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Modification of X-ray Atomic Scattering Factors in Electric Fields–Validation of the Shell Model

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(*Received* 11 *November* 1983; *accepted* 27 *July* 1984)

Abstract

Quantum-mechanical calculations of the modification of the X-ray scattering factor of an atom/ion in an electric field are compared with predictions of the semi-classical shell model. If the shell parameters are fitted to the dipole polarizability of the ion, the shell model is a very good representation of the scattering factor of the deformed ion, giving support to its use in estimating the effect of ionic deformation on X-ray diffuse scattering and X-ray Debye–Waller factors.

1. Introduction

Born (1942) was the first to consider the effect of modification of atomic scattering factors due to deformation of vibrating atoms and ions. More recently, Buyers & Smith (1966), Melvin, Pirie & Smith (1968) and Reid (1974*a*, *b*) have applied the shell model to investigate the effects of ionic deformation on X-ray diffuse scattering from alkali halides. In its simplest form the shell model, originally developed by Dick & Overhauser (1958) to account for dielectric properties of alkali halides, separates the ion into a core and a shell coupled by a spring and has, with various modifications, proved a very useful classical parametrization of inter-ionic force constants. However, its ability to describe modifications of atomic scattering due to ionic deformation is less clear. Melvin, Pirie & Smith (1968) and Reid (1974*a*, *b*) plausibly assign to the core and the shell quantum-mechanically calculated charge distributions characteristic of the inner and outer electrons in the ion and, using the core–shell displacements calculated from the lattice-dynamical shell-model calculations, estimate the resultant changes in diffuse X-ray intensity due to the modified scattering factors. Robertson & Reid (1979) have made similar applications of the shell model to X-ray scattering from Si, while Reid & Pirie (1980) and Reid (1983) have used the model to estimate the effect of ionic deformation on Debye–Waller factors. Although March & Wilkins (1978) have developed a method of calculating elastic X-ray scattering from solids in terms of non-rigid pseudoatoms, this quantum-mechanical approach cannot be readily compared with semi-classical shell-model specifications of charge deformation.

In this paper we attempt an evaluation of the effectiveness of the simple shell model in specifying charge deformation of atoms and ions by comparing quantum-mechanical calculations of perturbed X-ray atomic scattering factors with shell-model predictions for isolated atoms or ions in electric fields. § 2 compares the shell-model theory with the corresponding quantum-mechanical theory. § 3 discusses the Kirkwood–Pople–Schofield method of calculating perturbed wave functions, while § 4 analyses the results of the calculations. Finally, § 5 discusses the validation of the shell model in simulating dynamical deformation of atomic/ionic scattering factors, and potential application of such mechanical models to describe static modifications of scattering factors in low-symmetry environments.

2. Theory

The X-ray atomic scattering factor for an unperturbed atom with N electrons is given by

$$f_0 = \sum_{j=1}^{N} \int \psi_0^* \exp(i\chi \mathbf{S} \cdot \mathbf{r}_j)\psi_0 \, d\tau, \qquad (1)$$

where $\psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_j, \ldots, \mathbf{r}_N)$ is the many-electron wave function of the atom, $\mathbf{S} = \mathbf{s} - \mathbf{s}_0$ is the difference

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between unit vectors in the direction of the incident and scattered beams and $\chi = 2\pi/\lambda$, where λ is the X-ray wavelength. If $2\theta_s$ is the angle between the incident and the scattered beams, we define

$$K = (4\pi/\lambda)\sin\theta_s \qquad (2)$$

and, setting **S** in the Z direction,

$$f_0 = \sum_{j=1}^{N} \int \psi_0^* \exp(iKr_j\cos\theta_j)\psi_0\,d\tau. \qquad (3)$$

In the presence of an electric field **F**, the wave function is perturbed, but only the component of the field in the **S** direction will modify the scattering factor to linear order in the magnitude of the field. Following Buckingham (1964), we consider a field **F** in the direction of the scattering vector. Then

$$f = f_0 + if_1F + O(F^2), \qquad (4)$$

where

$$if_1F = 2F\sum_j \int \psi_0^* \exp(iK\hat{\mathbf{S}}\,.\,\mathbf{r}_j)\psi_1\,d\tau. \qquad (5)$$

and $F\psi_1$ is the change in the many-electron wave function to first order.

For small-angle scattering, *i.e.* K small,

$$f_1F \simeq -K\alpha F, \qquad (6)$$

where α is the dipole polarizability. Quantum mechanically the calculation of f_1 is therefore a natural extension of conventional atomic polarizability calculations.

