Modification of calculation of mineral unit cell contents

A SIMPLE modification can increase the versatility of the FORTRAN computer programme for the 'Calculation of mineral unit cell contents' (Howarth, 1966, p. 787). If the list of oxides for each chemical analysis is followed by a floating point number denoting the unit cell content of oxygen atoms, the programme can be adapted to calculate the results according to the values for different minerals without substitution of cards in the source programme. This enables a variety of minerals to be processed in one batch and permits the storing of the programme on disc or magnetic tape, saving valuable computer time. By an additional simple modification the programme can also be used to recalculate chemical analyses of rocks to a base of 100 cations.

In subsequent calculations of norms from the same data, the oxygens per unit cell number serves to identify the type of mineral so that the norm can be modified for special cases. For example, in an olivine analysis which is deficient in silica but contains alumina the alumina could be calculated as hercynite or picotite as these are frequently found as inclusions in olivine.

These features are incorporated in a computer programme developed in FORTRAN II D for the IBM 1620 computer at the University of St. Andrews. The programme was originally written in KDF 9 ALGOL for use on the English Electric KDF 9 computer at the University of Glasgow.

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Reference

Howarth (R. J.), 1966. Calculation of mineral unit cell contents: Fortran computer programme. Min. Mag., vol. 35, p. 787.

[Manuscript received 19 May 1966]

On the determination of 2V

In a recent article (Ehlers, 1966) describing a method of bringing a crystal into the Berek position for indirect determination of 2V, a preliminary part of the procedure (p. 959) discussed a technique of putting the crystal into the cardinal position. Professor D. Jerome Fisher