BUILDING NUCLEAR CRYSTAL STRUCTURE MODELS

D. JEROME FISHER, *University of Chicago*, and
E. H. STEVENS, *Colorado School of Mines*.

ABSTRACT

Herein appears a detailed description of a simplified method for building nuclear crystal structure models of any complexity. As a basis of explanation the building of a sanidine model serves as the guide; brief remarks are given on a muscovite model and color schemes.

Crystal structure models are valuable in introducing the beginning student to the intricacies of the subject, even though some advanced workers in the field may be able to dispense with them. Models of this kind are of two types, which may be designated as nuclear models and packing[1] models. The latter are commonly balls of sizes proportional to those of the atoms or ions concerned which are in contact with at least some of their neighbors; they are valuable to show types of packing, to elucidate morphotropic changes, and to indicate "cavities" in the structure. But some of them (e.g., quartz) are commonly built so that balls are linked together with rods where there is actually no coordination, and the interior of "tight" structures cannot readily be discerned. Nuclear models are made of balls of much smaller size, spaced relatively widely along a wire network; thus each ball can be taken to represent the nucleus of the atom or ion concerned. They are particularly useful in demonstrating coordination relations, bond angles, and types of bonding such as Machatschki advocated be used in classifying the silicates. They are excellent aids in clarifying the explanations of such physical properties as cleavage[2] and hardness. They may be used for graphically determining the necessary angles for making packing models, or for checking such calculations made analytically. The original calculations necessary to build the model are much simpler than is true for packing models. It is easy to indicate the unit cell on them. Another kind of model which may be regarded as a modification of the nuclear type may be called the polyhedral nuclear model; in this the coigns of polyhedra

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[1] Buerger, M. J., and Butler, R. D., A technique for the construction of models illustrating the arrangement and packing of atoms in crystals: *Am. Mineral.*, vol. **21**, pp. 150–172, 1936.

[2] For example, see Shappell, M. D., Cleavage of ionic minerals: *Am. Mineral.*, vol. **21**, pp. 75–102, 1936.

nuclear and of polyhedral nuclear models are much more common than are taken to represent the positions of ions.[3] Combinations of strictly the purely polyhedral kind, which are suitable for only such substances as silica.

The above discussion serves to indicate that no one type of model is entirely satisfactory for all purposes. For general use, and particularly for the instruction of beginning students, it is desirable to have different types of models of the same crystal structure. Where the structures are simple, with a small number of atoms in the unit cell, it is practicable to have both nuclear and packing models on the same scale. For more complicated models such as muscovite, which while the unit cell has but 76 atomic positions, must contain some 300 atomic positions if it is to be really effective in showing the sheet structure, it is impossible to make a nuclear model by the method herein described on a scale much smaller than 2.4 cms. to 1 Å. While the writers know of no packing model of muscovite, presumably one could be made to advantage on a scale considerably smaller than this.

The object of the present note is to describe a modification of the scheme given by Gruner,[4] thus enabling relatively untrained workers to build nuclear models of considerable complexity with a high degree of accuracy. A model can be made very easily by attaching balls to vertical pegs or rods at appropriate places. But for most structures, a model of this kind has its essential features obscured by these rods, which have no structural significance. The method herein described makes use of such rods during construction, but they are eliminated in the completed model.

For purposes of illustration, the building of a sanidine model according to the analysis of Taylor[5] will be described. Fig. 1 is a reduced copy of the plan used in building the model. It is really a projection of the

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[3] The ion commonly at the polyhedron center is ordinarily not visible, unless transparent material as glass or celluloid is used in fabricating the polyhedra. The polyhedra degenerate into planes in making this type of models of nitrates, carbonates, and of other substances with "plane" radicles; e.g., K_2PtCl_4. Polyhedral nuclear models are shown in the *Strukturbericht*, **1913–1928** (e.g., p. 234) and are figured very frequently in E. Schiebold: *Kristallstruktur der Silikate*, in vols. **11** and **12** of Ergebnisse der exakten Naturwissenschaften.

[4] Gruner, John W., A new method of building crystal structure models: *Am. Mineral.*, vol. **17**, pp. 35–37, 1932.

