quite good regions but others were much less clear. We show in Fig. 1 one of the better portions of a *FRODO* map (Jones, 1985) for RNA from our final phases, with the structure superimposed. We conclude that the results for RNA are rather marginal; to progress from the starting point we provide to a complete elucidation of the structure would probably be possible, but would certainly require prior stereochemical information and much experience in protein crystallography.

Concluding remarks

We are encouraged by the fact that for a structure of the size of RNA the automatic procedures we have so far devised can give results at the margin of being useful. One thing we have confirmed, although it is a well known effect, is that the accuracy of the data is very critical in work of this kind. When we repeat analyses using calculated data from the known structure then there results a remarkable improvement in phase estimates. We are hoping to strengthen our analytical methods but we hope that experimentalists will also be able to improve the quality of the data they provide.

We are most grateful to the Royal Society and the Chinese Academy of Sciences with whose support the collaborative research at Beijing and York is carried out. One of us (HQ) is also indebted to the Royal Society for the award of a Royal Fellowship. Direct-methods work at York is supported by the Science and Engineering Research Council, the Wellcome Trust and the Wolfson Foundation, to whom we give thanks.

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The Application of One-Wavelength Anomalous Scattering. II. An Analytical Approach for Phase Determination

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Abstract

An analytical method has been developed by which phase estimates may be uniquely determined from one-wavelength anomalous-scattering data; the method as described can be applied to structures containing one type of anomalous scatterer. The method has been tested on two structures. The first is an Hg derivative of a small protein, avian pancreatic polypeptide (App), crystallizing in space group $C2$ with one molecule of 36 amino-acid residues in the asymmetric unit. The second is a Pt derivative of ribonuclease Sa (RNA), crystallizing in space group $P2_12_12_1$ with two molecules of 96 amino-acid residues in the asymmetric unit. The phases for App give an electron density map which can easily be interpreted in terms of a model. For RNA the map is less clear but has strong similarities with the true map and could probably be interpreted. If anomalous scatterers are centrosymmetrically arranged then the analysis shows

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that there is a simple alternative process for calculating a map, called a B_P map, which directly shows a structural image.

Introduction

It is usually assumed that one-wavelength anomalous-scattering data can only give phases with an ambiguity and, indeed, much effort has been put into finding techniques for resolving the ambiguity (*e.g.* Kartha, 1961; Fan Hai-fu, Han Fu-son, Qian Jin-zi & Yao Jia-xing, 1984). Karle (1989) has demonstrated the use of exact linear equations for one-wavelength anomalous scattering, the effectiveness of which was illustrated with calculated data having a superimposed random error. However, it was much earlier shown by Okaya, Saito & Pepinsky (1955), and more recently demonstrated by Hao Quan & Woolfson (1989), that the ambiguity is not really present as long as the locations of the anomalous scatterers are known. The calculation of a map, the P_s function, which requires only knowledge of differences between anomalous intensities, $|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2$, shows vectors from each anomalous scatterer to each non-anomalous scatterer, and also vectors between anomalous scatterers of different types. If the positions of the anomalous scatterers are known then a superposition function will, in principle, show an image of the complete structure. However, the P_s map is antisymmetric and for each positive peak there is a negative peak in the opposite direction. Cancellation of positive and negative density destroys information and degrades the resultant image.

It occurred to us that it might be possible to find an analytical alternative to the P_s function approach and this development is described here.

Analysis

We shall consider the case of a structure containing N atoms in the unit cell with $N-m$ of them being anomalous scatterers. We shall take the scattering factors as f_j+if_j'' so that the real part includes that from anomalous scattering where it occurs. We may now write structure factors as

$$F(\mathbf{h})=\sum_{i=1}^{N}(f_i+if_i'')\exp(2\pi i\mathbf{h}\,.\,\mathbf{r}_i) \qquad (1)$$

and

$$F(\bar{\mathbf{h}})=\sum_{i=1}^{N}(f_i+if_i'')\exp(-2\pi i\mathbf{h}\,.\,\mathbf{r}_i). \qquad (2)$$

Following Okaya, Saito & Pepinsky (1955) we find

$$|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2=2\sum_{i=1}^{N}\sum_{j=1}^{N}(f_j''f_i-f_i''f_j)\times\sin[2\pi\mathbf{h}\,.\,(\mathbf{r}_i-\mathbf{r}_j)]. \qquad (3)$$

