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. Publication will be quicker if the contributions are without illustrations.*

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Seminvariants for space groups $I\bar{4}2m$ and $I\bar{4}2d$.

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Errors in the tables of seminvariants given by Karle & Hauptman [*Acta Cryst.* (1961). **14**, 217–223] are corrected.

There are two errors in the tables of seminvariants given by Karle & Hauptman (1961) which seem to have continued unnoticed (*e.g.* by Giacovazzo, 1974 and in *International Tables for X-ray Crystallography*, 1974). The space group $I\bar{4}2m$, No. 121 (*International Tables for X-ray Crystallography*, 1969) has its origin fixed by convention at positions with point symmetry $\bar{4}2m$. There are only two such distinct equivalent points in the unit cell, $0,0,0$ and $0,0,\frac{1}{2}$. The space group $I\bar{4}2d$, No. 122 (*International Tables*, 1969) has its origin fixed by convention at positions with point symmetry $\bar{4}$. There are four such distinct points in the unit cell, but they are not all equivalent. The disposition of symmetry elements about the equivalent points $0,\frac{1}{2},\frac{1}{4}$ and $0,\frac{1}{2},\frac{3}{4}$ differs from that about the equivalent points $0,0,0$ and $0,0,\frac{1}{2}$. The latter pair of points are thus the only permissible origins for this space group.

(Note that when conventional body-centred unit cells are chosen the points $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ and $\frac{1}{2},\frac{1}{2},0$ are translationally equivalent to the points $0,0,0$ and $0,0,\frac{1}{2}$, and are not distinct origins.)

It is therefore clear that for both $I\bar{4}2m$ and $I\bar{4}2d$ the seminvariant vector is (l), the seminvariant modulus is (2), and that these two space groups are not of type $3P_34$ but of type $3P_32$ in Karle & Hauptman's notation, $(l)-I(2)$ in Giacovazzo's notation.

References

Giacovazzo, C. (1974). *Acta Cryst.* A**30**, 390–395.

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Absorption correction for back reflexions in plate-shaped crystals of high absorption.

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A simple expression for the absorption correction, derived for an infinite plate intercepting the whole beam, has been shown to be applicable in the structure analysis of plate-shaped hexagonal polytypes of high absorption coefficient. The expression holds almost exactly for crystals which have even a slightly bigger cross section than the X-ray beam, while for crystals completely bathed in X-rays the expression, with slight modification, holds approximately.

Some authors have described more or less general methods for calculating the absorption corrections (*e.g.* Howells, 1950), while others have calculated the correction for suitably shaped crystals, *e.g.* Fitzwater (1961) for ellipsoidal crystals. However, as a result of one or more difficulties in the application of these methods, such as the tediosity of the method, the impossibility of grinding the crystal to a particular shape, the size of the crystal being bigger than the cross section of X-ray beam, some authors have preferred to devise their own simple treatments suited to particular cases (*e.g.* Ferrari, Braibanti & Tiripicchio, 1961). We have arrived at a simple expression for the absorption correction for the special case of back reflexions from highly absorbing platy crystals of a hexagonal polytype, such as CdI_2, PbI_2 and $CdBr_2$. Up until now in the absence of any suitable expression, the practice has been to omit the correction, *e.g.* in the crystal structure determination of 60, 11 and 4 polytypes of CdI_2, PbI_2 and $CdBr_2$ respectively, by different workers (Trigunayat & Verma, 1975). The expression is equally applicable to the plate-shaped crystals of other substances which have sufficiently high absorption coefficients. The underlying analytical treatment will be illustrated by the example of cadmium iodide crystals, typically 50–500 μm in thickness and 0·5 to 5·0 mm across, with **c** perpendicular to the plate.

Reflexions $01.l$ for the upper values of l, *viz.* $l=2n$ to $4n$