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A Unified Program for Phase Determination, Type 2*P*

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The new probability approach, in which the crystal structure is fixed and the Miller indices range uniformly but not independently over the integers, has yielded phase determining formulas with universal application to all the space groups. The formulation includes both the equal and unequal atom cases and takes special advantage of the symmetries characteristic of a particular space group.

The present paper is concerned with the centrosymmetric space groups comprising type 2*P*. A detailed procedure for phase determination in this type is described.

1. Introduction

The program initiated in a previous paper (Karle & Hauptman, 1959, hereafter referred to as 1*P*) is continued here. The application of the new probability methods, based on the Miller indices as random variables, is made to the space groups of type 2*P* (Hauptman & Karle, 1953, 1959). This type consists of the twenty primitive centrosymmetric space groups in the tetragonal system and the eight *C*-centered centrosymmetric space groups. It is to be emphasized that all the space groups are treated here with primitive unit cells. For the conventionally primitive space groups the unit cell corresponds to that found in the *International Tables* (1952). For the *C*-centered space groups the primitive unit cell is defined in our paper on the seminvariants (Hauptman & Karle, 1959). We present here a detailed procedure for phase determination in the space groups of type 2*P*, which utilizes the same general formula and, at the same time, makes use of relationships among the structure factors characteristic of each space group.

2. Notation

The same notation as appears in 1*P* (1959) is employed here.

3. Phase determining formulas

3·1. *Basic formulas*

$$B_{2,0}\colon\ \mathscr{E}_{\mathbf{h}}'^2 = 1+\frac{4\pi\sigma_2^2}{2^{(p+q+2)/2}pq\Gamma\left(\frac{p+1}{2}\right)\Gamma\left(\frac{q+1}{2}\right)\sigma_4}\times\langle\lambda_{p\mathbf{k}}\lambda_{q(\mathbf{h}+\mathbf{k})}\rangle_{\mathbf{k}}+R_{2,0}\,. \quad (3\cdot1\cdot1)$$

$$B_{3,0}\colon\ \mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2} = \frac{(2\pi)^{3/2}\sigma_2^3}{2^{(p+q+r+3)/2}pqr\Gamma\left(\frac{p+1}{2}\right)\Gamma\left(\frac{q+1}{2}\right)\Gamma\left(\frac{r+1}{2}\right)\sigma_4^{3/2}}\times\langle\lambda_{p\mathbf{k}}\lambda_{q(\mathbf{h}_1+\mathbf{k})}\lambda_{r(\mathbf{h}_1+\mathbf{h}_2+\mathbf{k})}\rangle_{\mathbf{k}}$$
$$-2\frac{\sigma_6}{\sigma_4^{3/2}}+\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'''_{\mathbf{h}_1}+\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_2}+\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_1+\mathbf{h}_2})+R_{3,0}\,. \quad (3\cdot1\cdot2)$$

3·2. *Integrated formulas*

$$I_{2,0}\colon\ \mathscr{E}_{\mathbf{h}}'^2 = 1+\frac{2\sigma_2^2}{C_1^2(t)\sigma_4}\langle\Lambda_{t\mathbf{k}}\Lambda_{t(\mathbf{h}+\mathbf{k})}\rangle_{\mathbf{k}}+R'_{2,0}\,. \quad (3\cdot2\cdot1)$$

$$I_{3,0}\colon\ \mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2} = \frac{\sigma_2^3}{C_1^3(t)\sigma_4^{3/2}}\langle\Lambda_{t\mathbf{k}}\Lambda_{t(\mathbf{h}_1+\mathbf{k})}\Lambda_{t(\mathbf{h}_1+\mathbf{h}_2+\mathbf{k})}\rangle_{\mathbf{k}}$$
$$-2\frac{\sigma_6}{\sigma_4^{3/2}}+\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'''_{\mathbf{h}_1}+\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_2}+\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}\mathscr{E}'''_{\mathbf{h}_1+\mathbf{h}_2})+R'_{3,0}\,. \quad (3\cdot2\cdot2)$$

In these formulas, p, q, r and t are restricted to be positive. Ordinarily they are given values in the range 2–4.

The remainder terms are given in the appendix § 6 and in 1*P* (1959). Equation (3·1·1) or (3·2·1) serves to determine the magnitudes of the structure factors $|\mathscr{E}'_{\mathbf{h}}|$ corresponding to the squared structure. By means of equation (3·1·2) or (3·2·2), the phases of these structure factors $\varphi'_{\mathbf{h}}$ may be determined. In the next section we describe in detail how these equations are to be used for the various space groups included in type 2*P*, the conventionally primitive centrosymmetric space groups in the tetragonal system and the conventionally *C*-centered centrosymmetric space groups which occur in the monoclinic and orthorhombic systems (Table 1, p. 14, Monograph I, 1953 and Hauptman & Karle, 1959).