We now define

$$F^0(\mathbf{h})=\sum_{i=1}^{N}f_i\exp(2\pi i\mathbf{h}\,.\,\mathbf{r}_i)=A^0(\mathbf{h})+iB^0(\mathbf{h}) \qquad (4)$$

where

$$A^0(\mathbf{h})=\sum_{i=1}^{m}f_i\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_i)+\sum_{i=m+1}^{N}f_i\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_i) \qquad (5)$$

and

$$B^0(\mathbf{h})=\sum_{i=1}^{m}f_i\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_i)+\sum_{i=m+1}^{N}f_i\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_i). \qquad (6)$$

We shall assume that all the anomalous scatterers are of the same kind, which means that there are no non-zero terms in (3) relating to interactions between anomalous scatterers. In such a circumstance (3) may be rewritten in the form

$$|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2=4\sum_{j=m+1}^{N}f_j''\sum_{i=1}^{m}f_i\sin[2\pi\mathbf{h}\,.\,(\mathbf{r}_i-\mathbf{r}_j)]. \qquad (7)$$

When all the anomalous scatterers are equal the ratio $g=f_i/f_i''$ is independent of site occupancy or thermal motion. This enables us to write

$$A^0(\mathbf{h})=\sum_{i=1}^{m}f_i\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_i)+ga(\mathbf{h}) \qquad (8)$$

and

$$B^0(\mathbf{h})=\sum_{i=1}^{m}f_i\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_i)+gb(\mathbf{h}) \qquad (9)$$

where

$$a(\mathbf{h})=\sum_{i=m+1}^{N}f_i''\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_i) \qquad (10)$$

and

$$b(\mathbf{h})=\sum_{i=m+1}^{N}f_i''\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_i). \qquad (11)$$

Since

$$\sum_{i=1}^{m}f_i\sin[2\pi\mathbf{h}\,.\,(\mathbf{r}_i-\mathbf{r}_j)]=\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_j)\sum_{i=1}^{m}f_i\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_i)-\sin(2\pi\mathbf{h}\,.\,\mathbf{r}_j)\sum_{i=1}^{m}f_i\cos(2\pi\mathbf{h}\,.\,\mathbf{r}_i) \qquad (12)$$

we have

$$4\sum_{j=m+1}^{N} f_j'' \sum_{i=1}^{m} f_i \sin[2\pi\mathbf{h}.(\mathbf{r}_i-\mathbf{r}_j)]$$
$$=4\sum_{j=m+1}^{N} f_j'' \cos(2\pi\mathbf{h}.\mathbf{r}_j)[B^0(\mathbf{h})-gb(\mathbf{h})]$$
$$-4\sum_{j=m+1}^{N} f_j'' \sin(2\pi\mathbf{h}.\mathbf{r}_j)[A^0(\mathbf{h})-ga(\mathbf{h})]$$
$$=4\{a(\mathbf{h})[B^0(\mathbf{h})-gb(\mathbf{h})]-b(\mathbf{h})[A^0(\mathbf{h})-ga(\mathbf{h})]\}$$
$$=4[a(\mathbf{h})B^0(\mathbf{h})-b(\mathbf{h})A^0(\mathbf{h})]. \quad (13)$$

Thus (7) can be written as

$$|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2=4[a(\mathbf{h})B^0(\mathbf{h})-b(\mathbf{h})A^0(\mathbf{h})] \quad (14)$$

or

$$\sin[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]=\frac{|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2}{4|F^0(\mathbf{h})|[a(\mathbf{h})^2+b(\mathbf{h})^2]^{1/2}} \quad (15)$$

where $\tan[\varphi(\mathbf{h})]=B^0(\mathbf{h})/A^0(\mathbf{h})$ and $\tan[\varepsilon(\mathbf{h})]=b(\mathbf{h})/a(\mathbf{h})$.

The angle $\varphi(\mathbf{h})$ is the phase of the structure factor of the protein with scattering factors equal to the total real part of the anomalous-scattering factor for the anomalous scatterers. Equation (15) gives the sine of the difference of angle φ and the phase of the heavy-atom substructure, ε. Since we only find the sine of the angle we are still left with a phase ambiguity.