We may contrast this with the corresponding shell-model formulation of Melvin, Pirie & Smith (1968). The charge density in the ion is given by

$$\rho(\mathbf{r}) = \rho_c(\mathbf{r}) + \rho_s(\mathbf{r}) \qquad (7)$$

i.e. the sum of core and shell charge distributions (Fig. 1) and the atomic scattering factor is then initially given by

$$f_0(\mathbf{K}) = f_c(\mathbf{K}) + f_s(\mathbf{K}). \qquad (8)$$

With a field **F** in the Z direction, let us assume a displacement of magnitude ω of shell with respect to the core, giving

$$f(K) = f_c(K) + f_s(K)\exp(-iK\omega). \qquad (9)$$

Expanding to include only terms linear in ω (and so F) we have

$$f(K) = f_0 + iFf_1, \qquad (9')$$

where

$$f_1(K)F = -K\omega f_s(K). \qquad (9'')$$

Now, $f_s(0) = Z_s$, where Z_s is the shell charge, and the shell model is parametrized so that

$$Z_s\omega = \alpha F.$$

Hence,

$$f_1(K)F = -K\alpha F f_s(K)/Z_s \qquad (10)$$

and for small K

$$f_1F \simeq -K\alpha F \qquad (6')$$

as before, *i.e.* the shell model and the quantum-mechanical model give identical results for small scattering vectors. We now wish to compare the two models at finite K with $f_s(K)$ in (9″) calculated from the outer-electron ground-state wave functions of the atom or ion, and ψ_1 in (5) calculated by the Kirkwood-Pople-Schofield method.

3. Kirkwood–Pople–Schofield calculation of perturbed wave functions

The Kirkwood-Pople-Schofield approach is a particularly simple method of calculating the wave functions of an atom or ion perturbed by an electric field. Its successes are reviewed by Thorhallson, Fisk & Fraga (1968) and Fraga, Karlowski & Sazenda (1976). The modified state wave function is expressed in the form

$$\psi = \psi_0\left[1 + \sum_j U(\mathbf{r}_j)\right], \qquad (11)$$

where the $\mathbf{r}_j$ are with respect to a coordinate system with the electric field in the Z direction. $U(\mathbf{r})$ is approximated by

$$U(\mathbf{r}) = F(\mu r + \nu r^2)\cos\theta \qquad (12)$$

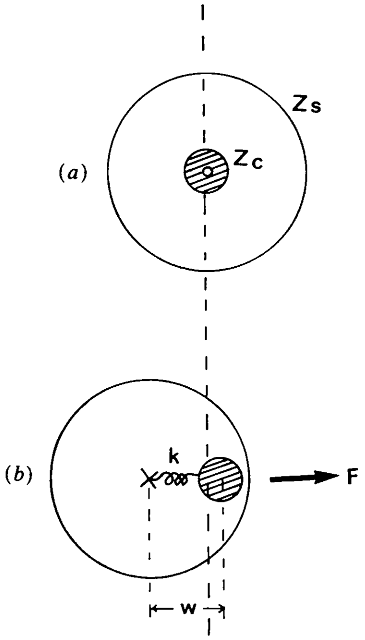

Fig. 1. Schematic diagram of the simple shell model of an ion (*a*) in the absence of a field, (*b*) in the presence of an electric field **F**.

and the μ and ν are determined variationally in terms of moments of the unperturbed charge distribution.

Then f_1 is given through (5) by

$$if_1 F = 2F \sum_i \sum_j \int \psi_0^* \exp(iK\hat{s}.\mathbf{r}_j) \times(\mu r_i + \nu r_i^2) \cos\theta_i \psi_0 \, d\tau. \qquad (13)$$

For the special case of a hydrogenic atom the i, j symbols are suppressed, $\mu = -1/Z$, $\nu = -1/2Z$, and the exact solution (Buckingham, 1964) is given in atomic units (a.u.) by

$$f_1 = -K\alpha(1 + K^2/4Z^2)^{-4}(1 + K^2/12Z^2). \qquad (14)$$

For a general N-electron system f_1 contains both diagonal terms ($i = j$) and off-diagonal terms ($i \neq j$), the latter arising directly from the antisymmetry constraint in ψ_0.

