)	5(2)	2^R, 0, $3_2{}^{RI}$; 1, 2^I, $2_2{}^R$.
6.6e	Trigonal plane hexagon		D_{3h}	S	5	5		7(5)	5(1)	2^R, 1, $4_2{}^{RI}$; 1, 1^I, $1_2{}^R$.
6.6f	Twisted trigonal prism		D_{3d}	S	5	5		4(2)	5(2)	2^R, 0, $2_2{}^R$; 2^I, 1, $3_2{}^I$.
6.6g	Twisted trigonal prism	(R+L)	D_3	S	5	5		8(5)	7(2)	3^R, 2^I, $5_2{}^{RI}$.
6.6h	Trigonal hexangular pyramid		C_{3v}	S	5	5		8(5)	8(3)	3^{RI}, 2, $5_2{}^{RI}$.
6.51a	Pentagonal pyramid		C_{5v}	S	3	6		9(6)	6(3)	3^{RI}, 0, $3_2{}^{RI}$, $3_2{}^R$.
6.42a	Tetragonal octahedron		D_{4h}	S	7	4		5(3)	5(2)	2^R, 0, 1^R, 1^R, $1_2{}^R$; 0, 2^I, 0, 1, $3_2{}^I$.
6.42b			V_d	S	7	4		11(8)	7(3)	3^R, 0, 3^{RI}, 1^R, $4_2{}^{RI}$.
6.42c	Rectangular bipyramid		V_h	A	15			6(3)	8	3^R, 1^R, 1^R, 1^R; 1, 3^I, 2^I, 3^I.
6.42d	Plane		V_h	A	15			6(3)	8	3^R, 1^R, 2^R, 0; 1, 3^I, 2^I, 3^I.
6.42e		(R+L)	V	A	15			15(11)	11	4^R, 4^{RI}, 3^{RI}, 4^{RI}.
6.42f			C_{2v}	A	15			15(10)	12	5^{RI}, 3^{RI}, 3^R, 4^{RI}.
6.42g			C_{2h}	A	15			6(2)	9	4^R, 2^R, 4^I, 5^I.
6.411a	Polar tetragonal octahedron		C_{4v}	S	7	4		11(7)	8(4)	4^{RI}, 0, 2^R, 1^R, $4_2{}^{RI}$.
6.411b	Polar rectangular bipyramid		C_{2v}	A	15			15(10)	13	5^{RI}, 4^{RI}, 2^R, 4^{RI}.
6.33a	Plane		D_{3h}	S	5	5		7(5)	6(2)	2^R, 1, $4_2{}^{RI}$; 0, 2^I, $1_2{}^R$.
6.33b	Plane		C_{3h}	S	5	5		8(5)	6(2)	3^R, 4^{RI}, 4^{RI}; 2^I, 1^R, 1^R.
6.33c	Pyramid or prism		C_{3v}	S	5	5		9(5)	9(4)	4^{RI}, 1, $5_2{}^{RI}$.
6.33d	Pyramid or prism	(R+L)	C_3	S	5	5		10(5)	10(5)	5^{RI}, 5^{RI}, 5^{RI}.
6.3111a	Trigonal bipyramid		C_{3v}	S	5	5		10(5)	10(5)	5^{RI}, 0, $5_2{}^{RI}$.
6.222a	Linear		$D_{\infty h}$	L	6	5		5(2)	6	$3A_{1g}{}^R$, $3A_{2u}{}^I$, $3E_{1u}{}^I$, $2E_{1g}{}^R$.
6.222b	Orthorhombic octahedron		V_h	A	15			6(3)	9	3^R, 1^R, 1^R, 1^R; 0, 3^I, 3^I, 3^I.
6.222c	Trapezoidal bipyramid		C_{2v}	A	15			15(9)	13	6^{RI}, 4^{RI}, 2^R, 3^{RI}.
6.222d	Plane		C_{2h}	A	15			6(1)	9	5^R, 1^R; 3^I, 6^I.
6.222e	Monoclinic octahedron		C_{2h}	A	15			6(2)	9	4^R, 2^R, 3^I, 6^I.
6.222f	Triangular prism		C_s	A	15			15(7)	15	8^{RI}, 7^{RI}.
6.222g	Monoclinic octahedron	(R+L)	C_2	A	15			15(7)	15	8^{RI}, 7^{RI}.
6.222h	Triclinic octahedron		C_i	A	15			6(0)	9	6^R, 9^I.
6.2211a	Orthorhombic octahedron		C_{2v}	A	15			15(9)	14	6^{RI}, 4^{RI}, 1^R, 4^{RI}.
6.2211b	Heptahedron		C_s	A	15			15(6)	15	9^{RI}, 6^{RI}.
6.2211c	Monoclinic octahedron	(R+L)	C_2	A	15			15(8)	15	7^{RI}, 8^{RI}.
6.21111a			C_s	A	15			15(5)	15	10^{RI}, 5^{RI}.
6.111111a	Linear		$C_{\infty v}$	L	6	5		11(5)	11	$6A_1{}^{RI}$, $5E_1{}^{RI}$.
6.111111b	Plane		C_s	A	15			15(4)	15	11^{RI}, 4^{RI}.
6.111111c	General		C_1	A	15			15(0)	15	15^{RI}.