We now return to the P_s function given by Okaya, Saito & Pepinsky (1955). This is

$$P_s(\mathbf{u})=\sum_{\mathbf{h}}[|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2]\sin(2\pi\mathbf{h}.\mathbf{u}). \quad (16)$$

It was shown by Hao Quan & Woolfson (1989) that the P_s function has positive peaks of weights $4f_j''f_i$ from each anomalous scatterer to each non-anomalous scatterer and negative peaks of the same weight in the reverse direction. If the cancellation of positive and negative peaks is not too severe then the function $|P_s(\mathbf{u})|$ will have peaks of weight $4f_j''f_i$ from each anomalous scatterer to each non-anomalous scatterer and in the reverse direction as well. The Fourier transform of $|P_s(\mathbf{u})|$ gives

$$\chi(\mathbf{h})=V^{-1}\int|P_s(\mathbf{u})|\cos(2\pi\mathbf{h}.\mathbf{u})$$
$$=4\sum_{j=m+1}^{N} f_j''\sum_{i=1}^{m} f_i\cos[2\pi\mathbf{h}.(\mathbf{r}_i-\mathbf{r}_j)]$$
$$=4[a(\mathbf{h})A^0(\mathbf{h})+b(\mathbf{h})B^0(\mathbf{h})]$$
$$-4g[a(\mathbf{h})^2+b(\mathbf{h})^2]. \quad (17)$$

This gives

$$\cos[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]=\frac{\chi(\mathbf{h})+4g[a(\mathbf{h})^2+b(\mathbf{h})^2]}{4|F^0(\mathbf{h})|[a(\mathbf{h})^2+b(\mathbf{h})^2]^{1/2}}. \quad (18)$$

Table 1. *Detailed molecular information for App and RNA crystals*

	App	RNA
Space group	$C2$	$P2_12_12_1$
Number of molecules/asymmetric unit	1	2
Number of amino-acid residues/molecule	36	96
Type of anomalous scatterers (a.s.)	Hg	Pt
Number of a.s. sites/unit cell	4	20
Resolution of data (Å)	2·04	2·50
Number of independent reflexions	2109	7008
Cell dimensions		
a (Å)	34·18	64·90
b (Å)	32·92	78·32
c (Å)	28·44	38·79
β (°)	105·3	

Combining equations (15) and (18) we find

$$\tan[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]=\frac{|F(\mathbf{h})|^2-|F(\bar{\mathbf{h}})|^2}{\chi(\mathbf{h})+4g[a(\mathbf{h})^2+b(\mathbf{h})^2]}. \quad (19)$$

From this equation the phases $\varphi(\mathbf{h})$ can be determined unambiguously since $\sin[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]$ and $\cos[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]$ must have the sign of the numerator and denominator of (19) respectively.

Test procedure

Equation (19) was tested with two known proteins – a small one, an Hg derivative of avian pancreatic polypeptide (App) (Glover, Moss, Tickle, Pitts, Haneef, Wood & Blundell, 1985) and a much larger one, a Pt derivative of ribonuclease Sa (RNA) (Dodson, Sevcik, Dodson & Zelinka, 1987). Details of the two crystals are given in Table 1. From anomalous differences,

$$\Delta F(\mathbf{h})=|F(\mathbf{h})|-|F(\bar{\mathbf{h}})|, \quad (20)$$

as input for the direct-methods program *MULTAN* the four Hg sites in App and the twenty Pt sites, with occupancies from 0·18 to 0·42, in RNA were found (Dodson *et al.*, 1987). These positions could then be used to find $a(\mathbf{h})$, $b(\mathbf{h})$ and $\varepsilon(\mathbf{h})$.

The diffraction data employed were provided in the form of $\overline{F(\mathbf{h})}=[|F(\mathbf{h})|+|F(\bar{\mathbf{h}})|]/2$ and $\Delta F(\mathbf{h})$, so (19) was taken in the form

$$\tan[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]=\frac{2\overline{F(\mathbf{h})}\Delta F(\mathbf{h})}{\chi(\mathbf{h})+4g[a(\mathbf{h})^2+b(\mathbf{h})^2]}. \quad (21)$$

In order to compensate for possible scaling errors in the data and approximations in the analysis – for example, the assumption that no information is lost in the $|P_s|$ map – we took steps to scale the top and bottom of the right-hand side of (21). These were

(i) Normalize $\overline{F(\mathbf{h})}$ to an absolute scale by Wilson statistics.

(ii) Normalize $\Delta F(\mathbf{h})$ by Wilson statistics taking into account only the contributions of the anomalous scatterers.

