

Fig. 1. Mass spectrum of xenon tetroxide.

spectrum of mercury. The fragmentation pattern varied very little with the energy of the ionizing beam of electrons.

The volatility of  $\text{XeO}_4$  was demonstrated by its very rapid distillation when a liquid nitrogen bath was replaced by one of dry ice.

The same reaction conducted in a test tube yields a gas with a strong pungent odor which gives a test with potassium iodide-starch paper. These properties could be caused by ozone; however, only a small peak was observed at mass 48 in the mass spectrometer.

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References and Notes

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3. Based on work performed under the auspices of the U.S. Atomic Energy Commission. We thank J. G. Malm for the sample of sodium perxenate and L. P. Moore for technical assistance.

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Computer Program for Printing Undeformed Fourier Maps

Abstract. *The program calculates the values of the function at those points where the computer can print them.*

A doubly periodic function that can be represented by a Fourier series with known coefficients is usually computed at  $m$  by  $n$  points in the mesh (two-dimensional period). The mesh, a parallelogram in the general case, has each of its sides subdivided into an integral number of parts,  $m$  or  $n$ . The

machine prints the results in a rectangular array, which is a deformed map of the mesh. The deformation has two sources: (i) the map cannot be true to scale in both directions and (ii) the parallelogram is transformed into a rectangle.

The purpose of the program is to print an array of numbers that can be contoured directly into a map, on which true distances and angles can be measured. Two cases can be considered. In one the mesh is orthogonal (a rectangle) and in the other it is non-orthogonal (a parallelogram).

*Orthogonal mesh.* For example,  $ca$  in the orthorhombic system, with  $c < a$ .

The problem is one of scale only. In general, for any convenient scale, say 1 Å to 2 inches,  $c$  will be a non-integral multiple  $M$  of the width of one machine-printed digit (or interval), and  $a$  will be another nonintegral multiple  $N$  of some interline spacing (single, double, . . .). The machine will be asked to calculate the values of the doubly periodic function precisely at the points where they can be printed. These points form a rectangular array, which we will call the "machine grid." Successive rows come at  $x = pa/M$ , where

$$p = 0, 1, 2, \dots, m, m + 1$$

and  $m < M < m + 1$ . Along each row, points come at  $z = rc/N$ , where

$$r = 0, 1, 2, \dots, n, n + 1$$

and  $n < N < n + 1$ .

The summation of the Fourier series at the points of the machine grid can be shortened thanks to a recurrence formula of H. Takahashi (1). To calculate either

$$C = \frac{1}{2} a_0 + \sum_{h=1}^H a_h \cos 2\pi hX$$

or

$$S = \sum_{h=1}^H a_h \sin 2\pi hX$$

(note that the coefficients  $a_h$  need not be the same in  $S$  as in  $C$ ), compute the following sequence of  $u_n$ 's:

$$\begin{aligned} u_0 &= a_H, \\ u_1 &= 2 u_0 \cos 2\pi X + a_{H-1}, \\ u_2 &= 2 u_1 \cos 2\pi X - u_0 + a_{H-2}, \\ &\dots, \\ u_n &= 2 u_{n-1} \cos 2\pi X - u_{n-2} + a_{H-n}, \\ &\dots, \\ u_{H-3} &= 2 u_{H-3} \cos 2\pi X - u_{H-4} + a_2, \\ u_{H-1} &= 2 u_{H-2} \cos 2\pi X - u_{H-3} + a_1, \\ u_H &= 2 u_{H-1} \cos 2\pi X - u_{H-2} + a_0, \end{aligned}$$

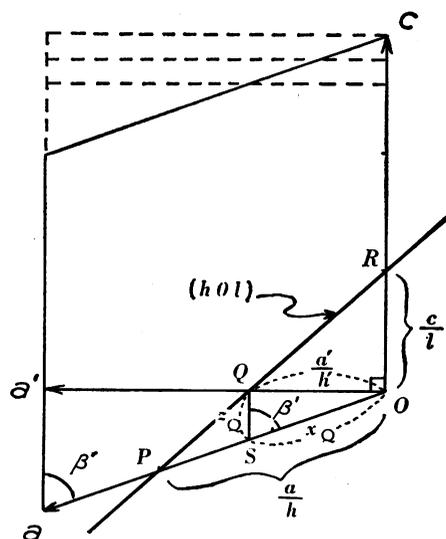


Fig. 1. Monoclinic mesh  $ca$ , with trace of  $(h0l)$  plane and intercepts of the latter on  $a$ ,  $a'$ , and  $c$ , equal to  $OP$ ,  $OQ$ , and  $OR$ , respectively.

but keep only the last three values. Then  $C$  or  $S$ , as the case may be, is given by,

$$C = \frac{1}{2} (u_H - u_{H-2})$$

or by

$$S = u_{H-1} \sin 2\pi X.$$

Although the Takahashi formula was proposed for a small computer and for calculations that made use of an integral number of subdivisions in the period (for example,  $M = m = 45, 60, 100, \dots$ ; with  $X = 1/M$ ), its main advantages are that it permits the use of a nonintegral number of subdivisions and that it eliminates the looking up of sine and cosine tables, which is usual in the Beevers-Lipson summation method.

*Non-orthogonal mesh.* For example,  $ca$  in the monoclinic system, with  $a < c$ .

The mesh is a parallelogram. In view of the fact that the translation repeat need not have the same shape as the mesh, we propose, for purposes of computation, that the repeat of the Fourier function be taken as a rectangle instead of a parallelogram. This result can be achieved by using non-integral Miller indices  $(h0l)$ . For example, the parallelogram  $ca$  can be replaced by the rectangle  $ca'$  (Fig. 1), where

$$a' = a \sin \beta'$$

and

$$a'/h' = x_0 \sin \beta',$$