MOLECULES WITH SEVEN ATOMS

6.6a. Regular octahedron. B : uoo, ūoo, ouo, oūo, oou, ooū. SF_6[26], SeF_6[26], TeF_6[26]. Modes of vibration, Fig. 3. Normal frequencies.[26]

6.6b. Regular plane hexagon. B : (o, v, o)$(\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, o)(\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, o)$(o, v̄, o)$(-\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, o)(-\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, o)$.

6.6c. Hexagonal pyramid. B : (ovw)$(\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, w)(\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)$(o, v̄, w)$(-\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)(-\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, w)$.

6.6d. Trigonal prism. B : (o, v, w)$(\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)(-\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)$(o, v, w̄)$(\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w̄)(-\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w̄)$.

6.6e. Trigonal plane hexagon. B : (ū, v, o)(u, v, o)$(\frac{1}{2}\sqrt{3}v+\frac{1}{2}u, -\frac{1}{2}v+\frac{1}{2}\sqrt{3}u, o)(\frac{1}{2}\sqrt{3}v-\frac{1}{2}u, -\frac{1}{2}v-\frac{1}{2}\sqrt{3}u, o)(-\frac{1}{2}\sqrt{3}v+\frac{1}{2}u, -\frac{1}{2}v-\frac{1}{2}\sqrt{3}u, o)(-\frac{1}{2}\sqrt{3}v-\frac{1}{2}u, -\frac{1}{2}v+\frac{1}{2}\sqrt{3}u, o)$.

6.6f. Twisted trigonal prism. B : (o, v, w)$(\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)(-\frac{1}{2}\sqrt{3}v, -\frac{1}{2}v, w)$(o, v̄, w̄)$(-\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, w̄)(\frac{1}{2}\sqrt{3}v, \frac{1}{2}v, w̄)$.

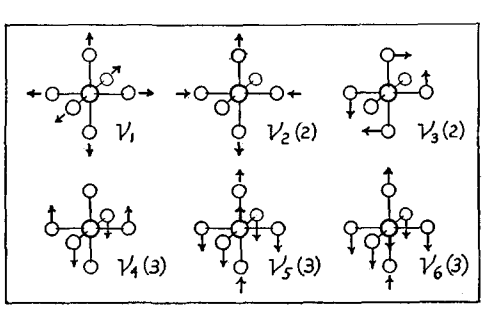

FIG. 3. Modes of vibration of 6.6a, regular octahedron.

6.6g. Twisted trigonal prism. B : (ū, v, w)(u, v, w̄)($\frac{1}{2}\sqrt{3}$v+$\frac{1}{2}$u, $-\frac{1}{2}$v+$\frac{1}{2}\sqrt{3}$u, w)($\frac{1}{2}\sqrt{3}$v−$\frac{1}{2}$u, $-\frac{1}{2}$v−$\frac{1}{2}\sqrt{3}$u, w̄)($-\frac{1}{2}\sqrt{3}$v+$\frac{1}{2}$u, $-\frac{1}{2}$v−$\frac{1}{2}\sqrt{3}$u, w)($-\frac{1}{2}\sqrt{3}$v−$\frac{1}{2}$u, $-\frac{1}{2}$v+$\frac{1}{2}\sqrt{3}$u, w̄).

