of the shape and dimensions of small crystals. The method could be applied with profit to the study of the size and shape of molecularly dispersed protein molecules, particularly those, such as horse haemoglobin, whose intramolecular order is independent of water (Perutz, 1949).

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Preliminary X-ray investigation of nitrogen triphenyl and phosphorus triphenyl.

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1. Single-crystal X-ray measurements

Nitrogen triphenyl crystallizes in plates bounded by (100) and $(\bar{1}00)$, with prominent inclined (101), $(10\bar{1})$ and {110} faces, and minor {010}, (201), (001) and $(00\bar{1})$ faces. Phosphorus triphenyl grows in crystals elongated along [001], bounded by {110} and terminated by {101} and {001}. Oscillation and rotation photographs about the principal crystallographic axes show that both compounds are monoclinic and have the unit-cell dimensions given in Table 1.

Table 1. *Single-crystal data*

(Accuracy of cell dimensions about 1 %; of monoclinic angle 0·5°.)

	a (A.)	b (A.)	c (A.)	β	No. of molecules per unit cell	Class	Space group
Nitrogen triphenyl	22·6	11·2	11·2	90°	8	Monoclinic hemihedral	*Pm*
Phosphorus triphenyl	11·6	15·1	8·57	93°	4	Monoclinic holohedral	*P*2/*a*

Table 2. *Powder photograph data*

Nitrogen triphenyl			Phosphorus triphenyl		
Interplanar spacing (A.)	Relative peak intensity	Indices	Interplanar spacing (A.)	Relative peak intensity	Indices
7·93	0·19	011, 210, 201	9·20	—	110
6·24	0·04	301, 310	8·62	0·30	001
5·61	0·21	020, 002, 400	7·64	0·39	020
4·93	0·43	220, 202, 401, 410	6·38	0·18	120
4·46	1·00	500, 302, 320	5·76	0·55	200
4·15	0·20	321, 312, 501, 510	4·90	0·80	201
3·93	0·36	022, 420, 402, 122	4·60	1·00	220, 130, 211
3·69	0·15	—	4·27	0·52	002
3·50	0·24	—	3·98	0·55	221
3·36	0·20	—	3·77	0·50	040, 022, 310
3·19	0·15	—	3·45	0·27	202, 311
2·97	0·06	—	3·28	0·11	032
2·84	0·10	—	3·08	0·09	222
2·76	—	—	2·86	0·11	400, 003, 232
2·69	—	—	2·75	0·09	113
2·48	—	—	2·66	0·18	023, 322
2·39	—	—			
2·28	—	—			
2 21	—	—			
2 07	0·04	—			

The X-ray reflexions with nitrogen triphenyl show no systematic absences; the space group is therefore one of *P*2, *Pm*, *P*2/*m*. From the external symmetry it seems that the most probable space group is *Pm*.

Phosphorus triphenyl exhibits absences in the reflexions $h0l$ when h is odd, so that the space group is either *Pa* or *P*2/*a*. The external form of the typical crystal suggests that the structure has a centre of symmetry, and the distributions of the intensities of reflexions $h0l$ and $hk0$ agree satisfactorily with the theoretical curve for a centrosymmetric projection (Howells, Phillips & Rogers, 1950). The space group is therefore more probably *P*2/*a*. Nitrogen triphenyl and phosphorus triphenyl are not isomorphous; in fact there is no isomorphous pair in the group composed of these compounds and the arsenic, antimony and bismuth triphenyls (Wetzel, 1942).

Patterson–Fourier syntheses have been performed for the projections of phosphorus triphenyl on (001) and (010). The intensities were estimated visually from zero-layer-line Weissenberg photographs. The first projection shows sharp peaks at (0, 0·416) and (0·500, 0·416); the

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latter one does not possess any clear maxima except on the x axis. Location of the four phosphorus atoms at the points (0, ±0·208, 0) and (0·500, ±0·208, 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.

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