4. Phase determining procedure

It is assumed that the $|\mathscr{E}_{\mathbf{h}}|$ have been calculated from the observed intensities. From these, the $|\mathscr{E}'_{\mathbf{h}}|$ are obtained by applying (3·1·1) or (3·2·1). In fact the $|\mathscr{E}'_{\mathbf{h}}|$ so computed may be made to cover a range of reflections extending beyond that of the original set of observations. We are here concerned only with the larger $|\mathscr{E}'_{\mathbf{h}}|$ and it is the phases of these whose values are to be determined. In the application of (3·1·2) or (3·2·2), the values of some $|\mathscr{E}'''_{\mathbf{h}}|$ may be required. These may be obtained from (3·1·1) or (3·2·1) in which $\mathscr{E}$ is replaced by $\mathscr{E}'$ and $\mathscr{E}'$ by $\mathscr{E}'''$, given sufficient data.

In the phase determining procedures to be described,

Table 1

For each of the centrosymmetric, conventionally C-centered space groups in the monoclinic system, the coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ are given in columns two and three and the coefficients of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ are given in columns four and five, as they would appear, in application, on the left side of (3·1·2) or (3·2·2), for selected values of $\mathbf{h}_1$ and $\mathbf{h}_2$. The notation $P(C2/m)$ refers to the primitive unit cell, instead of the conventionally centered one (cf. Hauptman & Karle, 1959)

	Coeff. of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$		Coeff. of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$	
$\mathbf{h}_1$	$h_1,\ h_1+\bar{h},\ l_1$	$h_1,\ \bar{h}_1+h,\ l$	$\frac{1}{2}(h+\bar{k}),\ \frac{1}{2}(\bar{h}+k),\ 0$	$h_1,\ h_1,\ 2l_1$
$\mathbf{h}_2$	$\bar{h}_1+h,\ \bar{h}_1,\ \bar{l}_1$	$\bar{h}_1+h,\ h_1,\ l$	$\frac{1}{2}(h+k),\ \frac{1}{2}(\bar{h}+k),\ 2l$	$\bar{h}_1+h,\ \bar{h}_1+k,\ 2\bar{l}_1+2l$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$h,\ \bar{h},\ 0$	$\bar{h},\ h,\ 2l$	$h,\ k,\ 2l$	$h,\ k,\ 2l$
			$h\equiv k\ (\mathrm{mod}\ 2)$	$h_1\equiv h\equiv k\ (\mathrm{mod}\ 2)$
$P(C2/m)$	$+1$	$+1$	$+1$	$+1$
$P(C2/c)$	$(-1)^{l_1}$	$(-1)^{l}$	$+1$	$+1$

it will be seen that the first steps concern the application of (3·1·2) or (3·2·2) with choices of indices which take full advantage of the space group symmetry. The final step is in the form of a general application which is the same for all the space groups.

The specification of the origin is carried out in conformance with the seminvariant theory previously developed (Hauptman & Karle, Monograph I, 1953; 1959). Origin specification in all space groups of a given type is the same. Thus, the method of origin specification for space group $C2/m$ serves as a model for the remaining ones of type $2P$.

In type $2P$, the phases φ_{hkl} which are structure seminvariants are of the form, $h\equiv k\ (\mathrm{mod}\ 2)$ and $l\equiv 0\ (\mathrm{mod}\ 2)$. In other words h and k are both odd or both even and l is even. This means that once the functional form for the structure factor has been chosen, the values of these phases are uniquely determined by the intensities alone. It is of interest to note in the procedures to follow how a single equation (3·1·2) or (3·2·2) used in conjunction with relationships among the structure factors, characteristic of the particular space group and the chosen functional form for the structure factor, does, in fact, lead to unique values for the structure seminvariants.

4·1. *Monoclinic system, C-centered*

We are concerned here with space groups $C2/m$ and $C2/c$. The special choices for $\mathbf{h}_1$ and $\mathbf{h}_2$, in addition to $\mathbf{h}_1=\mathbf{h}_2$, are shown in the second and third rows of Table 1. By means of the first of these, $\mathbf{h}_1=(h_1, h_1+\bar{h}, l_1)$ and $\mathbf{h}_2=(\bar{h}_1+h, \bar{h}_1, \bar{l}_1)$, equation (3·1·2) or (3·2·2) yields the value of $\mathscr{E}'^2_{h_1,\,h_1+\bar{h},\,l_1}\mathscr{E}'_{\bar{h}\bar{h}0}$ multiplied by the numerical coefficient given in the second column of Table 1. In this way the value of the phase $\varphi'_{\bar{h}\bar{h}0}$ is determined. Since h_1 and l_1 may be chosen arbitrarily, $\varphi'_{\bar{h}\bar{h}0}$ may possibly be determined in many ways. As always, the computations are performed for the larger values of $|\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}|$.

The second relationship, $\mathbf{h}_1=(h_1, \bar{h}_1+h, l)$ and $\mathbf{h}_2=(\bar{h}_1+h, h_1, l)$ leads to the value of the phase φ'_{hh2l} by means of the numbers listed in the third column of Table 1 and (3·1·2) or (3·2·2).

We note that $\varphi_{h\bar{h}0}$ and φ_{hh2l} are special types of phases which are seminvariants. By the use of these, it is possible to calculate the values of phases of a general type which are seminvariants $\varphi_{hkl}(h\equiv k\ (\mathrm{mod}\ 2), l\equiv 0\ (\mathrm{mod}\ 2))$, as is seen from columns four and five in Table 1. The phase $\varphi_{\mathbf{h}_2}$ of column five is of the form φ_{ggg} ($g\equiv$ even) and may be obtained as in $P\bar{1}$. The numbers in columns four and five are the coefficients of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ appearing in (3·1·2) and (3·2·2).