[5] Taylor, W. H., The structure cf sanidine and other feldspars: *Zeit. Krist.*, Vol. **85**, pp. 425–442. 1933. Also see Taylor, Darbyshire and Strunz: An *X*-ray investigation of the feldspars: *Zeit. Krist.*, Vol. **87**, pp. 464–498, 1934.

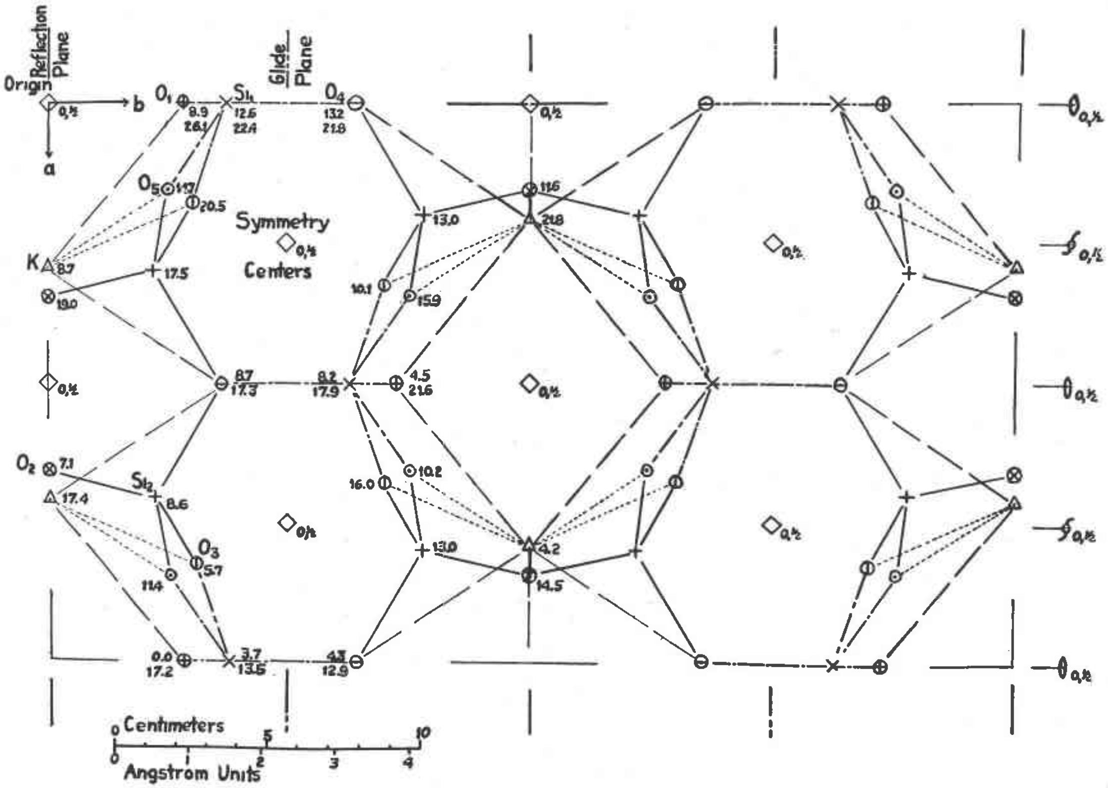

FIG. 1. Reduced copy of a plan of the unit cell of sanidine, projected onto a plane normal to the *c*-axis through the lower front edge of the unit cell. Explanation of the symbols used appears in the diagram. The eight points having abbreviations of elements near them are the ones given by the coordinates in the table of footnote 6. The other points are obtained from these by the symmetry, which is indicated. The glide planes $(010)_{\frac{1}{4},\frac{3}{4}}$ have translations $a/2$. The numbers indicating heights of the ions in centimeters omitted from the right half of the plan may be obtained from those given in the left half by operation of the reflection plane $(010)_{\frac{1}{2}}$. The symmetry axes and centers occur in the base and half way up the unit cell, as is indicated.

coordinates[6] of the ions of the sanidine unit cell on a plane through the lower front edge of the unit cell perpendicular the *c*-axis. The numbers near the points located refer to the heights of the ions concerned above the baseboard on which the plan is mounted with thumbtacks. These numbers[7] are given in terms of centimeters on the basis of 1 Å = 2.4 cms., or an enlargement of 240,000,000 times. This is somewhat smaller than the scale advocated by Gruner, and appears to be rather more satisfactory. It is based on the fact that with this scale an ordinary tennis ball can be used to represent an oxygen ion of radius 1.32Å.