For small K (13) reduces to $f_1 = -\alpha K$, where α is the value of the polarizability calculated by the Kirkwood–Pople–Schofield method, and in all the cases discussed here the α value implied by f_1 agrees well with those previously calculated more directly by Fraga *et al.* (1976). In all the calculations that follow (apart from H where analytic solutions are available) $f_1(K)$ and $f_s(K)$ are calculated from the Hartree–Fock wave functions of Clementi & Roetti (1974). In computing the shell scattering factors it is assumed that only the outermost *ns* and *np* wave functions contribute.

4. Results

(*a*) *Hydrogen*

Fig. 2 compares $|f_1|$ *v* K in a.u. for the exact solution given in (14), and the shell-model approximation assuming the single electron constitutes the shell charge.

$$f_1 = -K\alpha f_0(K) = -\frac{9K}{2(1 + + K^2/4)^2} \qquad (15)$$

with a polarizability α fitted to the same value 9/2 as in the exact representation, and f_0 as given by Buckingham (1964). The exact and shell-model estimates start off together linear in K, but the shell model continues to rise to give a maximum at $K = 1$ a.u.$^{-1}$, a much higher value than for the exact solution. The shell model does not therefore give a good representation of f_1 for a hydrogenic atom for $K \gtrsim 0{\cdot}5$ a.u.$^{-1}$, but of course applying the shell model to a single-electron atom is not close to the original spirit of the model, and comparison with quantum-mechanical solutions for a many-electron atom is the relevant test.

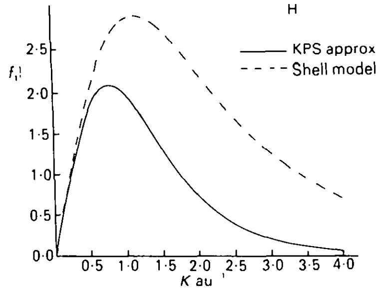

Fig. 2. Graph of $|f_1|$(the magnitude of the modified X-ray scattering factor per unit applied field) *vs* scattering vector K in a.u.$^{-1}$ for the hydrogen atom. In atomic units the unit of field is 51·4 V Å^{-1}; the unit of scattering vector is 1·89 Å^{-1}.

(*b*) *Neon-like atoms/ions*

Fig. 3(*a*) compares $|f_1|$ *vK* in a.u. for the quantum-mechanical model and the shell model for Ne with the shell model assigned the same polarizability as

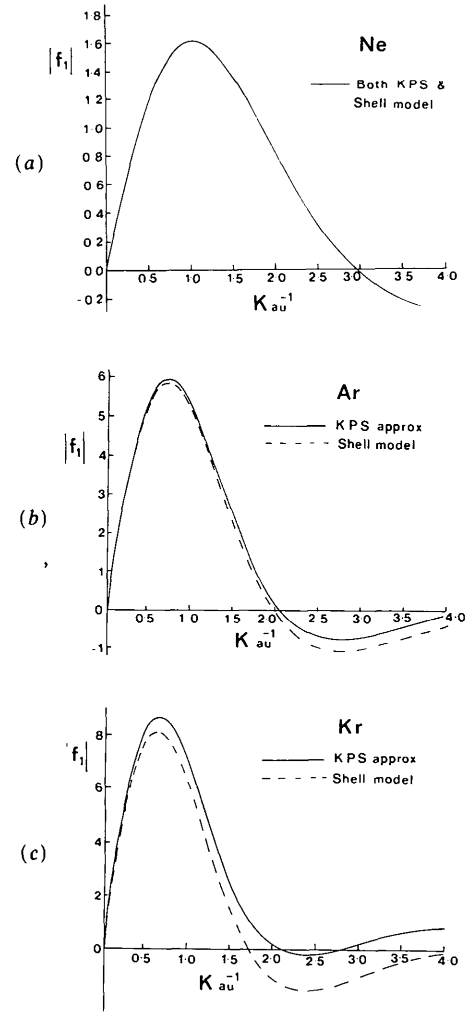

Fig. 3. Comparison of $|f_1|$ (the magnitude of modified X-ray scattering factor per unit applied field) *versus* scattering vector K in a.u.$^{-1}$ for the shell model and the quantum-mechanical model of Kirkwood, Pople & Schofield. (*a*) Ne; (*b*) Ar; (*c*) Kr.

that given by the Kirkwood-Pople-Schofield calculation. For both calculations the wave functions of Clementi & Roetti (1974) are used. The correspondence between the two curves is astonishingly good throughout the full relevant range of K. The level of agreement is very similar for Mg^{2+}, Na^{+} and F^{-}.