For the purpose of specifying the origin, a linearly semi-independent pair of phases φ'_α and φ'_β, having large corresponding $|\mathscr{E}'|$, is chosen. The values of these $\varphi'_{\mathbf{h}_i}$ are then specified arbitrarily (i.e. 0 or π), thus fixing the origin. Systematic application of equation (3·1·2) or (3·2·2) then permits the determination of the phases $\varphi'_{\mathbf{h}}$ of all the remaining $\mathscr{E}'_{\mathbf{h}}$ of interest, using previously determined or specified phases as necessary.

An example of a linearly semi-independent pair of phases is φ_{gug} and φ_{ggu} ($u\equiv$ odd). We recall that phases of the type φ_{ggg} and φ_{uug} may be obtained directly from the intensities before an origin specification has been made. Additional phases are obtainable from these by suitable choice of $\mathbf{h}_1$ and $\mathbf{h}_2$ in (3·1·2) or (3·2·2). It is readily seen that any phase is accessible, once the origin specification has been made. This follows from the fact that starting with the specified phases and those of the form φ_{ggg} and φ_{uug}, it is possible to express an arbitrary vector $\mathbf{h}$ (whose components have any parity) in the form $\mathbf{h}_1+\mathbf{h}_2$ where $\varphi_{\mathbf{h}_1}$ and $\varphi_{\mathbf{h}_2}$ are known. For example, $\varphi_{\mathbf{h}}=\varphi_{ugg}$ is obtainable from suitable phases $\varphi_{\mathbf{h}_1}=\varphi_{gug}$ and $\varphi_{\mathbf{h}_2}=\varphi_{uug}$, where $\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$. The remaining types, φ_{uuu}, φ_{guu} and φ_{ugu} are similarly obtained.

4·2. *Orthorhombic system, C-centered*

The special choices of $\mathbf{h}_1$ and $\mathbf{h}_2$ characteristic of the C-centered centrosymmetric space groups of the orthorhombic system are shown in the second and third rows of Table 2. By means of these and (3·1·2) or (3·2·2), the values of many of the phases which are seminvariants may be found. The substitution of $\mathbf{h}_1$ and $\mathbf{h}_2$ of Table 2 into (3·1·2) or (3·2·2) yields, for the left sides, $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ times the coefficients listed in all but the last column. The numbers in the last column are the coefficients of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$, illustrating how a

Table 2

For each of the centrosymmetric, conventionally C-centered space groups in the orthorhombic system, the coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ are given in columns two to seven and the coefficients of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}$ are given in column eight, as they would appear, in application, on the left side of (3·1·2) or (3·2·2). The notation $P(Cmcm)$ refers to the primitive unit cell, instead of the conventionally centered one (cf. Hauptman & Karle, 1959)

	Coeff. of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$						Coeff. of $\mathscr{E}'_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}_2}\mathscr{E}'_{\mathbf{h}}$
$\mathbf{h}_1$	h_1, k_1, l	$h_1, \bar{h}_1+h, l_1$	$h_1, \bar{h}_1+h, l$	$h_1, h_1+\bar{h}, l$	h, k, l_1	$h, \bar{h}+h_1, l_1$	$\frac{1}{2}(h+k), \frac{1}{2}(\bar{h}+k), 0$
$\mathbf{h}_2$	$\bar{h}_1, \bar{k}_1, l$	$\bar{h}_1+h, h_1, \bar{l}_1$	$\bar{h}_1+h, h_1, l$	$\bar{h}_1+h, \bar{h}_1, l$	$h, k, \bar{l}_1$	$h+\bar{h}_1, \bar{h}_1, l_1$	$\frac{1}{2}(h+\bar{k}), \frac{1}{2}(\bar{h}+k), 2l$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$0, 0, 2l$	$h, h, 0$	$h, h, 2l$	$h, \bar{h}, 2l$	$2h, 2k, 0$	$h, \bar{h}, 0$	$h, k, 2l$ $h \equiv k \pmod 2$
$P(Cmcm)$	$(-1)^l$	$+1$	$(-1)^l$	$+1$	$(-1)^{l_1}$	$(-1)^{l_1}$	$+1$
$P(Cmca)$	$(-1)^{h_1+k_1+l}$	$(-1)^h$	$(-1)^l$	$(-1)^h$	$(-1)^{h+k+l_1}$	$(-1)^{l_1}$	$+1$
$P(Cmmm)$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
$P(Cccm)$	$+1$	$(-1)^{l_1}$	$(-1)^l$	$(-1)^l$	$+1$	$(-1)^{l_1}$	$+1$
$P(Cmma)$	$(-1)^{h_1+k_1}$	$(-1)^h$	$+1$	$(-1)^h$	$(-1)^{h+k}$	$+1$	$+1$
$P(Ccca)$	$(-1)^{h_1+k_1}$	$(-1)^{h+l}$	$(-1)^l$	$(-1)^{h+l}$	$(-1)^{h+k}$	$(-1)^{l_1}$	$+1$

general seminvariant phase may be obtained from special ones already known.

