latter one does not possess any clear maxima except on the x axis. Location of the four phosphorus atoms at the points $(0, \pm 0{\cdot}208, 0)$ and $(0{\cdot}500, \pm 0{\cdot}208, 0)$ is consistent with the Patterson peaks observed. Work is being continued on the structure of phosphorus triphenyl.

2. Powder-photograph data

Powder photographs of nitrogen triphenyl and phosphorus triphenyl, taken in a 19 cm. camera of the Bradley–Jay type, show rather broad Debye–Scherrer arcs, for the low absorbing power of the two compounds results in the whole specimen contributing to each diffracted beam. Table 2 gives the interplanar spacings, relative peak intensities (estimated from microphotometer traces), and indices of the low-order lines. As Groth (1906–19, vol. 5, p. 274) points out, nitrogen triphenyl is pseudo-tetragonal with $a \fallingdotseq 2b \fallingdotseq 2c$. Hence different indices often give the same interplanar spacing within the experimental error. The indices of the higher-order lines are therefore omitted.

My thanks are due to Dr A. J. C. Wilson, under whose direction this work was carried out; to Miss I. E. Lewis for assistance with the powder photography; and to the Chemistry Department of this College for supplying the compounds.

References

Groth, P. (1906–19). *Chemische Krystallographie*. Leipzig: Engelmann.

Howells, E. R., Phillips, D. C. & Rogers, D. (1950). *Acta Cryst.* **3**, 210.

Wetzel, J. (1942). *Z. Krystallogr.* **104**, 305.

Acta Cryst. (1950). **3**, 318

Some formulas for the X-ray scattering from atoms in various spatial probability distributions.

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Introduction

In a previous paper by the present authors (King & Lipscomb, 1950), a formula was derived for the X-ray scattering from an atom in hindered rotation about an axis not passing through its center. In this note, formulas will be given for the average complex scattering powers of atoms with the positions of their centers distributed with uniform probability over the interior of a circular disk, the interior of a sphere, or along a circular arc. Such formulas may prove useful in computing structure factors for assumed models of crystals containing atoms in motion or disorder. There are certain general conditions under which one may calculate the intensity of coherent scattering from a crystal from the square of the spatial average of the amplitude (Zachariasen, 1944, Chap. 4). We have compared the average intensity with the square of the average amplitude for a crystal containing independently disordered rigid groups, such that definite phase relations exist among the motions of atoms within each group. If in the crystal there are N such groups, each containing n atoms, then whenever $N \gg n^2$ it is legitimate under these general conditions to average the amplitude.

Notation

Let $\mathbf{k}$ = the position vector of the center of the disk, sphere, or arc.

$\mathbf{h}$ = the reciprocal-lattice vector of the reflection considered.

v = the radius of the disk, sphere, or arc.

f = the atomic scattering factor of the given atom taken with its center at the origin.

ψ = the angle between the normal to the plane of the disk or arc and the vector $\mathbf{h}$.

$\bar{g}$ = the average complex scattering power of the atom.

θ_1, θ_2 = the position angles of the ends of the arc, measured from the projection of $\mathbf{h}$ on the plane of the arc.

$a = 2\pi\,|\mathbf{h}|\,v\sin\psi$.

$x = 2\pi\,|\mathbf{h}|\,v$.

Formulas

The formula derived for the value of $\bar{g}$ for an atom having the position of its center distributed with uniform probability over a circular disk is

$$\bar{g} = f\exp(2\pi i\mathbf{h}.\mathbf{k})\,(2/a)\,J_1(a).$$

The formula for $\bar{g}$ for an atom having the position of its center distributed with uniform probability over the interior of a sphere is

