(Tableau 3); cependant dans l'étude infra-rouge menée parallèlement, un déplacement faible de la fréquence de vibration de valence de O–H a été observé et la présence de liaisons hydrogène importantes estainsi exclue.

Conclusion

Les études radiocristallographiques et infra-rouges entreprises parallèlement font apparaître dans la série $M^IFe(CrO_4)_2.2H_2O$ l'existence d'un seul motif structural, la chaîne $n[Fe(CrO_4)_2.2H_2O]^-$, mais de symétrie plus ou moins grande suivant M^I. Deux types structuraux ont été déterminés: le type potassium, le plus symétrique, correspondant aux éléments monovalents M^I de grand rayon ionique ($M^I = K$, Tl, NH_4) et le type sodium, moins symétrique où M^I a un petit rayon ionique ($M^I = Na$). Le Tableau 4 indique les caractéristiques cristallographiques des divers composés dont nous disposons.

Les calculs nécessaires à ce travail ont été effectués au C.I.R.C.E. (C.N.R.S.).

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Formulas for the Cosine Seminvariants, $\cos(\varphi_1+\varphi_2)$*

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Expressions for the cosines of those structure seminvariants, $\varphi_1+\varphi_2$, which are linear combinations of two phases, are found in terms of the observed magnitudes, $|E|$, of the normalized structure factors. These formulas have found important application in some recent crystal structure determinations.

1. Introduction

Explicit formulas for the cosines of single phases which are structure seminvariants (the so-called $\sum_1$ formulas) were first found almost twenty years ago (Hauptman & Karle, 1953). Again, expressions for the cosines of those invariants which are linear combinations of three phases were obtained some fifteen years ago (Hauptman & Karle, 1957; Vaughan, 1958). However, despite the fact that the space-group dependent linear combinations of two phases which are structure seminvariants have been known since 1953 (Hauptman & Karle), explicit formulas for their cosines in terms of the magnitudes of the normalized structure factors have been discovered only recently (Hauptman, 1971). A brief sketch of the derivation is presented here only for the space group $P2$. Analogous formulas and generalizations in the space groups $P2_1$ and $P2_12_12_1$ are merely quoted.

2. Space group $P2$

In the space group $P2$, $\varphi_{h_1k_1l_1}+\varphi_{h_2k_2l_2}$ is a structure seminvariant (or invariant) if and only if h_1+h_2 and l_1+l_2 are both even and k_1+k_2 is zero. Only the special case that $k_1=k_2=0$ is considered here although the more general case is readily treated in the same way.

If there are N identical atoms in the unit cell then the normalized structure factor E_{hkl} is defined by means of

$$E_{hkl}=\frac{2}{N^{1/2}}\sum_{\mu=1}^{N/2}\cos 2\pi(hx_\mu+lz_\mu)\exp(2\pi iky_\mu) \quad (2.1)$$

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whence it follows that

$$|E_{hkl}|^2=\frac{4}{N}\sum_{\substack{\mu,\nu\\1}}^{N/2}\cos 2\pi(hx_\mu+lz_\mu)\cos 2\pi(hx_\nu+lz_\nu)\times\exp\left(2\pi ik(y_\mu-y_\nu)\right). \tag{2.2}$$

If the double sum (2.2) is decomposed into two parts, a simple sum, when $\mu=\nu$, and a residual double sum, when $\mu\neq\nu$, one obtains, after some simplification,

$$|E_{hkl}|^2-1=\frac{1}{N^{1/2}}E_{2h02l}+\frac{4}{N}\sum_{\substack{\mu\neq\nu\\1}}^{N/2}\cos 2\pi(hx_\mu+lz_\mu)\cos 2\pi(hx_\nu+lz_\nu)\times\cos 2\pi k(y_\mu-y_\nu). \tag{2.3}$$

Multiplying (2.3) by the like equation obtained by replacing h by h' and l by l'; decomposing the resulting quadruple sum into two (equal) double sums, four (equal) triple sums, and a residual quadruple sum; and finally averaging over all integers k, one finds that only the double sum survives the averaging process so that finally

$$\begin{aligned}\langle(|E_{hkl}|^2-1)(|E_{h'kl'}|^2-1)\rangle_k=&\frac{1}{N}E_{2h02l}E_{2h'02l'}\\&+\frac{4}{N^2}\sum_{\substack{\mu\neq\nu\\1}}^{N/2}\{\cos 2\pi[(h+h')x_\mu+(l+l')z_\mu]\\&+\cos 2\pi[(h-h')x_\mu+(l-l')z_\mu]\}\\&\times\{\cos 2\pi[(h+h')x_\nu+(l+l')z_\nu]+\cos 2\pi[(h\\&-h')x_\nu+(l-l')z_\nu]\}.\end{aligned} \tag{2.4}$$