The procedure is completed by specifying the origin and determining the remaining phases of interest in the same way as for $C2/m$ and $C2/c$.

4·3. *Tetragonal system*

The special choices of $\mathbf{h}_1$ and $\mathbf{h}_2$ characteristic of the centrosymmetric space groups in the tetragonal system are shown in the first two rows of Tables 3 and 4. By means of these and (3·1·2) or (3·2·2), the values of many of the phases which are seminvariants may be found. The substitution of $\mathbf{h}_1$ and $\mathbf{h}_2$ of Tables 3 and 4 into (3·1·2) or (3·2·2) yields, for the left sides, $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ times the coefficients listed in the appropriate columns.

The procedure is completed by specifying the origin and determining the remaining phases of interest in the same way as for $C2/m$ and $C2/c$.

5. Concluding remarks

It is clear from the foregoing that this paper should be read in conjunction with 1P (1959). This avoids the necessity for redefining symbols and repeating remarks which are applicable to all the space groups.

Tables 1, 2, 3 and 4 contain the main choices of interest among $\mathbf{h}_1$, $\mathbf{h}_2$ and $\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$ for the particular sets of space groups involved. However, no attempt has been made to be exhaustive and the investigator may well find additional relationships of significance in application.

As a general rule, it is seen that the phase determining procedures offer many ways to calculate the value of a particular phase. This feature, together with the fact that the calculation of the right sides of (3·1·2) and (3·2·2) should yield not only the sign of the left side, but also its magnitude, serves as a good internal consistency check as the phase determination proceeds.

As mentioned in 1P (1959) the calculation of an $\mathscr{E}'^2$ map in the case of unequal atoms may be a particularly useful adjunct to the procedure since it exaggerates the Patterson peaks arising from the heaviest atoms.

6. Appendix

The correction terms for the formulas listed in § 3 are given here and in 1P (1959). As a general rule, for larger N, these terms make a very small contribution. In any specific instance, the investigator can judge for himself their importance.

We define:

Table 3

The coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ given by the left side of (3·1·2) or (3·2·2), for selected values of $\mathbf{h}_1$ and $\mathbf{h}_2$, and for each of four space groups of the tetragonal system

$\mathbf{h}_1$	h_1k_1l	$\frac{1}{2}(h+k), \frac{1}{2}(\bar{h}+k), l_1$	hkl_1	$\frac{1}{2}(h+k), \frac{1}{2}(\bar{h}+k), l$
$\mathbf{h}_2$	$\bar{h}_1\bar{k}_1l$	$\frac{1}{2}(h+\bar{k}), \frac{1}{2}(h+k), \bar{l}_1$	$hk\bar{l}_1$	$\frac{1}{2}(h+\bar{k}), \frac{1}{2}(h+k), l$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$	$0\,0\,2l$	$h \quad k \quad 0$ $h+k \equiv 0 \pmod 2$	$2h2k0$	$h \quad k \quad 2l$ $h+k \equiv 0 \pmod 2$
$P4/m$	$+1$	$+1$	$+1$	$+1$
$P4_2/m$	$+1$	$(-1)^{l_1}$	$+1$	$(-1)^l$
$P4/n$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{h+k}$	$(-1)^{\frac{1}{2}(h-k)}$
$P4_2/n$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h-k)+l_1}$	$(-1)^{h+k}$	$(-1)^{\frac{1}{2}(h+k)+l}$

$$
\begin{aligned}
{}_3R^{(0)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}\left(\mathscr{E}'''_{002l}+\mathscr{E}'''_{h+\bar{h},\bar{h}+k,0}+\mathscr{E}'''_{h+k,h+k,0}\right)\\
&-\frac{2\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{\sigma_4}{4\sigma_2^2}\left((p-2)(p-4)+(q-2)(q-4)\right)\mathscr{E}'^2_{\mathbf{h}}\\
&+\frac{2\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\
&+\frac{\sigma_4}{16\sigma_2^2}\left((p-2)(q-2)+2(p-2)(p-4)\right.\\
&\left.+2(q-2)(q-4)\right)+\ldots, \qquad (6{\cdot}1)
\end{aligned}
$$

$$
\begin{aligned}
{}_4R^{(0)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}\left(\mathscr{E}'''_{002l}+2\mathscr{E}'''_{h+k,\bar{h}+k,0}\right)\\
&-\frac{2\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{\sigma_4}{4\sigma_2^2}\left((p-2)(p-4)+(q-2)(q-4)\right)\mathscr{E}'^2_{\mathbf{h}}\\
&+\frac{2\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\
&+\frac{\sigma_4}{16\sigma_2^2}\left((p-2)(q-2)+2(p-2)(p-4)\right.\\
&\left.+2(q-2)q-4)\right)+\ldots, \qquad (6{\cdot}2)
\end{aligned}
$$

Table 4

The coefficients of $\mathscr{E}'^2_{\mathbf{h}_1}\mathscr{E}'_{\mathbf{h}}$ given by the left side of (3·1·2) or (3·2·2), for selected values of $\mathbf{h}_1$ and $\mathbf{h}_2$, and for each of sixteen space groups of the tetragonal system.