$$\bar{g} = f\exp(2\pi i\mathbf{h}.\mathbf{k})\,(3/x^3)\,(\sin x - x\cos x).$$

Table 1. *Values of* $A(a, \theta)$

	$\theta=15°$	$30°$
$a=0{\cdot}5$	$-0{\cdot}0152+0{\cdot}1242i$	$-0{\cdot}0264+0{\cdot}2406i$
$1{\cdot}0$	$-0{\cdot}0564+0{\cdot}2187i$	$-0{\cdot}0984+0{\cdot}4271i$
$1{\cdot}5$	$-0{\cdot}1110+0{\cdot}2608i$	$-0{\cdot}1959+0{\cdot}5177i$
$2{\cdot}0$	$-0{\cdot}1621+0{\cdot}2404i$	$-0{\cdot}2908+0{\cdot}4922i$
$2{\cdot}5$	$-0{\cdot}1925+0{\cdot}1625i$	$-0{\cdot}3544+0{\cdot}3567i$
$3{\cdot}0$	$-0{\cdot}1896+0{\cdot}0458i$	$-0{\cdot}3639+0{\cdot}1420i$
$3{\cdot}5$	$-0{\cdot}1490-0{\cdot}0819i$	$-0{\cdot}3090-0{\cdot}1035i$
$4{\cdot}0$	$-0{\cdot}0758-0{\cdot}1900i$	$-0{\cdot}1944-0{\cdot}3244i$
	$\theta=45°$	$60°$
$a=0{\cdot}5$	$-0{\cdot}0306+0{\cdot}3414i$	$-0{\cdot}0266+0{\cdot}4196i$
$1{\cdot}0$	$-0{\cdot}1149+0{\cdot}6130i$	$-0{\cdot}1006+0{\cdot}7621i$
$1{\cdot}5$	$-0{\cdot}2320+0{\cdot}7598i$	$-0{\cdot}2061+0{\cdot}9658i$
$2{\cdot}0$	$-0{\cdot}3524+0{\cdot}7529i$	$-0{\cdot}3203+0{\cdot}9964i$
$2{\cdot}5$	$-0{\cdot}4446+0{\cdot}5955i$	$-0{\cdot}4182+0{\cdot}8540i$
$3{\cdot}0$	$-0{\cdot}4823+0{\cdot}3222i$	$-0{\cdot}4780+0{\cdot}5717i$
$3{\cdot}5$	$-0{\cdot}4502-0{\cdot}0094i$	$-0{\cdot}4854+0{\cdot}2084i$
$4{\cdot}0$	$-0{\cdot}3478-0{\cdot}3303i$	$-0{\cdot}4362-0{\cdot}1639i$
	$\theta=75°$	$90°$
$a=0{\cdot}5$	$-0{\cdot}0154+0{\cdot}4692i$	$0{\cdot}4862i$
$1{\cdot}0$	$-0{\cdot}0585+0{\cdot}8594i$	$0{\cdot}8932i$
$1{\cdot}5$	$-0{\cdot}1212+1{\cdot}1068i$	$1{\cdot}1572i$
$2{\cdot}0$	$-0{\cdot}1915+1{\cdot}1756i$	$1{\cdot}2423i$
$2{\cdot}5$	$-0{\cdot}2564+1{\cdot}0644i$	$1{\cdot}1466i$
$3{\cdot}0$	$-0{\cdot}3041+0{\cdot}8050i$	$0{\cdot}9021i$
$3{\cdot}5$	$-0{\cdot}3266+0{\cdot}4555i$	$0{\cdot}5668i$
$4{\cdot}0$	$-0{\cdot}3211+0{\cdot}0876i$	$0{\cdot}2121i$

The formula for $\bar{g}$ for an atom having the position of its center distributed with uniform probability along a circular arc is

$$\bar{g}=f\exp(2\pi i\mathbf{h}.\mathbf{k})\,[J_0(a)+\{A(a,\theta_2)-A(a,\theta_1)\}/(\theta_2-\theta_1)],$$

where $$A(a,\theta)=\sum_{m=1}^{\infty}(2/m)\,i^mJ_m(a)\sin m\theta.$$

The function $A(a,\theta)$ is periodic in θ with the period 2π. In addition, it has the properties:

$$A(a,\pi+\theta)=A^*(a,\theta);\quad A(a,\pi-\theta)=-A^*(a,\theta);$$
$$A(a,-\theta)=-A(a,\theta);\quad A(a,n\pi)=0;\quad A(0,\theta)=0.$$

Hence it is necessary only to tabulate values of the A function for the range, $\theta=0$ to $\theta=\frac{1}{2}\pi$. A table of values of $A(a,\theta)$ is given in Table 1.