After carrying out the indicated multiplication, the double sum in (2.4) is seen to consist of four terms each of the form

$$\frac{4}{N^2}\sum_{\substack{\mu\neq\nu\\1}}^{N/2}\cos 2\pi(h_1x_\mu+l_1z_\mu)\cos 2\pi(h_2x_\nu+l_2z_\nu) \tag{2.5}$$

and it is necessary now to evaluate this double sum in terms of normalized structure factors E. To this end write [from (2.1)]

$$E_{h_10l_1}=\frac{2}{N^{1/2}}\sum_{\mu\neq 1}^{N/2}\cos 2\pi(h_1x_\mu+l_1z_\mu), \tag{2.6}$$

$$E_{h_20l_2}=\frac{2}{N^{1/2}}\sum_{\nu=1}^{N/2}\cos 2\pi(h_2x_\nu+l_2z_\nu). \tag{2.7}$$

Multiplying (2.6) and (2.7); decomposing the resulting double sum into a simple sum (when $\mu=\nu$) and a residual double sum (when $\mu\neq\nu$); and employing (2.1) to replace the simple sum by its value in terms of normalized structure factors, one finally obtains

$$\begin{aligned}\frac{4}{N}\sum_{\substack{\mu\neq\nu\\1}}^{N/2}&\cos 2\pi(h_1x_\mu+l_1z_\mu)\cos 2\pi(h_2x_\nu+l_2z_\nu)\\&=E_{h_10l_1}E_{h_20l_2}-\frac{1}{N^{1/2}}E_{h_1+h_20l_1+l_2}\\&\quad-\frac{1}{N^{1/2}}E_{h_1-h_20l_1-l_2},\end{aligned} \tag{2.8}$$

the desired expression for the double sum (2.5) which is needed in (2.4). Substituting from (2.8) into (2.4) after replacing first, h_1, l_1, h_2, l_2 by $h+h'$, $l+l'$, $h+h'$, $l+l'$ respectively; second, h_1, l_1, h_2, l_2 by $h+h'$, $l+l'$, $h-h'$, $l-l'$ respectively; third, h_1, l_1, h_2, l_2 by $h-h'$, $l-l'$, $h+h'$, $l+l'$ respectively; and fourth, h_1, l_1, h_2, l_2 by $h-h'$, $l-l'$, $h-h'$, $l-l'$ respectively, one finds, after some simplification and neglecting terms of order $1/N^{1/2}$,

$$\begin{aligned}E_{h+h'0l+l'}E_{h-h'0l-l'}\simeq&\frac{N}{2}\langle(|E_{hkl}|^2-1)(|E_{h'kl'}|^2-1)\rangle_k\\&-\tfrac{1}{2}E_{2h02l}E_{2h'02l'}-\tfrac{1}{2}E^2_{h+h'0l+l'}\\&-\tfrac{1}{2}E^2_{h-h'0l-l'}.\end{aligned} \tag{2.9}$$

Making the substitution

$$\left.\begin{aligned}h+h'=h_1,\ l+l'=l_1,\\ h-h'=h_2,\ l-l'=l_2,\end{aligned}\right\} \tag{2.10}$$

where $h_1\pm h_2$ and $l_1\pm l_2$ are all even, one finally obtains the basic formula for the cosine seminvariant $\cos(\varphi_{h_10l_1}+\varphi_{h_20l_2})$,

$$\begin{aligned}E_{h_10l_1}E_{h_20l_2}=&|E_{h_10l_1}E_{h_20l_2}|\cos(\varphi_{h_10l_1}+\varphi_{h_20l_2})\\\simeq&\frac{N}{2}\langle(|E_{(h_1+h_2)/2\ k\ (l_1+l_2)/2}|^2-1)\\&\times(|E_{(h_1-h_2)|2\ k\ (l_1-l_2)/2}|^2-1)\rangle_k\\&-\tfrac{1}{2}E_{h_1+h_20l_1+l_2}E_{h_1-h_20l_1-l_2}-\tfrac{1}{2}(E^2_{h_10l_1}+E^2_{h_20l_2}).\end{aligned} \tag{2.11}$$