	$\mathbf{h}_1$	hk_1l_1	$h_1k\,l_1$	h_1k_1l	$\frac{1}{2}(h+k),\frac{1}{2}(\bar{h}+k),l_1$	$h\;k\;l_1$	$h\;k_1l$
	$\mathbf{h}_2$	$h\bar{k}_1\bar{l}_1$	$\bar{h}_1k\,\bar{l}_1$	$\bar{h}_1\bar{k}_1l$	$\frac{1}{2}(h+\bar{k}),\frac{1}{2}(h+k),\bar{l}_1$	$h\;k\;\bar{l}_1$	$h\;\bar{k}_1l$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$		$2h\,0\,0$	$0\;2k\,0$	$0\;0\;2l$	$h,\quad k,\quad 0$	$2h2k0$	$2h02l$
					$h+k\equiv 0\pmod 2$		
	$P4/mmm$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
	$P4/mcc$	$(-1)^{l_1}$	$(-1)^{l_1}$	$+1$	$+1$	$+1$	$(-1)^{l}$
	$P4/nbm$	$(-1)^{k_1}$	$(-1)^{h_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h-k)}$	$(-1)^{h+k}$	$(-1)^{h}$
	$P4/nnc$	$(-1)^{k_1+l_1}$	$(-1)^{h_1+l_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{h+k}$	$(-1)^{h+l}$
	$P4/mbm$	$(-1)^{h+k_1}$	$(-1)^{h_1+k}$	$+1$	$+1$	$+1$	$(-1)^{h+k_1}$
	$P4/mnc$	$(-1)^{h+k_1+l_1}$	$(-1)^{h_1+k+l_1}$	$+1$	$+1$	$+1$	$(-1)^{h+k_1+l}$
	$P4/nmm$	$(-1)^{h}$	$(-1)^{k}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{h+k}$	$(-1)^{k_1}$
	$P4/ncc$	$(-1)^{h+l_1}$	$(-1)^{k+l_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)}$	$(-1)^{h+k}$	$(-1)^{k_1+l}$
	$P4_2/mmc$	$+1$	$+1$	$+1$	$(-1)^{l_1}$	$+1$	$+1$
	$P4_2/mcm$	$(-1)^{l_1}$	$(-1)^{l_1}$	$+1$	$(-1)^{l_1}$	$+1$	$(-1)^{l}$
	$P4_2/nbc$	$(-1)^{k_1}$	$(-1)^{h_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)+l_1}$	$(-1)^{h+k}$	$(-1)^{h}$
	$P4_2/nnm$	$(-1)^{k_1+l_1}$	$(-1)^{h_1+l_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)+l_1}$	$(-1)^{h+k}$	$(-1)^{h+l}$
	$P4_2/mbc$	$(-1)^{h+k_1}$	$(-1)^{h_1+k}$	$+1$	$(-1)^{l_1}$	$+1$	$(-1)^{h+k_1}$
	$P4_2/mnm$	$(-1)^{h+k_1+l_1}$	$(-1)^{h_1+k+l_1}$	$+1$	$(-1)^{k+l_1}$	$+1$	$(-1)^{h+k_1+l}$
	$P4_2/nmc$	$(-1)^{h}$	$(-1)^{k}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)+l_1}$	$(-1)^{h+k}$	$(-1)^{k_1}$
	$P4_2/ncm$	$(-1)^{h+l_1}$	$(-1)^{k+l_1}$	$(-1)^{h_1+k_1}$	$(-1)^{\frac{1}{2}(h+k)+l_1}$	$(-1)^{h+k}$	$(-1)^{k_1+l}$

Table 4 (*cont.*)

