

to maintain a diametric position. The clamp has a maximum opening of 10 in. and can accommodate samples 10 in. wide; specimens weighing up to 40 lb have been handled.

In use it is wise to clamp the rock with its centre of gravity approximately at the mid-point of the sphere of which this device constitutes one circular plane. Adjustment of A_2 is made first to get the horizontal location line approximately to its original position, and then both A_2 and A_1 are adjusted together to obtain an accurate horizontal position and also to get the dip arrow to its original attitude. Finally the geographical position can be regained by rotation of the wheel about A_3 to the correct compass bearing.

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*Deriving the formula of a mineral
from its chemical analysis*

IN a recent note with the above title, Gabrielle Donnay (1964) has seemingly overlooked a most useful method that is applicable to complex silicates, phosphates, sulphates, &c., even though the unit cell may be large and the chemical analysis may indicate numerous cationic and anionic components.

The basic principle of this method stems from the Bragg concept: Such structures are composed of a sea of oxygen atoms in symmetrical array, and the interstices are filled (more or less) by cations. In turn the oxygen atoms surrounding these cations give rise to Pauling's polyhedra that establish simultaneously the co-ordination numbers of the cations. One basic assumption is involved in the calculation of the structural formula by this procedure: The number of oxygens packed in one structural unit must be an integer.¹ There can be no 'holes' among the regular oxygen positions and no 'excess' (McConnell, 1958), and all symmetrical sites for oxygen must be accounted for, either by oxygen or by OH, H₂O, or halogens.

Accepting this fundamental premise, one can calculate the number of oxygens in the unit cell directly from the chemical analysis, the density, and the volume of the unit cell (McConnell, 1954*a*; McConnell and Verhoek, 1963). From crystallographic data on analogous structures it is usually feasible to arrive at an integer that is highly credible.

Assuming that the number of oxygens is known, it can be corrected appropriately for substitution of halogen atoms; no effort should be made at this juncture to surmise the number of hydrogen atoms. One now knows the number of negative electrical charges for the average unit cell, and can allocate equivalent cationic charges to them in so far as the valences of the cations are known. (The ratios of the cations to be used for this purpose are the same as those of the chemical analysis, of course.)

In very complex situations, such as ettringite (McConnell and Murdoch, 1962), it may be necessary to make additional assumptions concerning co-ordination numbers, but for schallerite (McConnell, 1954*a*) such information was not required. Possibly the simplest example of the procedure is that used to calculate the refractive indices of garnets from the ionic refractivities, chemical analyses, and unit-cell dimensions (McConnell, 1964).

Through the introduction of additional assumptions more specialized methods of calculation can be obtained, as was done for montmorillonite (McConnell, 1951), but the basic method remains the same: The number (integer) of oxygens per unit cell is determined. Correcting for halogens that may occur by substitution, the total number of negative electrical charges per unit cell (n) is ascertained. The atomic ratios of the cations multiplied by their valences are summed, and this summation (s) is re-evaluated so as to balance the negative charges. These re-evaluated ratios of cationic charges (each having been multiplied by n/s) are now divided by the valences for the individual cations in order to obtain the number of each cation per unit cell. Hydrogen is dealt with in the same manner as are the other cations, and the mode of occurrence of the protons can frequently be judged solely on the basis of the chemical data (see the results on ortho-antigorite (McConnell, 1954*b*)). Other situations may require supplemental information obtained by d.t.a., IR absorption, or other means.

Special complications may arise in cases where neither the crystallographic nor the chemical data are adequate to completely resolve the question of the precise structural formula. Such an example is calcium lipscombite (McConnell, 1963), but the applicability of these fairly

simple procedures to a hexagonal unit cell with a volume approximating 9000 Å³ (ettringite) demonstrates its great usefulness.

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 — and MURDOCH (J.), 1962. *Min. Mag.*, vol. 33, p. 59.
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¹ This assumption does not necessarily preclude the substitution of H₃O⁺ (or H₂O) for a cation, such as K⁺. Under such circumstances, this oxygen, together with its associated protons, would be additive to those of the symmetrical sites of the 'oxygen lattice'.

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BOOK REVIEWS

WYCKOFF (R. W. G.) *Crystal Structures*. Vol. 2. 2nd edn, New York, London, Sydney (Interscience Publishers), 1964. viii+588 pp. illus. Price: 180s.

This volume of 'Crystal Structures' covers inorganic substances of the types R_nX_m (other than RX and RX_2), $R(MX_2)_n$ and $R_n(MX_3)_p$, but unlike the first edition it postpones $R_n(MX_4)_p$ to Vol. 3. The text has been largely rewritten and brought up to date, with references up to late 1962, and with increased bibliographic coverage (by about 15 %) for the years up to 1955 that were covered by the first edition. The amount of material presented has thus been increased by about 80%, but as a result of the change of format from the loose-leaf style the shelf space required has been reduced by 25 % without any loss of detail or clarity.

The first edition was very troublesome to consult because the text, figures, and tables were in separate sections, the summary tables for