Table 2. *Phase errors for App given by the analytical method, arranged in descending order of* $\alpha|F_o|$

F_o: observed structure factor
α: figure of merit from equation (22)
NR: number of reflexions in the group
$\alpha|F_o|$: minimum $\alpha|F_o|$ in the group
WME: $\alpha|F_o|$-weighted mean phase error
ME: mean phase error

NR	$\alpha\|F_o\|$	WME (°)	ME (°)
200	2574	34·92	35·31
400	1579	33·01	31·93
600	1120	33·15	32·64
800	839	33·51	33·63
1000	629	33·80	34·47
1200	478	33·65	33·77
1400	336	33·78	34·28
1600	220	34·08	35·72
1800	121	34·33	37·42
2000	42	34·54	40·29
2109	0	34·57	41·80

Table 3. *Phase errors for RNA given by the analytical method, arranged in descending order of* $\alpha|F_o|$

F_o: observed structure factor
α: figure of merit from (22)
NR: number of reflexions in the group
$\alpha|F_o|$: minimum $\alpha|F_o|$ in the group
WME: $\alpha|F_o|$-weighted mean phase error
ME: mean phase error

NR	$\alpha\|F_o\|$	WME (°)	Me (°)
500	10 748	43·64	44·62
1000	6847	45·57	47·24
1500	4852	47·33	50·06
2000	3612	49·00	53·10
2500	2810	50·52	55·80
3000	2261	51·51	57·98
3500	1800	52·47	60·08
4000	1409	53·33	62·23
4500	1084	53·96	63·93
5000	816	54·50	65·69
5500	567	54·91	67·34
6000	346	55·17	68·74
6500	162	55·36	70·57
7008	0	55·42	72·22

(iii) Scale $\chi(\mathbf{h})$ to make the mean squared values of the top and bottom equal, on the assumption that the distribution of values of $\varphi(\mathbf{h})-\varepsilon(\mathbf{h})$ is random so that $\overline{\sin^2[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]}$ is equal to $\overline{\cos^2[\varphi(\mathbf{h})-\varepsilon(\mathbf{h})]}$.

From (19) we can also derive a figure of merit for the phase estimate based on the magnitudes of the numerator and denominator. This is

$$\alpha(\mathbf{h}) = ([|F(\mathbf{h})|^2 - |F(\mathbf{h})|^2]^2 + \{\chi(\mathbf{h}) + 4g[a(\mathbf{h})^2 + b(\mathbf{h})^2]\}^2)^{1/2}. \quad (22)$$

Test results

Phases $\varphi(\mathbf{h})$ derived from (21) have been compared with the true phases calculated from the known structures and a digest of the phase errors is given in Tables 2 and 3 for App and RNA respectively. The reflexions have been taken in the order of $\alpha(\mathbf{h})|F_o(\mathbf{h})|$ where $|F_o(\mathbf{h})|$ is the observed structure amplitude. We have also calculated conventional correlation coefficients between electron density maps calculated with the $\varphi(\mathbf{h})$'s, namely A maps, and the true phases. A weighting scheme, similar to that proposed by Sim (1960) was used in calculating the map. Each Fourier term had a weight

$$\frac{I_1[k\alpha(\mathbf{h})|F_o(\mathbf{h})|]}{I_0[k\alpha(\mathbf{h})|F_o(\mathbf{h})|]},$$

where I_1 and I_0 are modified Bessel functions and k is a scale factor chosen arbitrarily to give an equal number of reflexions with weights greater than 0·5 and less than 0·5.

In the case of App the mean phase error for all the 2109 reflexions within the 2·04 Å sphere of observation was 41·80° but with $\alpha|F_o|$ weighting this was reduced to 34·57°. The A map resembled the true map fairly closely with a correlation coefficient of 0·61. In Fig. 1 we compare a part of the three-dimensional map and the true model plotted by *FRODO* (Jones, 1985). There is little doubt that this map would lead to a complete structure determination.