	$\mathbf{h}_1$	h_1kl	$\frac{1}{2}(h+k),\frac{1}{2}(\bar{h}+k),l$	$h_1,\;h+\bar{h}_1,l_1$	$h_1,\;\bar{h}+h_1,l_1$	$h_1,\;h+\bar{h}_1,l$	$h_1,\;\bar{h}+h_1,l$
	$\mathbf{h}_2$	$\bar{h}_1kl$	$\frac{1}{2}(h+\bar{k}),\frac{1}{2}(h+k),l$	$h+\bar{h}_1,\;h_1,\;\bar{l}_1$	$h+\bar{h}_1,\;\bar{h}_1,\;\bar{l}_1$	$h+\bar{h}_1,\;h_1,\;l$	$h+\bar{h}_1,\;\bar{h}_1,\;l$
$\mathbf{h}=\mathbf{h}_1+\mathbf{h}_2$		$02k2l$	$h,\quad k,\quad 2l$	$h,\quad h,\quad 0$	$h,\quad \bar{h},\quad 0$	$h,\quad h,\quad 2l$	$h,\quad \bar{h},\quad 2l$
			$h+k\equiv 0\pmod 2$				
	$P4/mmm$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$
	$P4/mcc$	$(-1)^{l}$	$+1$	$(-1)^{l_1}$	$(-1)^{l_1}$	$(-1)^{l}$	$(-1)^{l}$
	$P4/nbm$	$(-1)^{k}$	$(-1)^{\frac{1}{2}(h+k)}$	$+1$	$(-1)^{h}$	$(-1)^{h}$	$+1$
	$P4/nnc$	$(-1)^{k+l}$	$(-1)^{\frac{1}{2}(h-k)}$	$(-1)^{l_1}$	$(-1)^{h+l_1}$	$(-1)^{h+l}$	$(-1)^{l}$
	$P4/mbm$	$(-1)^{h_1+k}$	$+1$	$(-1)^{h}$	$(-1)^{h}$	$(-1)^{h}$	$(-1)^{h}$
	$P4/mnc$	$(-1)^{h_1+k+l}$	$+1$	$(-1)^{h+l_1}$	$(-1)^{h+l_1}$	$(-1)^{h+l}$	$(-1)^{h+l}$
	$P4/nmm$	$(-1)^{h_1}$	$(-1)^{\frac{1}{2}(h-k)}$	$(-1)^{h}$	$+1$	$+1$	$(-1)^{h}$
	$P4/ncc$	$(-1)^{h_1+l}$	$(-1)^{\frac{1}{2}(h-k)}$	$(-1)^{h+l_1}$	$(-1)^{l_1}$	$(-1)^{l}$	$(-1)^{h+l}$
	$P4_2/mmc$	$+1$	$(-1)^{l}$	$(-1)^{l_1}$	$(-1)^{l_1}$	$(-1)^{l}$	$(-1)^{l}$
	$P4_2/mcm$	$(-1)^{l}$	$(-1)^{l}$	$+1$	$+1$	$+1$	$+1$
	$P4_2/nbc$	$(-1)^{k}$	$(-1)^{\frac{1}{2}(h-k)+l}$	$(-1)^{l_1}$	$(-1)^{h+l_1}$	$(-1)^{h+l}$	$(-1)^{l}$
	$P4_2/nnm$	$(-1)^{k+l}$	$(-1)^{\frac{1}{2}(h-k)+l}$	$+1$	$(-1)^{h}$	$(-1)^{h}$	$+1$
	$P4_2/mbc$	$(-1)^{h_1+k}$	$(-1)^{l}$	$(-1)^{h+l_1}$	$(-1)^{h+l_1}$	$(-1)^{h+l}$	$(-1)^{h+l}$
	$P4_2/mnm$	$(-1)^{h_1+k+l}$	$(-1)^{k+l}$	$+1$	$+1$	$+1$	$+1$
	$P4_2/nmc$	$(-1)^{h_1}$	$(-1)^{\frac{1}{2}(h-k)+l}$	$(-1)^{h+l_1}$	$(-1)^{l_1}$	$(-1)^{l}$	$(-1)^{h+l}$
	$P4_2/ncm$	$(-1)^{h_1+l}$	$(-1)^{\frac{1}{2}(h-k)+l}$	$(-1)^{h}$	$+1$	$+1$	$(-1)^{h}$

$$
\begin{aligned}
{}_5R^{(0)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{2h00}+\mathscr{E}'''_{02k0}+3\mathscr{E}'''_{002l}+\mathscr{E}'''_{h+\bar{k},\,h+\bar{k},\,0}\\
&+\mathscr{E}'''_{h+k,\,h+k,\,0}+2\mathscr{E}'''_{h+k,\,\bar{h}+k,\,0})\\
&-\frac{6\sigma_8^{1/2}}{\sigma_2\sigma_4^{1/2}}(p+q-4)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}-\frac{3\sigma_4}{4\sigma_2^2}((p-2)(p-4)\\
&+(q-2)(q-4))\mathscr{E}'^2_{\mathbf{h}}+\frac{9\sigma_6}{\sigma_2\sigma_4}(p+q-4)\\
&+\frac{3\sigma_4}{16\sigma_2^2}((p-2)(q-2)+2(p-2)(p-4)\\
&+2(q-2)(q-4))+\ldots, \qquad (6{\cdot}3)
\end{aligned}
$$

$$
\begin{aligned}
{}_3R^{(0)}_{3,0} = &-\frac{\sigma_4^{1/2}}{8\sigma_2}((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}\\
&+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_1, \qquad (6{\cdot}4)
\end{aligned}
$$

where

$$
\begin{aligned}
\varrho_1 = &-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1}(\mathscr{E}'''_{h_1,\,k_1,\,l_1+2l_2}+\mathscr{E}'''_{\bar{h}_2+k_1+k_2,\,h_1+h_2+\bar{k}_2,\,l_1}\\
&+\mathscr{E}'''_{h_2+k_1+k_2,\,h_1+h_2+k_2,\,l_1})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_2}(\mathscr{E}'''_{h_2,\,k_2,\,2l_1+l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,\bar{h}_1+k_1+k_2,\,l_2}\\
&+\mathscr{E}'''_{h_1+h_2+k_1,\,h_1+k_1+k_2,\,l_2})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}(\mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,\bar{l}_1+l_2}+\mathscr{E}'''_{h_2+k_1,\,h_1+k_2,\,l_1+l_2}\\
&+\mathscr{E}'''_{h_2+\bar{k}_1,\,\bar{h}_1+k_2,\,l_1+l_2})+\ldots, \qquad (6{\cdot}5)
\end{aligned}
$$

$$
\begin{aligned}
{}_4R^{(0)}_{3,0} = &-\frac{\sigma_4^{1/2}}{8\sigma_2}((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}\\
&+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_2, \qquad (6{\cdot}6)
\end{aligned}
$$