(*c*) *Argon-like atoms/ions*

Fig. 3(*b*) makes a similar comparison for Ar, where the agreement is still very good; Ca^{2+}, K^{+} and Cl^{-} behave very similarly.

(*d*) *Krypton-like atoms/ions*

Fig. 3(*c*) shows that, although the position of the maximum in $|f_1|$ is well reproduced in Kr, there are moderate discrepancies between the models at large K; Sr^{2+}, Rb^{+} and Br^{-} show similar trends.

It might be expected that the position of the maximum in $|f_1|$ would decrease with increasing atom/ion size. Fig. 4 shows a graph of the quantum-mechanical results for $|f_1/\alpha|$ *versus* K for a range of atoms and ions. Because of the universal scaling of f_1 with α at low K, all these curves begin with unit gradient. K_{MAX} varies as $R^{-\gamma}$, where R is the atomic/ionic radius, and γ varies from $\gamma \sim 2{\cdot}8$ (neutral atoms), to $\gamma \sim 1{\cdot}6$ (negative ions), while the maximum value of f_1 varies as $\alpha R^{-\gamma^1}$, where the values of γ^1 are similar (although slightly smaller) than the γ values above. Be careful not to be misled by Fig. 4; Na^{+} has a very low polarizability, and so its maximum deformed scattering factor is less than for many other ions (Table 1). Of course the values of α are in themselves R dependent, so that $(f_1)_{\mathrm{MAX}}$ varies approximately as $\alpha^{3/4}$. It is important to put the magnitude of the effect into some perspective–a singly charged ion 2·5 Å from the atom/ion concerned would produce maximum deformation f_1 values varying from 0·03 (Na^{+}) to 0.7 (Br^{-}). It is also relevant to compare f_1 with the unperturbed scattering factor f_0. The maximum values of f_1/f_0 are given in Table 1: large atomic number is less important, but negative ions are still favoured over neutrals or positive ions.

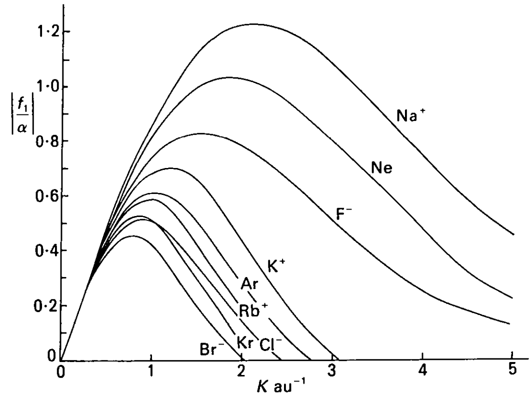

Fig. 4 Comparison of quantum-mechanically calculated curves of $|f_1/\alpha|$ *vs* scattering vector K in a.u.$^{-1}$ for a wide range of closed-shell systems. Note the universal unit initial gradient and the shift in the position of the maximum with atomic size.

Table 1. *Values of the maximum magnitude of the deformation in atomic scattering factor per unit field,* $|f_1|_{\mathrm{Max}}$ *and* $|f_1/f_0|_{\mathrm{Max}}$, *for various atoms and ions*

Field unit 51·4 V Å^{-1}

Atom/ion	$\lvert f_1\rvert_{\max}$	$\lvert f_1/f_0\rvert_{\max}$
Na^{+}	0·8	0·10
Ne	1·6	0·19
F^{-}	4·6	0·51
K^{+}	3·5	0·23
Ar	5·9	0·38
Cl^{-}	13·0	0·79
Rb^{+}	5·5	0·17
Kr	8·7	0·26
Br^{-}	17·3	0·51

It is well known that the polarizability of some ions in crystals varies with crystalline environment - see for example Maessen & Schmidt (1981). In Fig. 5 we have a similar effect in the comparison of the modification of the X-ray scattering factor for an 0^{2-} ion subjected to an external field F in addition to stabilizing potential wells of various depths [$V_0 = 0{\cdot}5$, 1·0, 1·5, 2·0 atomic units (1 atomic unit = 27·2 eV)]; here the wave functions of Harker (1974) have been used. The different initial gradients reflect polarizability differences, and the positions of the maximum of the curves reflect different effective ionic radii in the various potentials.