For RNA, since there are 1746 independent atomic positions to be determined and the twenty anomalous scatterers had various occupancies, the method was faced with a real challenge. Although the mean phase error for the 7008 reflexions within 2·5 Å resolution was 72·22° the $\alpha|F_o|$ weighted mean phase error was only 55·42° showing that the phase error was strongly correlated with the weights used. The weighted map has a correlation coefficient of 0·42 when compared with a true density map and a portion of it is shown in Fig. 2; the agreement is far from perfect but the chacteristics of the true model can be seen. However,

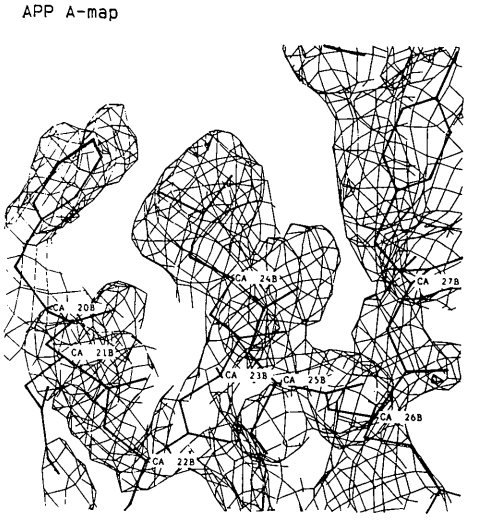

Fig. 1. Part of a *FRODO* map for App with the true model superimposed.

there is no doubt that prior stereochemical information would be required to interpret this map successfully.

A special case

Let $\mathbb{F}$ denote Fourier transformation. Then from (4) we have

$$\rho(\mathbf{r}) = \mathbb{F}[A^0(\mathbf{h}) + iB^0(\mathbf{h})] \tag{23}$$

where $\rho(\mathbf{r})$ differs slightly from the true electron density because of the contribution of the real part of anomalous scattering in the equation.

In similar fashion we can write

$$\rho(-\mathbf{r}) = \mathbb{F}[A^0(\mathbf{h}) - iB^0(\mathbf{h})]. \tag{24}$$

Subtracting (24) from (23) gives

$$\mathbb{F}[iB^0(\mathbf{h})] = [\rho(\mathbf{r}) - \rho(-\mathbf{r})]/2. \tag{25}$$

The positive regions of $\mathbb{F}[iB^0(\mathbf{h})]$, which we call a B_P map, contain all the information about the structure except for those arrangements where $\rho(\mathbf{r})$ overlaps $\rho(-\mathbf{r})$, *i.e.* centrosymmetric with respect to the chosen origin.

In general we cannot obtain a B_P map from one-wavelength anomalous-scattering data. However, if the anomalous scatterers happen to be in a centrosymmetric arrangement then $b(\mathbf{h}) = 0$ and from (14) we find

$$B^0(\mathbf{h}) = [|F(\mathbf{h})|^2 - |F(\bar{\mathbf{h}})|^2]/4a(\mathbf{h}). \tag{26}$$

In this case the B_P map can be calculated directly. The Hg atoms in App form a centrosymmetric arrangement and hence, by means of (26), we were able to calculate $\mathbb{F}^{-1}[iB^0(\mathbf{h})]$. Setting the negative density to zero gave the map B_P which is dominated by density representing the true structure. With density added at the Hg sites the B_P map was compared with the true density for the Hg derivative; the correlation coefficient was 0·62. The phase comparisons are shown in Table 4. There is a mean phase error of 40·81° but this reduces to 37·49° when weights $|F_oF_c|$ are taken, where F_c is the Fourier coefficient of the B_P map. For App the B_P map has a similar quality to that obtained by the procedure involving the use of (21) but the process is much simpler to apply.

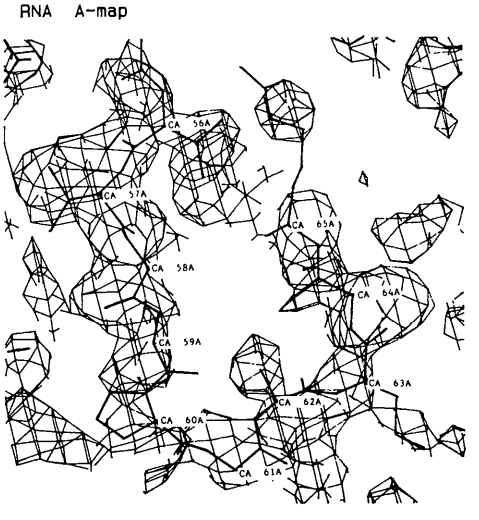

Fig. 2. Part of a *FRODO* map for RNA with the true model superimposed.

