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Calculation of mineral unit cell contents: FORTRAN computer programme

A COMPUTER programme for the calculation of cell contents of such minerals as micas, hornblendes, olivines, feldspars, pyroxenes, and garnets has been developed for the IBM 1620 computer. From the basic chemical analysis the cell content is recalculated on the basis of 24 oxygen atoms into the form:



The programme may be easily adapted for groups in which OH is zero by dividing the result calculated to O_{24} by 6 (olivines), 3 (feldspars), 8 (pyroxenes), or 4 (garnets), or by altering one card in the source programme. The sole restriction is that not more than 9999 data cards may be processed at once. Floating point arithmetic is used throughout, the atomic ratios in the unit cell are corrected to 0.01. The programme is written in FORTRAN II. The programme execution time is less than 50 sec per data card on the IBM 1620. Any similar computer with storage of 20 K or more could be used. The programme has been checked against hand-calculated data provided by Dr. B. E. Leake, Bristol University.

The programme is available from IBM and is listed under File Number 8.3.004 in the Catalogue of Programs for the IBM 1620 Data Processing System.

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