Fig. 1. Calculation cycle of the machine, using Booth's method of steepest descents

The machine is electrically driven, and the drive is automatically controlled, stopping after completion of a predetermined sequence of operations. Taking into account the setting times, it is about thirty times faster than manual methods. The output is of sufficient power to drive a registering pen mechanism. If desired, absolute values can be plotted automatically, each coded by means of a small kink in the curve; positive values have the kink upwards, negative downwards. A plot of F values is shown in Fig. 2.

Although this machine was designed for calculation of structure factors, it can be used for Fourier synthesis of the electron density. As the lengths of the cosine arms are not readily adjustable, it is best to set all their lengths equal. The structure factors can then be represented as a sum of two vectors of unit length, differing in phase. The machine is run separately for each set of unit vectors and the results added. A unidimensional continuous electron density tracing is then obtained.

Fig. 2. Automatic recording of $F(00l)$ values of strontium laurate for l up to 74 (odd values of l absent). Scale: $F(000) = 1040$ electrons

'Ecofix' girders and 'Meccano' were used for parts where high accuracy was not required; this reduced the cost of the machine considerably and enabled us to build it in less than six months.

I wish to thank Mr. E. T. Sanders for machining the more accurate components.

V. VAND

Research Department,
Lever Brothers and Unilever, Ltd.,
Port Sunlight, Cheshire.
July 27.

¹ Booth, A. D., *Nature*, **160**, 196 (1947).

² Vand, V., *Nature*, **161**, 600 (1948).

Quadrupole Rotation-Vibration Spectrum of the Hydrogen Molecule

It is usually considered that molecular hydrogen does not have an infra-red rotation-vibration spectrum. However, such a spectrum may be expected as a forbidden transition made possible by the change of quadrupole moment during the vibration¹. The predicted intensity of this spectrum is so low that a path of the order of 10 km. at atmospheric pressure is required to obtain it in absorption^{1,2}.

Using a pipe of 22 m. length and letting the light pass through it up to 250 times³ at a pressure of 10 atmospheres, it was possible to obtain equivalent path-lengths up to 55 km. atmospheres. Under these conditions a number of lines of the 2-0 and 3-0 bands of the hydrogen quadrupole spectrum were indeed observed. The accompanying table compares the observed wave numbers with those predicted from the ultra-violet hydrogen spectrum¹. The bands have only S , Q and O branches. Because of the small moment of inertia of the hydrogen molecule, only the first few lines of the S and Q branches are sufficiently intense for observation. No lines of the O branches were found.

Wave-numbers of quadrupole lines of H_2

Band	Line	ν (predicted)	ν (observed)
2-0	$S(0)$	8,403	8,406.36
2-0	$S(1)$	8,601	8,604.26
2-0	$S(2)$	8,782	8,785.54
2-0	$Q(1)$	8,072	8,075.42
3-0	$S(0)$	12,080	12,084.66
3-0	$S(1)$	12,261	12,265.55
3-0	$S(2)$	12,420	12,424.44
3-0	$Q(1)$	11,760	11,764.96

The slight systematic difference of observed and predicted wave-numbers is due to the much lower wave-number accuracy in the vacuum ultra-violet and the lack of standards in this region. It is hoped to obtain improved rotational and vibrational constants of the hydrogen molecule in the ground-state from the wave-numbers of the quadrupole lines.

It appears that the spectrum here observed is the first example of quadrupole radiation in molecular spectra.

G. HERZBERG

Yerkes Observatory,
Williams Bay, Wis.
Aug. 24.

¹ See Herzberg, G., *Astrophys. J.*, **87**, 428 (1938).

² James, H. M., and Coolidge, A. S., *Astrophys. J.*, **87**, 438 (1938).

³ Bernstein, H. J., and Herzberg, G., *J. Chem. Phys.*, **16**, 30 (1948).