5. Discussion

The primary objective of this paper is to evaluate the effectiveness of the semi-classical shell model in describing modifications of X-ray scattering factors. This has been done by comparing results for the idealized situation of an isolated atom or ion in an external electric field. The correspondence between quantum-mechanical calculations and the shell model is remarkable, particularly for Ne-like and Ar-like systems. Only for the rather artificial application to

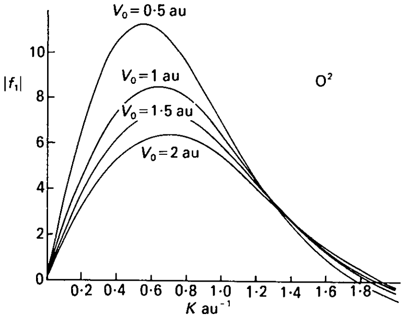

Fig. 5. Comparison of $|f_1|$ with scattering vector K in a.u.$^{-1}$ for 0^{2-} ion in stabilizing potential wells of various depths, calculated from the wave functions of Harker (1974).

H is there any large discrepancy, although Kr-like ions show some deviations at large scattering vector. It appears that the modification of the atomic scattering factor is not a very sensitive function of the details of the modified charge distribution. It is crucial to use the correct polarizability α, because both the initial gradient and the maximum value of $|f_1|$ scale with α. This is, of course, the very empirical quantity to which the shell model is fitted. Thereafter, the maximum value of $|f_1|$, and the decrease towards zero, is controlled to lowest-order approximation by atom/ion size. Describing the shell charge distribution crudely by displacement of the outer electron charge distributions of the undeformed ion appears to be adequate, and good correspondence with quantum-mechanical model results. It is interesting that the modification of the atomic scattering factor does not depend on the value assumed for the shell charge, another factor that gives some confidence in the approach. These results may also be interpreted in a negative way; if one somehow inverts scattering intensities from deformed ions to predict deformed charge distributions, it is likely that the resultant predictions will have the correct electric moment, but there is little information in these scattering intensities to get the detailed charge deformation right.

If $f(K)$ were calculated from (9) instead of (9′) there would be additional contributions of order of F^2 and higher in the shell-model calculations. In this way the shell-model approach takes account of higher-order polarizability effects, not considered in this quantum-mechanical model, but these contributions will be small. The KPS method takes account of charge deformation of all electrons in the atom or ion, but by far the largest response is from the outer s and p electrons, that have been assigned to the shell.

When ions vibrate in solids, their deformation is controlled by the local electric field (the effect that has been directly tested in this paper) and by overlap forces. Although the latter effect has not been examined here the insight we have gained on the way modified X-ray scattering factors depend on empirical quantities such as α and R would suggest that the shell model will give a good first-order description of deformation of scattering factors in such more complicated environments. We have only tested closed-shell systems directly; the application of these methods to systems such as Si may not be quite so easily justified, but the emprical fitting of the shell model is likely to build in the correct general deformation characteristics. More sophisticated forms of the shell model, *e.g.* the breathing shell model, will still have these basic strengths, and in addition will incorporate some further effects beyond the dipole approximation, which are certainly not negligible. Non-dipole contributions to atomic scattering factors in H have been previously considered by Matthew & Gravano (1979).

This suggests that the substantial body of work on deformation coupling on X-ray scattering factors and Debye–Waller factors by Melvin, Pirie & Smith (1968), Reid (1974*a*, *b*), Robertson & Reid (1979) and Reid & Pirie (1980) is well founded quantum mechanically. It gives support to their conclusion that the 'vibration' of the outer-electron charge distributions is much smaller than for the core electrons, and that this may lead to effective Debye–Waller factors B deviating by a few per cent from those of the ion cores for low-order reflections.

Much work has also been carried out in the study of the static modification of atomic scattering factors in molecules and crystalline environments; this has generally been quantum-mechanically based, but it would be attractive also to have mechanical models of the type discussed here to describe such changes in f_0 in terms of empirical parameters (nearest-neighbour distance, ionicity, polarizabilities *etc.*). In the work presented here it is important to note that the dynamical deformations scale with the *in situ* polarizability, *i.e.* contraction or expansion of the atomic/ionic wave functions in crystalline environments leads to a change in deformation properties as discussed here in the case of O^{2-}. The question is 'Can this initial static change in charge distribution itself be modelled mechanically?' The difficulty is that such effects usually depend on higher-order polarizabilities, which are less well known empirically or theoretically. The breathing shell model (Schroder, 1966) does allow for radial deformation of ions during vibration relative to the initial static-charge distribution of the ion in the crystal. It will be of interest to consider further ways of parametrizing such models to describe further variations in shell-charge distributions with crystalline potential, and this will be attempted in later work.

