It appears that the compounds investigated belong to a group of isostructural crystals, approximating to cubic morphology, whose composition can be represented by

$$\{(R')_n(R'')_{4-n}\mathrm{N}\}_2M^{\mathrm{IV}}X_6$$
$$\{(R')_n(R'')_{4-n}\mathrm{N}\}_2M^{\mathrm{VI}}\mathrm{O}_2X_4\,,$$

where R' and R'' can represent CH_3, C_2H_5, C_3H_7 or C_4H_9. The alkyl radicals may be replaced by hydrogen. The ammonia nitrogen may be substituted by phosphorus or antimony. The tetravalent elements Si, Ti, Ru, Pd, Ir, Os, Pt, Sn, Pb, Se, Te, Po, U and Pu, as well as the uranyl and plutonyl groups, have been encountered in place of M. The halogens F, Cl, Br or I have appeared for X.

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Tables of Absorption Factors for Spherical Crystals

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Correction of single-crystal X-ray diffraction intensity measurements for absorption in the crystal is greatly simplified if the crystal is ground into a sphere. The factor by which the intensity of a diffraction beam is reduced by absorption is a function then only of the dimensionless product of the linear absorption coefficient and the radius of the sphere, and the Bragg angle 2θ. Tables are given in this paper which give the absorption factor in terms of the two variables. The tables are analogous to the standard tables for cylinders.

In the accurate measurement of intensities of diffraction beams produced by small single crystals as used for structure analysis, one of the most troublesome problems encountered is that of properly accounting for the effect of absorption. Such crystals generally have a special geometric shape, and the effect is a geometric function of the diffraction angle, the angular position of the crystal in the beam and the shape of the crystal itself. Various attempts have been made to solve this problem systematically (Howells, 1950) but the solution for a large number of reflections will always be extremely tedious and time consuming.

If the crystal can be ground into the shape of a sphere, as Bond (1951) has recently done, the problem is greatly simplified. In this case, the absorption is a geometric function only of the diffraction angle 2θ, and the radius of the sphere R. This function has now been computed by us and is reported in this paper. The tables below are analogous to those for cylindrical specimens given in the *International Tables for the Determination of Crystal Structures* (1935, vol. 2, p. 581). The present tables were calculated from these data as originally derived by Claasen (1930). The tables for cylinders have been recalculated by Bradley (1935) but his results do not differ in any part from those of Claasen by more than 1% and usually much less. For practical purposes there is no choice between these two sets of tables.

The computation was accomplished by an approximate integration in which the absorption effect was summed over twenty cylindrical elements of the hemisphere, so chosen that the total volume of the elements is to a close approximation the same as that of the sphere, and so that the radii of the elements

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Table 1. *Absolute values of* 100*A for* $\mu R=0$–5