[6] Taylor, *Op. cit.*, p. 430. Taylor's values, in Ångstrom units, are given below, together with the corresponding values in cms., based on the scale 1 Å = 2.4 cms.

Ion	Number in unit cell	Axial Coordinates							
		x		x'	y		z		z'
		Å	cms.	cms.	Å	cms.	Å	cms.	cms.
O$_1$	4	0	0	0	1.79	4.3	0	0	8.9
O$_2$	4	5.53	13.3	11.9	0	0	1.68	4.0	7.1
O$_3$	8	6.90	16.6	14.9	1.97	4.7	1.68	4.0	5.7
O$_4$	8	0	0	0	4.12	9.9	1.78	4.3	13.2
O$_5$	8	1.28	3.1	2.8	1.61	3.9	2.96	7.1	14.7
K	4	2.47	5.9	5.3	0	0	0.99	2.4	8.7
Si$_1$	8	0	0	0	2.40	5.8	1.54	3.7	12.6
Si$_2$	8	5.90	14.2	12.7	1.43	3.4	2.47	5.9	8.6

These coordinates are in terms of a unit cell with $a:b:c = 8.45:12.90:7.15$Å $= 20.28:30.96:17.16$ cms. $= 0.655:1:0.554$ (axial ratio), and $\beta = 63°54'$. The x coordinates are measured parallel to the inclined a-axis; hence each value must be multiplied by sin β to change it to x', which is the corresponding distance in the horizontal plane. Thus the apparent length of the a-unit becomes 20.28 cms.$\times$sin $\beta = 18.25$ cms. in the plane of the drawing, Fig. 1. The z coordinates are measured parallel to the vertical c-axis, but from the inclined plane forming the base of the unit cell; to change these to z', which are the corresponding distances measured from the horizontal plane, each value of z must be increased by adding cot $\beta \times (18.25\text{-}x'$ cms.).

In the above table coordinates are given for only 8 ions. The coordinates of all additional ions within the unit cell are obtained from the original set through the operations of the symmetry shown in Fig. 1.

The axial coordinates given by Wyckoff (*Structure of Crystals Supplement*, **1935**, p. 126) appear to differ from those in the above table because the former are stated in terms of decimal parts of the unit cell dimensions. In some papers the positions of the unique ions of a unit cell are described in terms of angular coordinates θ_1, θ_2, and θ_3. These are used in structure determinations for calculating the scattering power (F) of the various ions. These can be converted to axial coordinates by means of the following formulae: $\theta_1 = 2\pi x/a$; $\theta_2 = 2\pi y/b$; $\theta_3 = 2\pi z/c$.

[7] In building the model it is convenient to add 5 cms. to each of these numbers to allow room for working below the base of the unit cell.

By means of a drill press, holes of a diameter to fit tightly B. and S. gauge no. 11 brass wire (just under 3/32 inches in diameter) are bored at the indicated points in the baseboard to a depth of 1.6 cms. Lengths of this wire corresponding to the largest number by each hole (adding 1.6 cms. in each case) are driven into the baseboard forming the peg model shown in Fig. 2A. At this stage the top of each peg represents the center of the highest ion in each position that is to appear in the model. While the plan of Fig. 1 outlines but a single unit cell, the model as actually built is somewhat larger than this. This extension laterally is easily carried out by means of translations of the plan in the *a*- or *b*-directions