However, the right side of (2.11) contains the term

$$-\tfrac{1}{2}E_{h_1+h_20l_1+l_2}E_{h_1-h_20l_1-l_2} \tag{2.12}$$

only the magnitude of which is, in general, known. Since

$$\left.\begin{aligned}(h_1+h_2)+(h_1-h_2)=2h_1\\ (l_1+l_2)+(l_1-l_2)=2l_1\end{aligned}\right\} \tag{2.13}$$

are both even, (2.12) is itself a structure seminvariant and (2.11) may be employed, with h_1 replaced by (h_1+h_2), h_2 by (h_1-h_2), l_1 by (l_1+l_2), and l_2 by (l_1-l_2) to yield an expression for (2.12) which however depends on the structure seminvariant

$$E_{2h_102l_1}E_{2h_202l_2}. \tag{2.14}$$

Hence (2.11) may be employed again to determine an expression for (2.14). Proceeding iteratively in this fashion one finally obtains the desired formula in the form of two rapidly converging series:

$$\begin{aligned}E_{h_10l_1}E_{h_20l_2}=&|E_{h_10l_1}E_{h_20l_2}|\cos(\varphi_{h_10l_1}+\varphi_{h_20l_2})\\\simeq&\frac{N}{2}\langle(|E_{(h_1+h_2)/2\ k\ (l_1+l_2)/2}|^2-1)\end{aligned}$$

$$\times(|E_{(h_1-h_2)/2\ k\ (l_1-l_2)/2}|^2-1)$$
$$-\tfrac{1}{2}(|E_{h_1k l_1}|^2-1)\,(|E_{h_2k l_2}|^2-1)$$
$$+\tfrac{1}{4}(|E_{h_1+h_2\ k\ l_1+l_2}|^2-1)\,(|E_{h_1-h_2\ k\ l_1-l_2}|^2-1)-\ldots\rangle_k$$
$$-\tfrac{1}{2}(E^2_{h_1 0 l_1}+E^2_{h_2 0 l_2})+\tfrac{1}{4}(E^2_{h_1+h_2\ 0\ l_1+l_2}+E^2_{h_1-h_2\ 0\ l_1-l_2})$$
$$-\tfrac{1}{8}(E^2_{2h_1\ 0\ 2l_1}+E^2_{2h_2\ 0\ 2l_2})+\ldots, \tag{2.15}$$

in which $h_1\pm h_2$ and $l_1\pm l_2$ are all even.

3. Space group $P2_1$

The analogue of (2.15) in the space group $P2_1$ is, surprisingly enough, simply

$$E_{h_1 0 l_1}E_{h_2 0 l_2}=|E_{h_1 0 l_1}E_{h_2 0 l_2}|\cos(\varphi_{h_1 0 l_1}+\varphi_{h_2 0 l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^k(|E_{(h_1+h_2)/2\ k\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ k\ (l_1-l_2)/2}|^2-1)\rangle_k, \tag{3.1}$$

in which $h_1\pm h_2$ and $l_1\pm l_2$ are all even. More generally, if $h_1\pm h_2$ and $l_1\pm l_2$ are even, then

$$E_{h_1k_1l_1}E_{h_2\bar{k}_1l_2}=|E_{h_1k_1l_1}E_{h_2k_1l_2}|\cos(\varphi_{h_1k_1l_1}+\varphi_{h_2\bar{k}_1l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^k(|E_{(h_1+h_2)/2\ k\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ k_1-k\ (l_1-l_2)/2}|^2-1)\rangle_k. \tag{3.2}$$

It should be noted that, if $k_1\neq 0$, then k ranges over the negative as well as the positive integers in (3.2) while in (3.1), the special case $k_1=0$ of (3.2), it is sufficient that k range over only the non-negative integers. Finally, it should be emphasized that (3.1) and (3.2) are useful in practice only if the magnitudes of the calculated cosine invariants are extremely large so that one may infer that the values of certain cosines, $\cos(\varphi_{h_1k_1l_1}+\varphi_{h_2\bar{k}_1l_2})$, are ± 1.