			θ		
μR	0°	22½°	45°	67½°	90°
0	100·0	100·0	100·0	100·0	100·0
0·1	86·2	86·2	86·3	86·9	87·2
0·2	74·2	74·2	74·3	74·8	75·3
0·3	64·6	64·6	64·7	65·5	66·1
0·4	56·0	56·0	56·7	58·0	58·9
0·5	48·9	49·0	50·2	52·0	53·1
0·6	42·2	42·4	44·1	46·2	47·6
0·7	36·8	37·2	39·1	41·5	43·2
0·8	32·1	32·6	34·8	37·4	39·3
0·9	28·1	28·7	31·3	34·0	35·9
1·0	24·5	25·2	28·1	31·0	33·0
1·1	21·5	22·4	25·6	28·5	30·6
1·2	18·9	20·0	23·3	26·3	28·6
1·3	16·7	17·9	21·4	24·5	26·7
1·4	14·7	15·9	19·6	22·8	25·0
1·5	13·1	14·3	18·0	21·5	23·6
1·6	11·5	12·8	16·6	20·1	22·2
1·7	10·2	11·6	15·4	19·0	21·0
1·8	9·10	10·5	14·3	17·9	19·9
1·9	8·14	9·53	13·4	16·9	18·9
2·0	7·31	8·74	12·5	16·1	18·1
2·1	6·53	7·97	11·7	15·2	17·3
2·2	5·85	7·29	10·9	14·5	16·5
2·3	5·28	6·73	10·3	13·8	15·9
2·4	4·76	6·21	9·77	13·2	15·2
2·5	4·30	5·75	9·25	12·6	14·7
2·6	3·88	5·32	8·77	12·1	14·1
2·7	3·52	4·96	8·35	11·6	13·6
2·8	3·21	4·63	7·96	11·2	13·1
2·9	2·90	4·33	7·60	10·8	12·6
3·0	2·67	4·05	7·26	10·4	12·2
3·1	2·44	3·81	6·95	10·0	11·8
3·2	2·24	3·59	6·66	9·71	11·4
3·3	2·05	3·38	6·38	9·39	11·1
3·4	1·89	3·19	6·14	9·11	10·8
3·5	1·74	3·02	5·90	8·83	10·5
3·6	1·61	2·87	5·69	8·57	10·2
3·7	1·49	2·73	5·49	8·33	9·91
3·8	1·38	2·60	5·30	8·09	9·67
3·9	1·28	2·47	5·12	7·86	9·41
4·0	1·19	2·35	4·94	7·65	9·18
4·1	1·11	2·24	4·81	7·44	8·95
4·2	1·03	2·14	4·66	7·25	8·73
4·3	0·960	2·05	4·57	7·05	8·52
4·4	0·899	1·97	4·39	6·88	8·33
4·5	0·841	1·89	4·27	6·72	8·15
4·6	0·787	1·82	4·15	6·56	7·97
4·7	0·738	1·75	4·03	6·41	7·80
4·8	0·693	1·69	3·93	6·27	7·65
4·9	0·650	1·63	3·83	6·12	7·49
5·0	0·613	1·57	3·73	6·00	7·34

Table 2. *Relative values of A for large values of* μR

			θ		
μR	0°	22½°	45°	67½°	90°
5·0	8·35	21·4	50·8	81·7	100
5·5	6·87	20·0	49·5	81·1	100
6·0	5·75	18·9	48·4	80·6	100
6·5	4·89	18·1	47·5	80·2	100
7·0	4·23	17·3	46·8	79·9	100
7·5	3·67	16·7	46·1	79·5	100
8·0	3·26	16·1	45·5	79·3	100
9·0	2·56	15·2	44·5	78·8	100
10·0	2·07	14·6	43·8	78·3	100
11·0	1·72	14·1	43·3	78·0	100
12·0	1·44	13·7	42·6	77·7	100
13·0	1·22	13·4	42·2	77·5	100
14·0	1·06	13·1	41·8	77·3	100
15·0	0·923	12·8	41·6	77·1	100
20·0	0·513	11·9	40·2	76·9	100
25·0	0·317	11·4	39·7	76·7	100
30·0	0·227	11·2	39·2	76·5	100
40·0	0·124	10·7	38·6	76·3	100
50·0	0·078	10·5	38·2	76·1	100
75·0	0·034	10·2	37·8	75·9	100
100·0	0·019	10·2	37·5	75·8	100
200·0	0	10·0	37·2	75·6	100
	0	9·8	36·9	75·5	100

increase in equal increments. Thus, the elements, as shown in Fig. 1, are made narrower near the poles of the sphere where their absorption effect changes most rapidly. The diffraction intensity given by each element is proportional to *va*, where *v* is the volume of each element equal to $(\mu r)^2h$, and *a* is the absorption factor of the element, taken directly from the tables for cylindrical specimens given in the *International Tables* (1935). μ is the linear absorption coefficient of the crystal and always occurs in the absorption functions as a dimensionless product with *r*. The radius of the element *r* corresponds to the radius of the spherical section determined by the equal increments on the equatorial radius of the sphere. The height of the element *h* is determined as half the sum of the distances from the spherical section of the element in question to the spherical sections of the elements immediately above and below. Thus, the sum of the volumes of the elements is nearly equal to the volume of the sphere *V* and the final absorption factor *A* is computed by

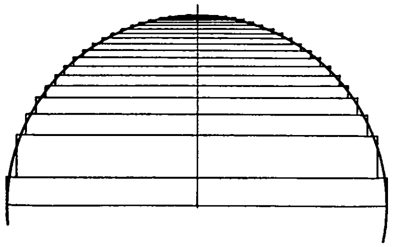

Fig. 1. Division of hemisphere into cylindrical elements.

$$A=\frac{\Sigma va}{V}.$$

Relative values of *a* for large values of μr, as given in the *International Tables*, were put on an absolute basis by using the formula

$$a = \sum_{n=1}^{n=\infty} \frac{\alpha_n}{(\mu r)^n}$$

where the coefficients α_n for $\theta = 90°$ are all taken as zero except $\alpha_1 = 0{\cdot}311$ and $\alpha_2 = 0{\cdot}014$. Absolute values of a for other values of θ were derived from the values for $\theta = 90°$ as calculated above and the relative values as tabulated in the *International Tables*. The final absorption factor A for spherical crystals was then expressed relative to $A = 100$ for $\theta = 90°$ as in the cylindrical case.