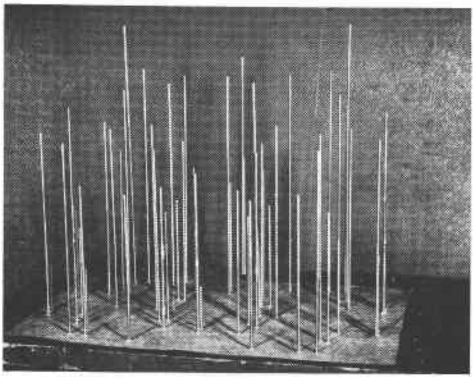

Fig. 2A

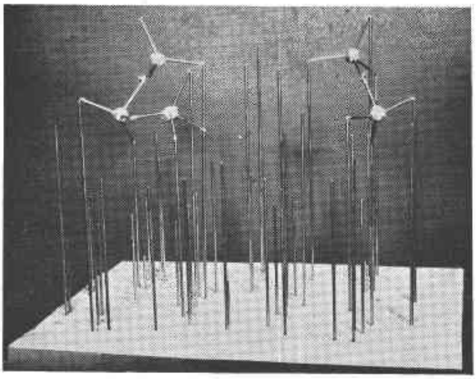

Fig. 2B

Fig. 2. *A* (above): Peg model of sanidine, initial stage. *B* (below): The same, after completing five SiO_4^{-4}-tetrahedra. Plastic wood balls indicate the positions of the five Si^{+4}-ions.

by distances equal to the unit in these directions, the length of the a-unit of course being foreshortened and so appearing as sin β times the true a-unit.

It was found to be easier and more accurate to make rods representing coordinations long enough to tie 3 ions together, no more no less. Thus the higher SiO_4^{-4}-tetrahedra were built first by cutting pieces of brass rod a trifle longer than 7.78 cms. (to allow for the overlap at the silicon ions), and bending them in the middle at angles of slightly under $109\frac{1}{2}°$.

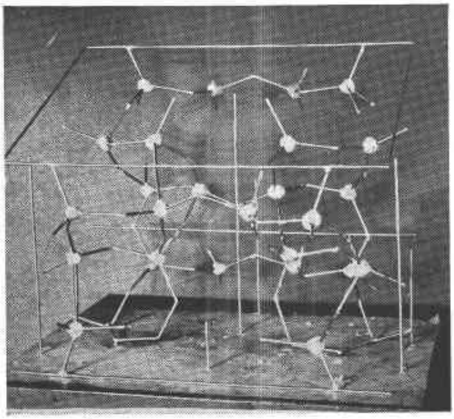

FIG. 3A

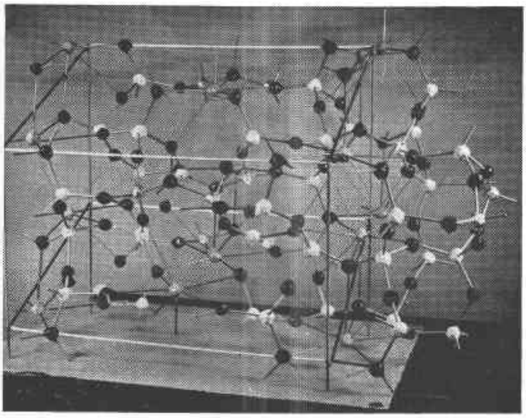

FIG. 3B

FIG. 3. *A* (above): Same as Fig. 2*B* except that all of the SiO_4^{-4}-tetrahedra of the unit cell have been completed and parts of the unit cell are outlined. *B* (below): The completed sanidine model. The morphological c-axis is vertical; the 2-fold, horizontal.

Before any soldering many rods were so cut and bent by gripping in a small vise, or simply holding in a pair of pincers and pressing the free side down against a board or the table top. Two such rods crossing at the bends serve to build the framework of a SiO_4^{-4}-tetrahedron. One rod is held by an end at the top of an "oxygen peg" with its bend on the top of a silicon peg and while in this position its far-end is soldered to the top of a suitable oxygen peg, using a flux on the top of the peg and the end of the rod. The peg whose top marks the position of the Si^{+4}-ion is then with a pair of nippers cut off at the next lower level shown on the plan, after marking the proper place with a pencil line, located by measuring up from the baseboard the indicated distance. Another bent rod is held across the first one so that the bends meet at the Si^{+4}-ion position and the two ends rest on the tops of the proper oxygen pegs. After fluxing, the two rods are soldered together at their bends which location marks the position of the Si^{+4}-ion at the center of the SiO_4^{-4}-tetrahedron. It is also advisable to "tack down" with solder one of the free ends of the second bent rod at the top of one of its oxygen pegs. The two oxygen pegs which now have the ends of two bent rods resting on but not attached to them are next cut down to their lower levels as was done for the silicon peg. To one of the free ends of the wire SiO_4^{-4}-tetrahedron thus completed is soldered the end of a new bent rod while its bend rests on the top of a Si^{+4}-peg and its other end is held at the top of a suitable oxygen peg. Then this second tetrahedron is finished in the manner described above. Fig. 2B shows the condition of the model after five such tetrahedra have been completed. Plastic wood balls have been added marking the positions of the Si^{+4}-ions. Moreover in two places where the two rods from an O^{-2}-ion position to two Si^{+4}-ions make a large angle (about 160°) with each other, small cross-pieces have been soldered at the junction of the two bent rods, so that when later the plastic wood ball representing an O^{-2}-ion is added, it will have no tendency to slip.

