

the $V_{\text{Ni}}:V_{\text{Mg}}$ values of the compounds listed in table I, excluding the spinels. The range of values is considerable and the very high and the very low probably derive from faulty data. The mean is 0.970 and this may be employed to estimate a Ni^{2+} ionic radius of 0.64 Å relative to Ahrens value of 0.66 Å for Mg^{2+} .

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[Manuscript received 5 December 1968]

MINERALOGICAL MAGAZINE, JUNE 1969, VOL. 37, NO. 286

A Fortran IV computer programme for the rapid computation of indexed X-ray d -spacings, Q -values, and Bragg angles

THIS programme is a general routine that, given a set of cell parameters and the wavelength of X-rays, produces an ordered list of indexed d -spacings, Q -values ($Q = 1/d^2$), 2θ , and 4θ for any prescribed crystal lattice.

All crystal lattices, including both monoclinic settings, and the rhombohedral system, are handled. Input cell parameters may be direct or reciprocal, and optional features include the generation of systematic absences for any space group, which is initiated by punching the international space group symbol (or lattice symbol) on to a data card. Provision is made for users to add a routine to produce additional absences due to special positioning in any particular space group. Systematic absences may be removed from the output list to provide a condensed list of observable reflections.

Operation of the programme is extremely simple, data for each job being punched on to three cards. Attention has been paid to printed format and the programme may be used for batchwise production of extensive reference catalogues as easily as for single jobs. The user has complete control over such variables as output lines per page and per job. Useful data such as the direct and reciprocal cell parameters and cell volumes are also printed out.

The programme is fitted with adequate internal error checks, and has been extensively tested. Card decks are available under the code name APOL, together with a write-up/users' manual in two versions: one suitable for I.B.M. 7090/94 machines, and the other suitable for I.B.M. 360 machines. Both versions are written in Fortran IV language and require about 15 000 words of core storage. Requests for these should be sent to Dr. I. S. Kerr at the following address.

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[Manuscript received 6 November 1968]

MINERALOGICAL MAGAZINE, JUNE 1969, VOL. 37, NO. 286

The oxyapatite (voelckerite) problem

THE problem of the existence of an apatitic isotype with the composition $\text{Ca}_{10}\text{O}(\text{PO}_4)_6$ was raised again with the introduction of the name voelckerite (Rogers, 1912); it had first arisen in 1883 (Voelcker). To say that the problem has not been completely resolved during the past half-century, would be an understatement, despite attempts by several highly competent mineralogists.

Today, there seems to be little doubt about the existence of hydroxyl- and/or halogen-deficient apatites ($\text{OH} + \text{F} + \text{Cl} < 2$); the current question is whether there are vacancies in some of the structural sites that are occupied by F in ordinary $\text{Ca}_{10}(\text{PO}_4)_6\text{F}_2$ (these (a) sites are located at $\pm(0, 0, \frac{1}{4})$, according to conventional selection of the origin, whereas Cl is in (b) sites $(0, 0, \frac{1}{2})$).

As indicated by Merker and Wondratschek (1960) for synthetic $\text{Pb}_{10}(\text{PO}_4)_6\text{O}$, there must be a doubling of *c* for the unit cell when occupancy of half of the (a) or (b) sites is ordered.¹

Most recent advocates for vacancies in the (a) sites are Sudarsanan and Young (1968), whereas Ito (1968, pp. 902–3) states: 'The above observations suggest that there is only one oxyapatite . . . in which the loss of hydroxyl ion is compensated by cation replacement, and the stabilized oxyapatite contains 26 oxygens in each unit cell, as originally postulated by . . . ?'

¹ Concerning their 'oxyppyromorphite', however, they state: 'Es ist möglich, dass etwas OH in das Gitter des Oxyppyromorphits eingebaut wird, vielleicht ist ein solcher Einbau sogar für die Stabilität des Oxyppyromorphit-Gitters wesentlich' (p. 29).