4. Space group $P2_12_12_1$

There is a great variety of formulas for the cosine invariants, $\cos(\varphi_1+\varphi_2)$, in the space group $P2_12_12_1$. Only twelve of these are listed here. If $k_1\pm k_2$ and $l_1\pm l_2$ are even,

$$E_{0k_1l_1}E_{0k_2l_2}=|E_{0k_1l_1}E_{0k_2l_2}|\cos(\varphi_{0k_1l_1}+\varphi_{0k_2l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^{h+(k_1+k_2)/2}(|E_{h\ (k_1+k_2)/2\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{h\ (k_1-k_2)/2\ (l_1-l_2)/2}|^2-1)\rangle_h \tag{4.1}$$
$$\simeq\frac{N}{2}\langle(-1)^{h+(k_1-k_2)/2+l_1}(|E_{h\ (k_1+k_2)/2\ (l_1-l_2)/2}|^2-1)$$
$$\times(|E_{h\ (k_1-k_2)/2\ (l_1+l_2)/2}|^2-1)\rangle_h. \tag{4.2}$$

If $l_1\pm l_2$ and $h_1\pm h_2$ are even,

$$E_{h_1 0 l_1}E_{h_2 0 l_2}=|E_{h_1 0 l_1}E_{h_2 0 l_2}|\cos(\varphi_{h_1 0 l_1}+\varphi_{h_2 0 l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^{k+(l_1+l_2)/2}(|E_{(h_1+h_2)/2\ k\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ k\ (l_1-l_2)/2}|^2-1)\rangle_k \tag{4.3}$$
$$\simeq\frac{N}{2}\langle(-1)^{k+(l_1-l_2)/2+h_1}(|E_{(h_1-h_2)/2\ k\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{(h_1+h_2)/2\ k\ (l_1-l_2)/2}|^2-1)\rangle_k. \tag{4.4}$$

If $h_1\pm h_2$ and $k_1\pm k_2$ are even,

$$E_{h_1k_10}E_{h_2k_20}=|E_{h_1k_10}E_{h_2k_20}|\cos(\varphi_{h_1k_10}+\varphi_{h_2k_20})$$
$$\simeq\frac{N}{2}\langle(-1)^{l+(h_1+h_2)/2}(|E_{(h_1+h_2)/2\ (k_1+k_2)/2\ l}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ (k_1-k_2)/2\ l}|^2-1)\rangle_l \tag{4.5}$$
$$\simeq\frac{N}{2}\langle(-1)^{l+(h_1-h_2)/2+k_1}(|E_{(h_1+h_2)/2\ (k_1-k_2)/2\ l}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ (k_1+k_2)/2\ l}|^2-1)\rangle_l. \tag{4.6}$$

Next, if $l_1\pm l_2$ are even,

$$E_{0k_1l_1}E_{0k_1l_2}=|E_{0k_1l_1}E_{0k_1l_2}|\cos(\varphi_{0k_1l_1}+\varphi_{0k_1l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^{k+(l_1-l_2)/2}(|E_{0\ k\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{0\ k+k_1\ (l_1-l_2)/2}|^2-1)\rangle_k. \tag{4.7}$$
$$E_{h_10l_1}E_{h_10l_2}=|E_{h_10l_1}E_{h_10l_2}|\cos(\varphi_{h_10l_1}+\varphi_{h_10l_2})$$
$$\simeq\frac{N}{2}\langle(-1)^{h+h_1+l_1}(|E_{h\ 0\ (l_1+l_2)/2}|^2-1)$$
$$\times(|E_{h+h_1\ 0\ (l_1-l_2)/2}|^2-1)\rangle_h. \tag{4.8}$$

If $h_1\pm h_2$ are even,

$$E_{h_10l_1}E_{h_20l_1}=|E_{h_10l_1}E_{h_20l_1}|\cos(\varphi_{h_10l_1}+\varphi_{h_20l_1})$$
$$\simeq\frac{N}{2}\langle(-1)^{l+(h_1-h_2)/2}(|E_{(h_1+h_2)/2\ 0\ l}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ 0\ l+l_1}|^2-1)\rangle_l. \tag{4.9}$$
$$E_{h_1k_10}E_{h_2k_10}=|E_{h_1k_10}E_{h_2k_10}|\cos(\varphi_{h_1k_10}+\varphi_{h_2k_10})$$
$$\simeq\frac{N}{2}\langle(-1)^{k+k_1+h_1}(|E_{(h_2+h_1)/2\ k\ 0}|^2-1)$$
$$\times(|E_{(h_1-h_2)/2\ k+k_1\ 0}|^2-1)\rangle_k. \tag{4.10}$$