where

$$
\begin{aligned}
\varrho_2 = &-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1}(\mathscr{E}'''_{h_1,\,k_1,\,l_1+2l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+k_1+k_2,\,l_1}\\
&+\mathscr{E}'''_{h_2+\bar{k}_1+\bar{k}_2,\,h_1+h_2+k_2,\,l_1})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_2}(\mathscr{E}'''_{h_2,\,k_2,\,2l_1+l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_2}\\
&+\mathscr{E}'''_{h_1+h_2+k_1,\,\bar{h}_1+k_1+k_2,\,l_2})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}(\mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,\bar{l}_1+l_2}\\
&+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1,\,l_1+l_2}+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_2,\,l_1+l_2})+\ldots, \qquad (6{\cdot}7)
\end{aligned}
$$

and

$$
\begin{aligned}
{}_5R^{(0)}_{3,0} = &-\frac{3\sigma_4^{1/2}}{8\sigma_2}((r-2)\mathscr{E}'^2_{\mathbf{h}_1}+(p-2)\mathscr{E}'^2_{\mathbf{h}_2}\\
&+(q-2)\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_3, \qquad (6{\cdot}8)
\end{aligned}
$$

where

$$
\begin{aligned}
\varrho_3 = &-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1}(\mathscr{E}'''_{h_1+2h_2,\,k_1,\,l_1}+\mathscr{E}'''_{h_1,\,k_1+2k_2,\,l_1}\\
&+3\mathscr{E}'''_{h_1,\,k_1,\,l_1+2l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+k_1+k_2,\,l_1}\\
&+\mathscr{E}'''_{h_2+\bar{k}_1+\bar{k}_2,\,h_1+h_2+k_2,\,l_1}+\mathscr{E}'''_{h_1+h_2+\bar{k}_2,\,h_2+\bar{k}_1+\bar{k}_2,\,l_1}\\
&+\mathscr{E}'''_{h_1+h_2+k_2,\,h_2+k_1+k_2,\,l_1})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_2}(\mathscr{E}'''_{2h_1+h_2,\,k_2,\,l_2}+\mathscr{E}'''_{h_2,\,2k_1+k_2,\,l_2}\\
&+3\mathscr{E}'''_{h_2,\,k_2,\,2l_1+l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,h_1+k_1+k_2,\,l_2}\\
&+\mathscr{E}'''_{h_1+h_2+k_1,\,\bar{h}_1+k_1+k_2,\,l_2}+\mathscr{E}'''_{h_1+h_2+\bar{k}_1,\,\bar{h}_1+k_1+k_2,\,l_2}\\
&+\mathscr{E}'''_{h_1+k_1+k_2,\,h_1+h_2+k_1,\,l_2})\\
&-\frac{\sigma_8^{1/2}}{\sigma_4}\mathscr{E}'_{\mathbf{h}_1+\mathbf{h}_2}(\mathscr{E}'''_{h_1+\bar{h}_2,\,k_1+k_2,\,l_1+l_2}\\
&+\mathscr{E}'''_{h_1+h_2,\,k_1+\bar{k}_2,\,l_1+l_2}+3\mathscr{E}'''_{h_1+h_2,\,k_1+k_2,\,l_1+\bar{l}_2}\\
&+\mathscr{E}'''_{h_1+\bar{k}_2,\,h_2+k_1,\,l_1+l_2}+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+k_2,\,l_1+l_2}\\
&+\mathscr{E}'''_{h_2+k_1,\,h_1+k_2,\,l_1+l_2}+\mathscr{E}'''_{h_2+\bar{k}_1,\,h_1+\bar{k}_2,\,l_1+l_2})+\ldots. \qquad (6{\cdot}9)
\end{aligned}
$$

Next we define (where $C_n(t)$ is replaced by C_n):

$$
\begin{aligned}
{}_3R^{(1)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{002l}+\mathscr{E}'''_{h+\bar{k},\,\bar{h}+k,\,0}+\mathscr{E}'''_{h+k,\,h+k,\,0})\\
&+\frac{4\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}}-\frac{4\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)\\
&+\frac{\sigma_4}{16C_1^2\sigma_2^2}((2C_1-C_2)^2+4C_1(8C_1-6C_2+C_3))+\ldots, \qquad (6{\cdot}10)
\end{aligned}
$$

$$
\begin{aligned}
{}_4R^{(1)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{002l}+2\mathscr{E}'''_{h+k,\,\bar{h}+k,\,0})\\
&+\frac{4\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}}-\frac{4\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)\\
&+\frac{\sigma_4}{16C_1^2\sigma_2^2}((2C_1-C_2)^2+4C_1(8C_1-6C_2+C_3))+\ldots, \qquad (6{\cdot}11)
\end{aligned}
$$