Fig. 3A shows the appearance of the model when this process has been continued until all the SiO_4^{-4}-and AlO_4^{-5}-tetrahedra have been completed. Plastic wood balls mark the locations of the Si^{+4}- and Al^{+3}-ions, and the top as well as half of the base (in the *b*-axis direction) of the unit cell is shown by wires. The seven remaining pegs mark the positions of the K^{+1}-ions.

The unit cell with four molecules of $KAlSi_3O_8$ must carry four Al^{+3}-ions. The positions of these can not be differentiated from those of the Si^{+4}-ions by *X*-ray data. Since the sixteen (Si^{+4}-plus Al^{+3}-ions) occur at the points of two general positions designated Si_1 and Si_2, in the table in footnote 6, each of which carries eight ions, there is no way of putting four

Al^{+3}-ions in the unit cell without destroying some of its symmetry.[8] A statistical distribution must be assumed. In making a model one has the choice of using one color of ball to designate the two kinds of ions, or he may color all the balls in either one of the two general silicon positions half aluminum paint and half the color (white) used to designate silicon, or he may arbitrarily select half the balls of either position to represent Al^{+3}-ions. The last course was followed in painting the model depicted in Fig. 3B, and the four "Si_2 balls" nearer the center of the unit cell were so chosen, as close examination will show. This satisfies all elements of symmetry except the screw axes, glide planes, and the symmetry centers lying in the latter. It serves to emphasize how difficult it is to make a static model furnish a close picture of that dynamic body we call a crystal.[9]

Having completed the framework structure of the sanidine model, it is but a fill-in job to add the positions of the K^{+1}-ions. These occupy large spaces in the structure and coordinate with ten O^{-2}-ions. They are 6.8 cms. (2.84 Å.) from six of these and 7.6 cms. (3.16 Å.) from the other four. These two types of coordination are differentiated on Fig. 1. Accordingly two sizes of wire are used, both smaller than that used for the SiO_4^{-4}-framework (the stronger the bond, the coarser the wire in general).

Extension of the structure by methods already described a bit beyond the boundaries of the unit cell, addition of the remaining wires[10] to show the outline of the unit cell (those parallel the *c*-axis extend below the unit cell to serve as a base), completion of the plastic wood balls, and painting serve to finish the model to the form depicted in Fig. 3B. The whole process is so simple that given a plot such as shown in Fig. 1 any

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[8] This symmetry is indicated in Fig. 1. A diagram showing the symmetry of the unit cell viewed along the *b*-axis is given by Taylor, *op. cit.*, p. 428. One showing the symmetry looking along the *c*-axis appears on p. 100 of vol. 1 of the *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, **1935** (symbols used are explained on pp. 92–93.)

[9] Of course it must be realized that the exact atomic parameters of sanidine are not known. As Taylor says (*op. cit.*, pp. 431 et seq.); "the real symmetry of sanidine cannot be monoclinic holohedry; for the Al:Si ratio is always 1:3, so that the 16 (Al+Si) atoms which in this structure are divided into two groups of 8 Si_1 and 8 Si_2 without attempting to distinguish Si from Al, must really be divided into four groups of which three contain 4 Si each and one contains 4 Al." The evidence however favors lower monoclinic symmetry, rather than triclinic. Taken as monoclinic holohedral, sanidine is what Barth and Posnjak (*Jour. Wash. Acad. Sci.*, Vol. **21**, p. 257, 1931) have called a variate atom equipoint structure (also see Barth, *Am. Jour. Sci.*, **27**, 282, 1934), and what Strock (*Zeit. Krist.*, Vol. **93**, pp. 285–311, 1936) would classify as I. B. 2, a shared monocoordinate complete lattice defect structure.