6.6h. Trigonal hexangular pyramid. B : (ū, v, w)(u, v, w)($\frac{1}{2}\sqrt{3}$v+$\frac{1}{2}$u, $-\frac{1}{2}$v+$\frac{1}{2}\sqrt{3}$u, w)($\frac{1}{2}\sqrt{3}$v −$\frac{1}{2}$u, $-\frac{1}{2}$v−$\frac{1}{2}\sqrt{3}$u, w)($-\frac{1}{2}\sqrt{3}$v+$\frac{1}{2}$u, $-\frac{1}{2}$v −$\frac{1}{2}\sqrt{3}$u, w)($-\frac{1}{2}\sqrt{3}$v−$\frac{1}{2}$u, $-\frac{1}{2}$v+$\frac{1}{2}\sqrt{3}$u, w).

6.51a. Pentagonal pyramid. B : (o, v, w)(av, bv, w)(cv, −dv, w)(−cv, −dv, w)(−av, bv, w). B′ : (oow′). a, b, c, d as in 5.5a.

6.42a. Tetragonal octahedron. B : uoo, ūoo, ouo, oūo. B′ : oou′, ooū′.

6.42b. B : uow, ūow, ouw̄, oūw̄. B′ : oow′, oow̄′.

6.42c. Rectangular bipyramid. B : uvo, ūv̄o, ūvo, uv̄o. B′ : oow′, oow̄′.

6.42d. Plane. B : uvo, ūv̄o, ūvo, uv̄o. B′ : u′oo, ū′oo.

6.42e. B : uvw, uv̄w̄, ūvw̄, ūv̄w. B′ : oow′, oow̄′.

6.42f. B : uvw, uv̄w, ūv̄w, ūvw. B′ : u′ow′, ū′ow′. $(CH_2)_2O$.

6.42g. B : uvw, uv̄w, ūv̄w̄, ūvw̄. B′ : u′ow′, ū′ow̄′.

6.411a. Polar tetragonal octahedron. B : uow, ūow, ouw, oūw. B′ : oow′. B″ : oow″.

6.411b. Polar rectangular bipyramid. B : uvw, ūv̄w, ūvw, uv̄w. B′ : oow′. B″ : oow″.

6.33a. Plane. B : (o, v, o)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o). B′ : (o, v̄, o)($-\frac{1}{2}\sqrt{3}$v, $\frac{1}{2}$v, o)($\frac{1}{2}\sqrt{3}$v, $\frac{1}{2}$v, o).

6.33b. Plane. B : (o, v, o)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, o). B′ : (u′, v′, o)($\frac{1}{2}\sqrt{3}$v′−$\frac{1}{2}$u′, $-\frac{1}{2}$v′ −$\frac{1}{2}\sqrt{3}$u′, o)($-\frac{1}{2}\sqrt{3}$v′−$\frac{1}{2}$u′, $-\frac{1}{2}$v′+$\frac{1}{2}\sqrt{3}$u′, o).

6.33c. Pyramid or prism. B : (o, v, w)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w). B′ : (o, v′, w′)($\frac{1}{2}\sqrt{3}$v′, $-\frac{1}{2}$v′, w′)($-\frac{1}{2}\sqrt{3}$v′, $-\frac{1}{2}$v′, w′).

6.33d. Pyramid or prism. B : (o, v, w)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w). B′ : (u′, v′, w′)($\frac{1}{2}\sqrt{3}$v′−$\frac{1}{2}$u′, $-\frac{1}{2}$v′−$\frac{1}{2}\sqrt{3}$u′, w′)($-\frac{1}{2}\sqrt{3}$v′ −$\frac{1}{2}$u′, $-\frac{1}{2}$v′+$\frac{1}{2}\sqrt{3}$u′, w′).

6.3111a. Trigonal bipyramid. B : (o, v, w)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w). B′ : oow′. B″ : oow″. B‴ : oow‴. CH_3NCO.

6.222a. Linear. B : oow, oow̄. B′ : oow′, oow̄′. B″ : oow″, oow̄″.

6.222b. Orthorhombic octahedron. B : uoo, ūoo. B′ : ov′o, ov̄′o. B″ : oow″, oow̄″.

6.222c. Trapezoidal bipyramid. B : uow, ūow. B′ : u′ow′, ū′ow′. B″ : ov″w″, ov̄″w″.

6.222d. Plane. B : uvo, ūv̄o. B′ : u′v′o, ū′v̄′o. B″ : u″v″o, ū″v̄″o.