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References

KING, M. V. & LIPSCOMB, W. N. (1950). *Acta Cryst.* **3**, 155.
ZACHARIASEN, W. H. (1944). *Theory of X-ray Diffraction in Crystals*. New York: Wiley.

Acta Cryst. (1950). **3**, 319

La structure cristalline de $LaSi_2$.

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Zachariasen (1949) a montré que les siliciures d'uranium, de neptunium, de plutonium et de cérium sont isomorphes de $ThSi_2$ dont la structure a été établie par Brauer & Mitius (1942). Comme le thorium et les terres rares, dont le cérium est un représentant, sont isomorphes dans leurs borures, il est à supposer que toute la série des terres rares est isomorphe dans ses siliciures. Ce point a été vérifié sur $LaSi_2$ qui a donc pour groupe spatial $I4/amd$ avec les positions d'atomes suivantes:

$$(0,0,0),(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})+4\,\mathrm{La}\ \text{en}\ (0,0,0),(0,\tfrac{1}{2},\tfrac{1}{4}),$$
$$8\,\mathrm{Si}\ \text{en}\ (0,0,0\pm z),(0,\tfrac{1}{2},\tfrac{1}{4}\pm z),$$

où $z=0{,}417\pm0{,}01$.

Les paramètres sont $a=4{,}37_4$; $c=13{,}56_5$ A.

La densité calculée est $d=4{,}95$ g.cm.$^{-3}$.

Nous remercions Monsieur le professeur Dodero, qui le premier a réussi à préparer $LaSi_2$, d'avoir bien voulu nous confier un échantillon de cette substance.

Références

BRAUER, G. & MITIUS, A. (1942). *Z. anorg. Chem.* **249**, 325.
ZACHARIASEN, W. H. (1949). *Acta Cryst.* **2**, 94.

Acta Cryst. (1950). **3**, 319

A preliminary examination of the crystal structure of dimethyltelluronium diiodide, $Te(CH_3)_2I_2$.

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This substance was first prepared by Vernon (1920*a*, *b*, 1921), who obtained two forms corresponding to the formula deduced from the chemical analysis. Vernon postulated an isomerism, naming the two forms α- and β-dimethyltelluronium diiodide. Drew (1929), however, proved the non-existence of isomerism among these two forms, finding by means of chemical investigations that the β form is not isomeric with the α form, but is a complex substance having the same empirical formula; and he established for the β form the formula

$$Te(CH_3)_3I\,.\,Te(CH_3)I_3.$$

Vernon described the crystals of both forms, giving for the α form the following constants determined by goniometric measurement:—crystal system: monoclinic; class: holohedral; axial angle: 72° 21′; axial ratio:

$$a:b:c=0{\cdot}5578:1:0{\cdot}4310.$$

We have taken rotation patterns about the three axes and Weissenberg patterns about the b and c axes. The dimensions of the unit cell so determined were:

$$a=12.26\pm0{\cdot}03,\quad b=21{\cdot}89\pm0{\cdot}04,$$
$$c=9{\cdot}46\pm0{\cdot}04\ \text{A.};\quad \beta=72°\ 24'\pm10'.$$

These data give the axial ratios

$$a:b:c=0{\cdot}561\pm0{\cdot}03:1:0{\cdot}433\pm0{\cdot}03,$$

in agreement with Vernon's determinations.

When the diffraction spots in the Weissenberg photographs were indexed, the following interferences were observed: hkl in all orders; $h0l$ when $h=2n$; $0k0$ when $k=2n$. These data are consistent with the space group C^5_{2h}–$P2_1/a$.

The density of crystals, determined by Vernon, was 3·34 g.cm.$^{-3}$. From this and the unit-cell dimensions we calculated that the cell contains $11{\cdot}9\sim12$ molecules. No smaller cell can exist; if it did, the cell chosen could not be primitive. For atoms in general positions the space group C^5_{2h} presents a maximum multiplicity of 4. This induced us to suppose that the 12 molecules cannot all be identical.

The probability of this statement is consistent with the investigations of Drew for the β form; this author limited his observations to the β form and accepted for the α form the straight formula determined by analysis, basing his opinion uniquely on the method of chemical preparation. It is possible, therefore, that neither the α form nor the