[10] In some models it may be desirable to add a few fine wires to outline the edges of a polyhedron, the coigns of which mark the centers of a single kind of atom.

student with but slight technical ability can complete the job. Moreover, such a problem serves as an ideal introduction for students to the beauties and intricacies of the patterns on which crystals form. Some models of high symmetry such as the diamond are more difficult to make, since a superior quality of workmanship is needed to avoid mechanical distortion. In actual practice the silicon and oxygen positions are not in general completed before the other positions, and in no cases have plastic wood balls been added for part of the ions before the structure network was finished. The scheme followed in building the sanidine model was not one of expediency, but rather one to best illustrate exposition of the method.

In building models such as muscovite[11] with its sheets consisting of double layers of SiO_4^{-4}-tetrahedra (and possibly in making representations of band and chain structures as amphiboles and pyroxenes), it is time-saving to modify the method of model building as described for sanidine as follows. Lay out on a plan similar to Fig. 1 regular hexagons with sides 7.2 cms. long (where 2.4 cms. is equivalent to 1 Å.); the apices of these mark the positions of Si^{+4}-ions. Continue the pattern so that the hexagons fill "plane space." At the middle points of the hexagon sides mark the locations of O^{-2}-ions. Insert pegs extending 5.2 cms. above the baseboard in holes bored at these middle points; no holes need be made at the hexagon corners. Prepare rods like those described that were used in making the SiO_4^{-4}-tetrahedron framework of sanidine; i.e., 7.78+ cms. long bent in the middle at an angle of $109\frac{1}{2}°-$. Holding an end of one of these bent rods at a hexagon corner, with the portion of the rod held

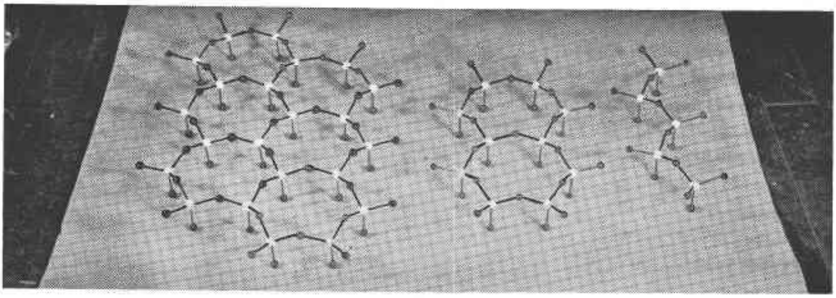

FIG. 4. SiO_4^{-4}-tetrahedra combined into a layer (left) forming one-half of a sheet, a band (or double chain), and a (single) chain (right), as seen in micas, amphiboles, and pyroxenes. The Si^{+4}-ions appear white; the bonds *within the structure*, black.

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[11] Jackson, W. W. and West, J., The crystal structure of muscovite: *Zeit. Krist.*, Vol. **76**, pp. 211 et seq, 1930. References to papers through 1934 describing crystal structures are given by Wyckoff, R. W. G., *The Structure of Crystals*, **1931**, and *Supplement*, **1935**.

being in a vertical position, rotate it till the other end of the rod touches the top of an oxygen peg and, after fluxing, solder this junction. Hold another bent rod under the rod just fastened down so that the two bends "hook" together, and solder at this point (position of a Si^{+4}-ion) while the two ends of the loose bent rod rest on the tops of two oxygen pegs at the middles of the hexagon sides. This completes one SiO_4^{-4}-tetrahedron of the layer, and continuance of this procedure results in the layer, or a band, or just a chain. Adding plastic wood balls and painting give the results shown in Fig. 4.

APPENDIX

The senior author has devoted some thought to coloring schemes. For simplicity the axial directions as shown by the outlines of the unit cell are painted red, white, and blue for *a*, *b*, and *c*, respectively. This may appeal to foreigners rather less than to our own American students. All O-Si-O bonds that form parts of framework, sheet, band, or chain structures are painted yellow; otherwise they are colored orange or, if the number of types of bonds is small so that these can all be differentiated by varying sizes of wire, left uncolored.

