necessary. A simple calculation based on the assumption that each atom has the same effect in determining the lattice constant as any other atom leads to a satisfactory system. On this assumption the lattice constant is given by the following equation:

$$a_0 = 1\cdot7888\left(\tfrac{3}{2}R_A+\tfrac{1}{2}R_B\right) . \qquad (1)$$

The factors $\frac{3}{2}$ and $\frac{1}{2}$ reflect the composition A_3B of the crystal.

The set of radii formulated for use with this equation is given in Table 1, and the values of a_0 calculated from them are compared with the observed values for the 32 compounds in Table 2. It is seen that for 21 of the compounds the deviation between the calculated and observed values is 0·004 Å or less. Only for 11 of the compounds is the deviation greater than 0·004 Å. The radii and equation used by Geller, in which the radii R_A and R_B are given equal weights instead of the weights 3:1, led to deviations with experiment of 0·01 Å or greater for 23 of the compounds. The mean deviation in lattice constant for the 32 compounds given in Table 1 is 0·004 Å, whereas Geller reported a mean deviation of 0·01 Å, over twice as great.

The effective radii for the β-wolfram structure used in preparing Table 2 are compared in Table 1 with the effective metallic radii for ligancy 12 reported a number of years ago (Pauling, 1947). It is seen that for most of the elements the two radii are in good agreement with one another, the mean deviation being 0·02 Å. The mean deviation between the effective radii suggested by Geller and the metallic radii for ligancy 12 is 0·04 Å.

It may be possible to find explanations for some of the differences between the effective radii for the β-wolfram structure and the standard metallic radii for ligancy 12. For example, the effective radii for Ti and Zr are about 0·05 Å smaller than the standard radii. The only compounds of Ti and Zr are those with Ir, Pt, Au, and Hg, all of which may be expected to transfer electrons to the hypoelectronic atoms Ti or Zr (Pauling, 1950), and in this way to lead to an increase in the number of bonding electrons for the crystal, and a decrease in the lattice constant. The decrease in the radii may be taken as evidence that this expected electron transfer has occurred.

There is no need to discuss Geller's arguments against the resonating-valence-bond theory in detail; one argument may serve as an example. Geller states 'The case of V_3Au is even more vivid. Pauling's radii would give 5·05 Å and Wells' 4·99 Å, 0·16 and 0·10 Å, respectively, too large'. In fact, the standard metallic radii for ligancy 12 (Pauling, 1947) lead to perfect agreement with experiment for V_3Au. These radii (Table 1) are 1·338 Å and 1·439 Å, respectively. When these values are substituted in equation (1) the value $a_0 = 4\cdot878$ Å is obtained, agreeing exactly with the reported experimental value 4·88 Å. The fallacy in Geller's argument is, of course, that of giving the radii of the small atom V and the large atom Au the same weight.

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The unit cell and space group of HCN tetramer.

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In a recent physical study of HCN tetramer by Webb, Frank & Schneider (1955), evidence was presented which supported the diaminomaleonitrile structure for that substance. The data presented in the present paper were obtained from a sample of HCN tetramer kindly provided by Dr Webb.

The material was recrystallized from isopropyl alcohol, and small single crystals were chosen for goniometric and X-ray examination. The crystals were six-sided needles with ill-formed terminations. Rotation and Weissenberg photographs showed that the substance was monoclinic, with

$$\mathbf{a} = 6\cdot47,\ \mathbf{b} = 18\cdot20,\ \mathbf{c} = 5\cdot23\ \text{Å},\ \beta = 123^\circ .$$

The forms of the needle are {010} and {021}. The density, as measured pycnometrically with carbon tetrachloride, is 1·409 g.cm.$^{-3}$; the density calculated for four molecules per unit cell is 1·388 g.cm.$^{-3}$. The absences on the Weissenberg photographs, namely, ($0k0$) with k odd and ($h0l$) with l odd, indicate that the space group is C_{2h}^5–$P2_1/c$. Since there are four molecules in the unit cell, no molecular symmetry is required.

On the Weissenberg photographs the reflection (041) is unusually intense, and on the **a**-axis rotation photograph this reflection is accompanied by streaks (not wheaks) in the direction of its normal. These observations suggest that the structure consists of planar, or nearly planar, molecules lying in planes roughly parallel to {041}, but since the outline of this plane in the unit cell is almost square, packing and hydrogen-bonding considerations alone were unable to lead to a trial structure. Obviously, the above discussion contains no evidence whatever for or against the diaminomaleonitrile structure for $(HCN)_4$—such evidence will be obtained in a complete crystal structure determination.

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Reference

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