If $k_1\pm k_2$ are even,

$$E_{h_1k_10}E_{h_1k_20}=|E_{h_1k_10}E_{h_1k_20}|\cos(\varphi_{h_1k_10}+\varphi_{h_1k_20})$$
$$\simeq\frac{N}{2}\langle(-1)^{h+(k_1-k_2)/2}(|E_{h\ (k_1+k_2)/2\ 0}|^2-1)$$
$$\times(|E_{h+h_1\ (k_1-k_2)/2\ 0}|^2-1)\rangle_h. \tag{4.11}$$
$$E_{0k_1l_1}E_{0k_2l_1}=|E_{0k_1l_1}E_{0k_2l_1}|\cos(\varphi_{0k_1l_1}+\varphi_{0k_2l_1})$$
$$\simeq\frac{N}{2}\langle(-1)^{l+l_1+k_1}(|E_{0\ (k_1+k_2)/2\ l}|^2-1)$$
$$\times(|E_{0\ (k_1-k_2)/2\ l+l_1}|^2-1)\rangle_l. \tag{4.12}$$

In addition to (4.1)–(4.12) there are the straightforward generalizations [analogous to (3.2) in the space group $P2_1$] which the interested reader is invited to derive for himself. Again, the formulas given here,

and their generalizations, have practical utility primarily in the case that the magnitudes of calculated cosines are so large as to imply that $\cos(\varphi_1+\varphi_2)=\pm 1$.

5. Applications

The formulas derived in this paper have been incorporated into recently secured techniques of crystal structure determination by direct methods and have played an important role in the solution of a number of crystal structures. Among these are:

(1) 2β,17β-diacetoxy-4-androsten-3-one, $C_{23}H_{32}O_5$, in the space group $P2_12_12_1$ (Duax, 1971);
(2) valinomycin, $C_{54}O_{18}N_6H_{90}$, in the space group $P2_1$ (Duax & Hauptman, 1971).

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Structure Cristalline de l'Hydrochlorothiazide, $C_7H_8ClN_3O_4S_2$

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The crystal and molecular structure of hydrochlorothiazide $C_7H_8ClN_3O_4S_2$ has been determined by X-ray diffraction techniques. The space group is $P2_1$ with two molecules per unit cell of dimensions $a=7{\cdot}419\pm0{\cdot}006$, $b=8{\cdot}521\pm0{\cdot}003$, $c=10{\cdot}003\pm0{\cdot}002$ Å and $\beta=111{\cdot}72°$. Three-dimensional intensity data were collected with a Hilger four-circle diffractometer. The structure was refined by least-squares methods to a final R value of 0·066 for 956 observed reflexions; the average standard deviations in bond lengths and angles not involving hydrogen atoms are about 0·015 Å and 1·0°. The molecule, apart from two nitrogen and the four oxygen atoms, is planar. A short N(sp^2)–C(sp^2) bond is observed (1·344 Å), which is explained by a delocalization of the nitrogen doublet towards the benzene ring. There are four intermolecular NH···O hydrogen bonds in the unit cell, in the range 2·88–2·94 Å. All other bonds are greater than the sum of the van der Waals radii.

Introduction

L'hydrochlorothiazide (dihydrochloro-6-sulfamoyl-7 benzothiadiazine-1,2,4 dioxyde-1,1) est un sulfamide diurétique de la série de la benzothiadiazine, dont le type est le chlorothiazide (Fig. 1). Ces composés agissent en inhibant un ou plusieurs des mécanismes de transport qui assurent la réabsorption du sodium par le tube rénal. Le chlorothiazide résulte de l'action de l'acide formique sur l'amino-3 chloro-1 benzène disulfonamide-4,6 ou salamid. La saturation de la double liaison située en 3-4 accroît environ dix fois l'activité salurétique du chlorothiazide et donne l'hydrochlorothiazide qui se forme également par cyclisation du salamid avec l'aldéhyde formique. En greffant des radicaux variés sur le carbone 3 de l'hydrochlorothiazide, on obtient toute une série de benzothiadiazines substituées à action diurétique renforcée, et parfois intense. On a remarqué que la substitution du groupement trifluorométhyle à l'atome de chlore en position 6 ne modifie pas sensiblement l'activité de la molécule (Bierbaum, Traverso & Whitehead, 1963; Gantt & Synek, 1961; Heinemann, Demartini & Laragh, 1959; Pignard, 1960). L'objet de ce travail est d'obtenir des informations sur la configuration de la molécule, principalement au voisinage de la liaison 3-4. Une étude radiocristallographique préliminaire de quelques thiazides a été publiée (Dupont & Dideberg, 1970).

Expérimentation

Les cristaux d'hydrochlorothiazide ont été obtenus à partir d'une solution de la substance dans l'éthanol. Celle-ci provient des laboratoires Merck, Sharp et Dohme (Haarlem, Nederland). L'hydrochlorothiazide est aussi soluble dans l'acétone, le méthanol et dans NH_3 dilué et sodé.

Les cristaux incolores se présentent sous forme de