Table 4. *Errors of App B_P map arranged in descending order of $|F_oF_c|$*

F_o: observed structure factor
F_c: calculated structure factor from B_P map
NR: number of reflexions in the group
$|F_oF_c|$: minimum $|F_oF_c|$ in the group
WME: $|F_oF_c|$-weighted mean phase error
ME: mean phase error

NR	$\|F_oF_c\|$	WME (°)	ME (°)
200	3947	35·83	34·31
400	2675	35·94	35·26
600	2020	36·83	37·15
800	1596	36·86	37·08
1000	1290	36·75	36·80
1200	1019	36·56	36·31
1400	805	36·73	36·78
1600	589	36·99	37·61
1800	364	37·26	38·71
2000	163	37·42	39·68
2109	0	37·49	40·81

Concluding remarks

In this paper we have presented two methods for the *ab initio* determination of phases in protein crystallography using one-wavelength anomalous-scattering data. The analytical method can be used for general cases but where the anomalous scatterers have a centrosymmetric arrangement the much simpler B_P map method may be used. Unlike the P_s-function method (Hao Quan & Woolfson, 1989) neither of these methods requires a superposition procedure to be used, which avoids density cancellation and a residue of ghost peaks. We are hoping that further investigations will greatly improve the quality of the information acquired by methods of this type.

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Complete Reduction Bases for the Principal Induced Representations of the Crystallographic Point Groups

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Abstract

An ordered partition P of a point group G is constructed in left cosets $H_{\ldots\beta\alpha} = \ldots B^\beta A^\alpha H$ related to a subgroup H by means of selected genitors $A, B, \ldots$:

$$P = \{H_{\ldots\beta\alpha} \mid \alpha = 1 \text{ to } a, \beta = 1 \text{ to } b, \ldots\},$$

$$ab\ldots = |G|/|H|.$$

This partition P spans a principal induced representation (PIR) $R(H:G)$ of G. Then a basis L of this PIR is built:

$$L = \{V_{\ldots kj} \mid j = 1 \text{ to } a, k = 1 \text{ to } b, \ldots\}$$

with

$$V_{\ldots kj} = \cdots \sum_{\beta=1}^{b} \sum_{\alpha=1}^{a} \exp[2i\pi(\cdots + k\beta/b + j\alpha/a)] H_{\ldots\beta\alpha}.$$

In many cases L is a complete reduction basis (CRB) of $R(H:G)$ for which all matrices are fully reduced. The possibility of obtaining such a CRB depends on the algebraic structure of the group G, on the considered subgroup H and on the choice of genitors $A, B, \ldots$. Methods are proposed using subgroup chain properties, invariant inductor subgroup properties, direct product properties etc. These methods have been applied to crystallographic point groups. Complete tables of CRBs are recorded for all PIRs of all crystallographic point groups except for a few PIRs of the point groups 432, $\bar{4}3m$ and $m\bar{3}m$.

Introduction

In practice the reduction of a reducible representation Γ of a group is not an easy task. The purpose is not only to determine the irreducible representations (IR) which are the components of Γ but also to find a basis of the representation vector space for which the matrices of Γ are all in a reduced form. When each irreducible component appears once only, the projection operators are usually used (Schonland, 1971; Bradley & Cracknell, 1972; Labarre, 1978); they lead to the required basis by a more or less laborious task. 'The problem is more complicated when the same IR appears several times in Γ.... There is no general method... one proceeds as best as one can, guiding oneself according to the form of the matrices of Γ' (Schonland, 1971).* In the case of induced representations, reduction methods have been proposed by Bradley & Cracknell (1972) which applied to representations induced by invariant subgroups.

In the present paper we will show that it is often possible in the case of a principal induced representation (PIR) of a point group G, to build a reduced basis; it is not necessary to use the group algebra $\mathcal{A}$ of G but a vector subspace Ω, the dimension of which is smaller than that of $\mathcal{A}$;† the vectors of this subspace are the cosets of the partition of G relating to the subgroup H inducing the PIR of G. It is not necessary for H to be invariant in G; no matrix diagonalization is needed in the reduction process; only the knowledge of the group multiplication table is required. An application of the method is to be able to propose basis vectors and reduced matrices for each IR of G.

I. Building the ordered partition

The PIR properties of a group are well known (Lomont, 1959; Murnagham, 1963; Kirillov, 1976).

* After the French edition.

† Except in the event of an inductor subgroup reduced to the identity element. In this case Ω is identical to $\mathcal{A}$.

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