The correspondence between quantum mechanics and the shell model of the idealized perturbation considered in this work gives confidence in the ability of the shell model to give a good first-order description of charge-deformation X-ray scattering effects that occur when ions vibrate in crystalline environments.

John Reid and John Pirie of the University of Aberdeen are acknowledged for stimulating discussions, and thanks are due to Professor Fraga for providing data on the modified wave functions for checking purposes. One of us (SY) wishes to thank the University of Basrah, Iraq, for financial support. We would also like to thank one of our referees for some interesting perspectives on the work.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

Acta Cryst. (1984). A**40**, 721

Space-group determination by dynamic extinction in convergent-beam electron diffraction: errata.

By M. TANAKA, H. SEKII and T. NAGASAWA, *Department of Physics, Faculty of Science, Tohoku University, Sendai 980, Japan*

(*Received* 1 *May* 1984; *accepted* 30 *May* 1984)

Abstract

Tables 13 and 17 of the paper by Tanaka, Sekii & Nagasawa [*Acta Cryst.* (1983), **A39**, 825–837] are not perfect. The correct tables are given.

The following corrections should be made to the paper by Tanaka, Sekii & Nagasawa (1983).

1. Table 13 should be replaced by Table 13 given here, since the case of general [*hk*0] incidence does not cover the special [110] incidence case.

2. Table 17 should be replaced by Table 17 given here. As a result, the numbers of distinguishable space groups should read 185 instead of 191 in the second sentence of the *Abstract* and in the first sentence of the second paragraph on p. 833. In the same paragraph, 16 pairs should read 19 pairs.

Table 13. *GM lines for point groups* 23 *and m*3

	Space group	Incident beam direction					
		[100] (cyclic)		[110] (cyclic)		[*hk*0] (cyclc)	
195	$P23$						
196	$F23$						
197	$I23$						
198		$00l$					
	$P2_13$	2_{13}	A_2 B_2	$00l$	A_2 B_2	$00l$	A_2 B_2
		$0k0$	B_3	2_{13}	B_3	2_1	B_3
		2_{12}					
199	$I2_13$						
200	$Pm3$						
	$P2/m\bar{3}$						
201		$00l$					
	$Pn3$	n_2				$\bar{k}h0$	A_2 B_2
	$P2/n\bar{3}$	$0k0$	A_3			n	A_3
		n_3					
202	$Fm3$						
	$F2/m\bar{3}$						
203		$00l$				$\bar{k}h0$	
	$Fd3$	d_2				$h+k=$	A_2 B_2
	$F2/d\bar{3}$	$0k0$	A_3			$4n+2$	A_3
		d_3				d	
204	$Im3$						
	$I2/m\bar{3}$						
205		$00l$	A_2 B_2	$00l$	A_2 B_2	$00l$	A_2 B_2
	$Pa3$	$a_2, 2_{13}$	A_3 B_3	2_{13}	B_3	2_1	B_3
	$P2_1/a\bar{3}$	$0k0$		$\bar{h}h0$	A_2 B_2	$\bar{k}h0$	A_2 B_2
		2_{12}	B_3	a_3	A_3	a	A_3
206	$Ia3$			$\bar{h}h0$	A_2 B_2	$\bar{k}h0$	A_2 B_2
	$I2_1/a\bar{3}$			a_3	A_3	a	A_3

Table 17. *Space groups indistinguishable by GM lines*

$[P3, (P3_1, P3_2)]$	$(P422, P4_222)$
$[P312, (P3_112, P3_212)]$	$(P42_12, P4_22_12)$
$[P321, (P3_121, P3_221)]$	$(P432, P4_232)$
$[P6, (P6_2, P6_4)]$	$(I4, I4_1)$
$[P622, (P6_222, P6_422)]$	$(I422, I4_122)$
$[P6_3, (P6_1, P6_5)]$	$(I432, I4_132)$
$[P6_322, (P6_122, P6_522)]$	$(F432, F4_132)$
$(P4, P4_2)$	$(I23, I2_13)$
$(P4/m, P4_2/m)$	$(I222, I2_12_12_1)$
$(P4/n, P4_2/n)$	

Reference

TANAKA, M., SEKII, H. & NAGASAWA, T. (1983). *Acta Cryst.* **A39**, 825–837.

0108-7673/84/060721-01$01.50