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

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:

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

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_{2h}^5–$P2_1/a$.

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_{2h}^5 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