TABLE 1. COLORS USED FOR DESIGNATING VARIOUS ELEMENTS

Color	*Radius (Å)	Elements
Pink	1.5 –2.2	(S, Se, Te)$^{-2}$, (Cl, Br, I)$^{-1}$, (F, OH**)$^{-1}$, Sb, Pb
Red	1.32	O^{-2}
Brown	1.3 –1.5	(Ba, Pb)$^{+2}$, K^{+1}, (NH$_4^{+1}$), Te, Ta
Orange	1.2 –1.3	La^{+3}, Sr^{+2}, Fe
Lemon chrome	.98–1.05	Na^{+1}, S
Ivory yellow	0.9 –1.2	Ce^{+4}, (Yt, Rare Earths)$^{+3}$, (Ca, Mn)$^{+2}$, Se
Light green	0.8 –0.9	Zr^{+4}, Sb^{+3}, (Fe, Co)$^{+2}$
Dark green	0.7 –0.8	Mn^{+3}, Mg^{+2}, Li^{+1}
Light blue	0.6 –0.7	Mo$^{+6,4}$, Sb^{+5}, Cb$^{+5,4}$, W^{+4}, (Ti, V)$^{+4,3}$, Fe^{+3}
Dark blue	0.4 –0.6	Mn$^{+7,4}$, V^{+5}
Lilac	0.2 –0.4	S^{+6}, (N, P)$^{+5}$, B^{+3}, Be^{+2}
White	0.39	Si^{+4}
Gray	0.47–1.35	As$^{+5,3}$, As
Black	0.15–0.77	C^{+4}, C
Aluminum	0.4 –1.13	Cr$^{+6,3}$, Sn^{+4}, Al^{+3}, (Ni, Zn, Cd, Hg)$^{+2}$, Ag^{+1}
Aluminum	1.3 –1.53	Pd, Ag, Sn, Os, Ir, Pt, Hg
Copper	0.7?–1.24	Cu^{+2}, Cu^{+1}, Cu
Brass	1.37–1.40	Au^{+1}, Au
Bronze	1.1?–1.77	Bi^{+3}, Bi

* As given in *Internationale Tabellen zur Bestimmung von Kristallstrukturen*, vol. **2**, pp. 611–614, 1935. Goldschmidt values used where available. C. N. 8 for atoms (except C).

** The radii of the F^{-1}- and OH^{-1}-ions are probably about 1.33 and 1.4 Å.respectively, but they are arbitrarily put with the "pink group" as it is desirable to include them with the electronegative ions, and yet they should be distinguished from O^{-2}.

There is no obvious systematic scheme of coloring the balls to represent the various elements which is likely to meet with general agreement. It is impractical and unnecessary to have 92 shades; moreover in case a single element occurs as ions of different valencies in a given mineral, as for example in the case of iron in silicates, it is necessary to differentiate between these. It is, however, obviously desirable that some uniform system be adopted.

Since it is probably not practicable to have balls of plastic wood of pronouncedly different sizes,[12] the attempt has been made to have color serve the double purpose of designating the element and giving some picture of its size, though actually a better size conception comes from the dimensions of the opening in which a given ball is centered. By making declining ionic or atomic radius go hand in hand with decreasing wave length, color is made to serve this double purpose, as is brought out in Table 1. The radii limits shown in this table may be taken as standard for 6–6 or 6–4 coordination at ordinary temperatures, but vary by plus 3 to minus 6–8 per cent for other coordinations. It is less practicable to use atomic radii as a basis for color separation in the thickly populated range from 1.2 to 1.5 Å. (orange and brown, Table 1). Aluminum paint is therefore substituted for silver-colored elements which occur as minerals, or which (as Cr, Ni, Zn, Cd) are in everyday use for plating, as well as for Al^{+3}. For the chromatic colors there is a close correspondence between size and wave length, although red is reserved for the all important O^{-2}, while yellow (lemon chrome) calls to mind the sodium flame, as well as elementary sulphur.

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[12] Wyckoff (*op. cit.*) in his drawings has used circles ("balls") which are in general too small for packing models but yet show great size differences. It is not practicable to make analogous models using plastic wood balls. Gruner (*op. cit.*) "makes each element a different size." He does not state the size variations, but at best it probably gives but a faint picture of actual size differences.