6.222e. Monoclinic octahedron. B : uvo, ūv̄o. B′ : u′v′o, ū′v̄′o. B″ : oow″, oow̄″.

6.222f. Triangular prism. B : uvw, uvw̄. B′ : u′v′w′, u′v′w̄′. B″ : u″v″w″, u″v″w̄″.

6.222g. Monoclinic octahedron. B : uvw, ūv̄w. B′ : u′v′w′, ū′v̄′w′. B″ : u″v″w″, ū″v̄″w″.

6.222h. Triclinic octahedron. B : uvw, ūv̄w̄. B′ : u′v′w′, ū′v̄′w̄′. B″ : u″v″w″, ū″v̄″w̄″.

6.2211a. Orthorhombic octahedron. B : uow, ūow. B′ : ov′w′, ov̄′w′. B″ : oow″. B‴ : oow‴.

6.2211b. Heptahedron. B : uvw, uvw̄. B′ : u′v′w′, u′v′w̄′. B″ : u″v″o. B‴ : u‴v‴o.

6.2211c. Monoclinic octahedron. B : uvw, ūv̄w. B′ : u′v′w′, ū′v̄′w′. B″ : oow″. B‴oow‴.

6.21111a. B : uvw, uvw̄. B′ : u′v′o. B″ : u″v″o. B‴ : u‴v‴o. B⁗ : u⁗v⁗o.

6.111111a. Linear. $B^{(i)}$: oow_i.

6.111111b. Plane. $B^{(i)}$: u_iv_io.

6.111111c. General. No symmetry. $B^{(i)}$: $u_iv_iw_i$.

TABLE VI. *Molecules with eight atoms.*

No.	Name	I	II	ν_1	ν_2	R	I.R.	Irreducible representations
7.7a	Plane heptagon	D_{7h}	S	2	8	3(2)	3(1)	1^R, 0, $2_2{}^I$, $2_2{}^R$, 2_2; 0, 1^I, 0, 1_2, 1_2.
7.7b	Heptagonal pyramid	C_{7v}	S	2	8	7(5)	4(2)	2^{RI}, 0, $2_2{}^{RI}$, $3_2{}^R$, 3_2.
7.52a	Pentagonal bipyramid	D_{5h}	S	4	7	5(3)	5(2)	2^R, 0, $3_2{}^I$, $2_2{}^R$; 2^I, 0, $1_2{}^R$, 1_2.
7.331a		C_{3v}	S	6	6	11(6)	11(5)	5^{RI}, 1, $6_2{}^{RI}$.
7.331b	Truncated trigonal bipyramid	C_{3v}	S	6	6	11(6)	11(5)	5^{RI}, 1, $6_2{}^{RI}$.
7.421a		C_{2v}	A	18		18(12)	15	6^{RI}, 5^{RI}, 3^R, 4^{RI}.

MOLECULES WITH EIGHT ATOMS

Only the type AB_7 is treated completely; the other structures listed were chosen because they seem the most probable physically. IF_7 presumably belongs to one of the classes below.

7.7a. Plane heptagon. B : (o, v, o)(gv, hv, o)(jv, kv, o)(ev, fv, o)(−ev, fv, o)(−jv, kv, o)(−gv, hv, o). g = sin φ, h = cos φ, j = sin 2φ, k = cos 2φ, e = sin 3φ, f = cos 3φ. φ = 2π/7.

7.7b. Heptagonal pyramid. B : (o, v, w)(gv, hv,

w)(jv, kv, w)(ev, fv, w)(−ev, fv, w)(−jv, kv, w)(−gv, hv, w). g, h, j, k, e, f as in 7.7a.

7.52a. Pentagonal bipyramid. B : (o, v, o)(av, bv, o)(cv, −dv, o)(−cv, −dv, o)(−av, bv, o). B′ : (oow′)(oow̄′).

7.331a, b. B : (o, v, w)($\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w)($-\frac{1}{2}\sqrt{3}$v, $-\frac{1}{2}$v, w). B′ : (o, v′, w′)($\frac{1}{2}\sqrt{3}$v′, $-\frac{1}{2}$v′, w′)($-\frac{1}{2}\sqrt{3}$v′, $-\frac{1}{2}$v′, w′). B″ : oow″.