To use the tables, calculate the value of μr and plot a graph of the corresponding values of A in the tables against the angle θ. The value of A for any angle can be read with sufficient accuracy from this graph. The table gives values of $100A$; for instance, when $r = 0{\cdot}05$ cm., $\mu = 20{\cdot}0$ cm.$^{-1}$, $\mu r = 1{\cdot}0$, a diffracted beam for which $\theta = 22\frac{1}{2}°$ is reduced by absorption to 25·2% of what it would have been had no absorption taken place.

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The Diffraction of X-rays by a Random Assemblage of Molecules Having Partial Alignment

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The medium considered consists of molecules or other like particles (e.g. micelles) of which one direction, called the molecular axis, has a probability distribution $D(\alpha)$ as in a fibre, i.e. depending only on the angle α between the molecular axis and a direction fixed in space, the fibre axis. Random orientation of the molecules about their molecular axes and random distribution of their centres is assumed. The intensity distribution for X-ray diffraction by this medium is expressed in Fourier space in terms of the intensity distribution (Patterson transform) of the single molecule. Two examples are given, one of which contains as a special case the previously determined effect of finite linear gratings in random orientation.

1. Introduction

The amplitude of coherent X-ray radiation scattered in the direction of a vector $\mathbf{k}$ from a molecule with density distribution $\varrho(\mathbf{x})$ referred to the origin $\mathbf{x}=0$ is given, if the usual constants are omitted, by the Fourier transform of the density,

$$F(\boldsymbol{\eta}) = \int \varrho(\mathbf{x}) \exp\left[-2\pi i(\boldsymbol{\eta}\mathbf{x})\right] dV_x ,$$

where $\boldsymbol{\eta} = \mathbf{k}-\mathbf{k}_0$ is a vector of reciprocal space, $\mathbf{k}_0$ a vector in the direction of the incident plane wave and $\mathbf{k}$, $\mathbf{k}_0$ are such that $|\mathbf{k}| = |\mathbf{k}_0| = \lambda^{-1}$, λ being the wave-length of the radiation.

The intensity of the scattered radiation is given by

$$G(\boldsymbol{\eta}) = F(\boldsymbol{\eta})F^*(\boldsymbol{\eta}) ,$$

which, being a function defined in reciprocal space, is called the *intensity function* of the molecule. It is the Fourier transform of the Patterson-folded density of the molecule,

$$P(\mathbf{x}) = \int \varrho^*(\mathbf{s})\varrho(\mathbf{s}+\mathbf{x}) dV_s . \qquad (1)$$

If the molecule were to take up another orientation in space, the intensity function would have a similar change of orientation in reciprocal space. Hence the resultant amplitude from an assemblage of N variously orientated similar molecules which are shifted from the origin by random vectors $\mathbf{x}_j$ is

$$\mathfrak{F}(\boldsymbol{\eta}) = \sum_{j=1}^{N} F_j(\boldsymbol{\eta}) \exp\left[-2\pi i(\boldsymbol{\eta}\mathbf{x}_j)\right] ,$$

where $F_j(\boldsymbol{\eta})$ denotes the amplitude function $F(\boldsymbol{\eta})$ orientated in reciprocal space to correspond to the orientation of the jth molecule. The intensity of the radiation is

$$\mathfrak{G}(\boldsymbol{\eta}) = \sum_{j=1}^{N} F_j(\boldsymbol{\eta})F_j^*(\boldsymbol{\eta}) + \sum_{j \neq k}\sum F_j(\boldsymbol{\eta})F_k^*(\boldsymbol{\eta}) \exp\left[-2\pi i(\boldsymbol{\eta}\,.\,\mathbf{x}_j-\mathbf{x}_k)\right] .$$

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