The ionic radius of nickel

COMPILATIONS of ionic radii in common use are due to Ahrens (1952) and Pauling (1960). According to both the Ni^{2+} ion is larger than the Mg^{2+} (Ahrens, Ni^{2+} 0·69 Å, Mg^{2+} 0·66 Å; Pauling, Ni^{2+} 0·72 Å, Mg^{2+} 0·65 Å), but a comparison of the unit cell volumes of many isomorphous nickel and magnesium compounds reveals that the nickel compound normally has a smaller cell volume. This provides sufficient evidence for a revision of the estimated relative ionic radii of nickel and magnesium.

The unit cell volumes of nineteen pairs of nickel and magnesium compounds that were believed to be isostructural were calculated from the data of the ASTM card index (1967). The ratio of the cell volume of the nickel compound to that of the magnesium compound, $V_{Ni}:V_{Mg}$, was then calculated (table I). In only two of the structures was the ratio greater than 1·00 and it is tentatively suggested that these two cases result from faulty data.

TABLE I. *Unit-cell-volume ratios of isostructural nickel and magnesium compounds*

Formula	MF_2	MCl_2	MBr_2	MI_2	$MOHCl$	$M(OH)_2$	MO	MCO_3	M_2SiO_4
$V_{Ni}:V_{Mg}$	1·060	0·971	0·919	0·836	1·151	0·952	0·974	0·971	0·971

Formula	MWO_4	$MMoO_4$	MSO_4	$MSeO_4$	MSb_2O_6	MNb_2O_6	MUO_4	Oxal.*	Perch.†
$V_{Ni}:V_{Mg}$	0·993	0·990	0·962	0·936	0·981	0·995	0·947	0·845	0·975

		Spinels					
Formula	Hyd.‡	MAl_2O_4	MFe_2O_4	MCr_2O_4	MGa_2O_4	M_2GeO_4	M_2SiO_4
$V_{Ni}:V_{Mg}$	1·000	0·979	0·979	0·995	0·993	0·990	0·937

* Oxalate, $M(COOH)_2.2H_2O$.   † Perchlorate, $M(ClO_4)_2.6H_2O$.
‡ Sulphate, $MSO_4.7H_2O$.

A further series of six spinel structures are listed in table I along with the calculated values of $V_{Ni}:V_{Mg}$, which are all less than 1·00. The spinel structure has lattice sites of four and six co-ordination and the compounds of nickel and magnesium will not be strictly isostructural since the magnesium ion will accept a greater degree of four co-ordination than the nickel ion, which is strongly favoured in sites with six co-ordination.

The diffraction patterns of other compounds are listed in the ASTM index without cell dimensions but an examination of the d-spacing of equivalent peaks indicates that the nickel compounds have smaller cell volumes.

The present data demonstrate *within the concept of an ion as a rigid sphere* with a fixed radius that the Ni^{2+} ion is smaller than the Mg^{2+} ion in halide and oxide lattices. An assessment of the size difference may be made by calculating the mean of

the $V_{Ni}:V_{Mg}$ 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+} onic radius of 0·64 Å relative to Ahrens value of 0·66 Å for Mg^{2+}.

Department of Geology   G. M. BIGGAR
University of Edinburgh
West Mains Road
Edinburgh, 9

REFERENCES

AHRENS (L. H.), 1952. *Geochimica Acta*, **2**, 155.
AMERICAN SOCIETY FOR TESTING AND MATERIALS (1967). *Powder Diffraction File, Inorganic Section.*
PAULING (L.), 1960. *The Nature of the Chemical Bond*, 3rd edn. (Cornell University Press).

[*Manuscript received 5 December 1968*]

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.