7.421a. B : uvw, ūv̄w, ūvw, uv̄w. B′ : u′ow′, ū′ow′. B″ : oow″.

TABLE VII. *Molecules with nine atoms.*

No.	Name	I	II	ν_1	ν_2	ν_3	R	I.R.	Irreducible representations
8.8a	Cube	O_h	Sp	2	2	5	4(3)	2	1^R, 0, 1_2^R, 2_3^R, 0; 0, 1, 1_2, 1_3, 2_3^I.
8.8b	Plane octagon	D_{8h}	S	5	8		4(3)	3(1)	1^R, 0, 1, 1, 1_2^R, 0, 2_2^R; 0, 1^I, 0, 1, 2_2^I, 2_2, 1_2.
8.8c	Octagonal pyramid	C_{8v}	S	5	8		7(5)	4(2)	2^{RI}, 0, 1, 2, 2_2^{RI}, 3_2, 3_2^R.
8.8d	Archimedian anti-prism	D_{4d}	S	5	8		7(5)	5(2)	2^R, 0, 1, 2^I, 3_2^I, 2_2^R, 3_2^R.
8.8e	Plane tetragonal octagon	D_{4h}	S	11	5		7(5)	5(1)	2^R, 1, 2^R, 2^R, 1_2^R; 1, 1^I, 1, 1, 4_2^I.
8.8f	Tetragonal parallelopiped	D_{4h}	S	11	5		7(5)	5(2)	2^R, 0, 1^R, 2^R, 2_2^R; 1, 2^I, 2, 1, 3_2^I.
8.8g	Twisted cube	D_4	S	11	5		14(11)	7(2)	3^R, 2^I, 3^R, 3^R, 5_2^{RI}.
8.8h	Tetragonal pyramid	C_{4v}	S	11	5		14(11)	8(3)	3^{RI}, 2, 3^R, 3^R, 5_2^{RI}.
8.8i	Twisted tetragonal parallelopiped	V_d	S	11	5		14(11)	8(3)	3^R, 2, 3^{RI}, 3^R, 5_2^{RI}.
8.8j	Rectangular parallelopiped	V_h	A	21			9(6)	9	3^R, 2^R, 2^R, 2^R; 3, 3^I, 3^I, 3^I.

MOLECULES WITH NINE ATOMS

Only the type AB_8 is considered. OsF_8[33] is said to belong to 8.8a or 8.8d.

8.8a. Cube. B : uuu, ūūū, ūuū, uūu, ūūu, uuū, uūū, ūuu.

8.8b. Plane octagon. B : (o, v, o)(mv, mv, o)(v, o, o)(mv, −mv, o)(o, v̄, o)(−mv, −mv, o)(v̄, o, o)(−mv, mv, o). m=$\frac{1}{2}\sqrt{2}$.

8.8c. Octahedral pyramid. B : (o, v, w)(mv, mv, w)(v, o, w)(mv, −mv, w)(o, v̄, w)(−mv, −mv, w)(v̄, o, w)(−mv, mv, w). m=$\frac{1}{2}\sqrt{2}$.

8.8d. Archimedian anti-prism. B : (uuw)(ūūw)(ūuw)(uūw)(pu, o, w̄)(o, pū, w̄)(pū, o, w̄)(o, pu, w̄). p=$\sqrt{2}$.

8.8e. Plane tetragonal octagon. B : uvo, ūv̄o, ūvo, uv̄o, vūo, v̄uo, vuo, v̄ūo.

8.8f. Tetragonal parallelopiped. B : uow, ūow̄, ūow, uow̄, oūw, ouw, ouw̄, oūw̄.

8.8g. Twisted cube. B : uvw, ūvw̄, ūv̄w, uv̄w̄, vūw, v̄uw, vuw̄, v̄ūw̄.

8.8h. Tetragonal octangular pyramid. B : uvw, ūv̄w, ūvw, uv̄w, vūw, v̄uw, vuw, v̄ūw.

8.8i. Twisted tetragonal parallelopiped. B : uvw, ūvw̄, ūv̄w, uv̄w̄, vūw̄, v̄uw̄, vuw, v̄ūw.

8.8j. Rectangular parallelopiped. B : uvw, ūv̄w̄, ūvw̄, uv̄w, ūv̄w, uvw̄, uv̄w̄, ūvw.

[33] H. Braune and S. Knoke, Naturwiss. **21**, 349 (1933).