$$
\begin{aligned}
{}_5R^{(1)}_{2,0} = &-\frac{\sigma_8^{1/2}}{\sigma_4}(\mathscr{E}'''_{2h00}+\mathscr{E}'''_{02k0}+3\mathscr{E}'''_{002l}+\mathscr{E}'''_{h+\bar{k},\,h+\bar{k},\,0}\\
&+\mathscr{E}'''_{h+k,\,h+k,\,0}+2\mathscr{E}'''_{h+k,\,\bar{h}+k,\,0})\\
&+\frac{12\sigma_8^{1/2}}{C_1\sigma_2\sigma_4^{1/2}}(2C_1-C_2)\mathscr{E}'_{\mathbf{h}}\mathscr{E}'''_{\mathbf{h}}\\
&-\frac{3\sigma_4}{2C_1\sigma_2^2}(8C_1-6C_2+C_3)\mathscr{E}'^2_{\mathbf{h}}\\
&-\frac{18\sigma_6}{C_1\sigma_2\sigma_4}(2C_1-C_2)+\frac{3\sigma_4}{16C_1^2\sigma_2^2}((2C_1-C_2)^2\\
&+4C_1(8C_1-6C_2+C_3))+\ldots, \qquad (6{\cdot}12)
\end{aligned}
$$

$$ {}_3R^{(1)}_{3,0} = \frac{\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)(\mathscr{E}'^2_{\mathbf{h}_1}+\mathscr{E}'^2_{\mathbf{h}_2}+\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_1 , \quad (6\cdot13) $$

$$ {}_4R^{(1)}_{3,0} = \frac{\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)(\mathscr{E}'^2_{\mathbf{h}_1}+\mathscr{E}'^2_{\mathbf{h}_2}+\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_2 , \quad (6\cdot14) $$

and

$$ {}_5R^{(1)}_{3,0} = \frac{3\sigma_4^{1/2}}{8C_1\sigma_2}(2C_1-C_2)(\mathscr{E}'^2_{\mathbf{h}_1}+\mathscr{E}'^2_{\mathbf{h}_2}+\mathscr{E}'^2_{\mathbf{h}_1+\mathbf{h}_2})+\varrho_3 . \quad (6\cdot15) $$

For space groups $C2/m$ and $C2/c$, we have

$$ R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0}+\ldots ; \quad i = 2, 3; \quad j = 0, 1 , \quad (6\cdot16) $$

where ${}_1R^{(0)}_{2,0}$, ${}_1R^{(0)}_{3,0}$, ${}_1R^{(1)}_{2,0}$ and ${}_1R^{(1)}_{3,0}$ are defined in 1*P* (1959).

For the six conventionally *C*-centered centrosymmetric space groups of the orthorhombic system, we have

$$ R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0}+{}_3R^{(j)}_{i,0}+\ldots ; \quad i = 2, 3; \quad j = 0, 1 . \quad (6\cdot17) $$

For space groups $P4/m$, $P4_2/m$, $P4/n$, and $P4_2/n$, we have

$$ R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0}+{}_4R^{(j)}_{i,0}+\ldots ; \quad i = 2, 3; \quad j = 0, 1 . \quad (6\cdot18) $$

For the sixteen remaining conventionally primitive centrosymmetric space groups in the tetragonal system, we have

$$ R^{(j)}_{i,0} = {}_1R^{(j)}_{i,0}+{}_5R^{(j)}_{i,0}+\ldots ; \quad i = 2, 3; \quad j = 0, 1 . \quad (6\cdot19) $$

It is seen that the remainder terms in the basic formulas are especially simple for the special case, $p = q = r = 2$. For this case, the formulas reduce to those obtainable by the algebraic methods proposed by us (1957).

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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Crystallographic data for benzenearsonic acid.

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Crystals of benzenearsonic acid were grown by room temperature evaporation of an alcohol solution. They appeared as transparent orthorhombic prisms, elongated in the direction subsequently designated as the *c* axis. The prism form {110} was well-developed, but the terminal faces occurred as curved surfaces so they could not be identified. The dimensions of the unit cell, measured from rotation and Weissenberg photographs are as follows (λ of Cu $K\alpha$ = 1·5418 Å):

$a_0 = 14{\cdot}90\pm0{\cdot}03$, $b_0 = 10{\cdot}49\pm0{\cdot}03$, $c_0 = 4{\cdot}69\pm0{\cdot}02$ Å .

The reported density is 1·760 g.cm.$^{-3}$ (Lange's *Handbook of Chemistry*, ninth edition). The density calculated for four molecules of $C_6H_7O_3As$ per unit cell is 1·830 g.cm.$^{-3}$. The observed extinctions ($h00$ present only with $h = 2n$, $0k0$ present only with $k = 2n$, and $00l$ present only with $l = 2n$) determine the space group as $P2_12_12_1$. Powder diffraction data for benzenearsonic acid, obtained with a Norelco diffractometer using nickel-filtered Cu $K\alpha$ radiation, is given in Table 1.

Table 1. *Powder diffraction data for benzenearsonic acid*

d (Å)	I/I_0	d (Å)	I/I_0
8·51	98	2·87	7
6·07	15	2·82	5
5·25	40	2·62	3
4·94	100	2·52	1
4·51	5	2·49	2
4·29	5	2·42	2
4·13	6	2·27	3
3·97	4	2·25	3
3·75	26	2·20	3
3·62	20	2·15	2
3·51	1	2·09	6
3·41	3	2·03	3
3·24	3	1·98	2
3·18	22	1·94	3
3·05	2	1·91	2

Work on this substance is being continued to obtain the detailed structure of the crystal and the molecule.