

THE AMERICAN MINERALOGIST

JOURNAL OF THE MINERALOGICAL SOCIETY OF AMERICA

Vol. 23

AUGUST, 1938

No. 8

DATA FOR THE CONSTRUCTION OF MODELS ILLUSTRATING THE ARRANGEMENT AND PACKING OF ATOMS IN CRYSTALS

(FORMULA TYPES A, AB, AND AB₂)

M. J. BUERGER AND ROBERT D. BUTLER,

*Massachusetts Institute of Technology, Cambridge, Massachusetts,
and Lehigh University, Bethlehem, Pennsylvania.*

INTRODUCTION

In a recent paper,¹ the writers have presented a technique for the construction of models illustrating both the arrangement and the packing of atoms in crystals. Models of some sixty-odd crystal structure types have been constructed by the methods discussed. In most of the structure types, the positions of the atoms are sufficiently general to require a very considerable expenditure of effort in the several calculations necessary before an acceptable model can be constructed. The present paper gives the results of such calculations as have been made to date for certain simple structures. A later paper will present data for more complex structures.² Those wishing to duplicate such models may utilize the data herewith presented and proceed with the construction without further calculation.

As discussed in the first paper, certain relatively minor parameter adjustments have been made in almost all cases. For the benefit of those wishing to ascertain to what extent these minor changes have affected the accuracy of representing the actual crystal structure, the adjustments are outlined for each model.

The drilling coördinates could be best presented by a series of labelled plan views of the atoms in question, similar to figures 5 and 8 of the original paper. In order to save expense, however, a tabular method of presentation has been adopted. This lists for each ball the ρ and ϕ co-

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 Data have already been published for models of some of the silicates: Dorris, J. E., Frondel, Clifford, Güssow, W. C., Lopez, V. M., Lord, C. S., Parrish, William and Shimer, J. A., Atomic packing models of some common silicate structures: *Am. Mineral.*, vol. 23, pp. 65-84, 1938.

ordinates of each hole to be drilled, the ball to which the bond from each hole extends, and the key coordinate of the hole in the neighboring ball to which the bond extends. The latter facilitates orientation during construction. The number of balls of each kind required for a model is also given in the tabulation. The column presenting this is headed "Number of balls required for one unit cell model." In this case, a "one unit cell model" contains the atomic contents of one unit cell plus certain extra atoms. The latter are usually required to give mechanical support or rigidity to the cell contents, or are desirable in order to fill out the environment of the atoms in the cell. The designations "F" and "C" refers to models based upon face-centered and C-centered cells. They have been used where the smallest unit cell shows too little of the structure to be representative. Among hexagonal crystals, the designation "hex" indicates that the model contains 3 diamond-shaped hexagonal cell units, arranged to display the hexagonal symmetry of the model.

Under the discussion for each structure is given the source of the data used by the writers. This is not necessarily the publication of the original worker, as many of the data have been compiled in the standard reference works: *Strukturbericht*^{3,4,5,6} I, II, III, and IV, (briefly referred to as S_I, S_{II}, S_{III} and S_{IV}), Wyckoff's *The Structure of Crystals*⁷ (briefly referred to as W), Wyckoff's *Supplement*⁸ (briefly referred to as WS) and Bragg's *The Atomic Structure of Minerals*⁹ (briefly referred to as B).

The space group of the structures is also given, for even if the reference showing the general plan of the structure is not available, it is possible to construct models from a knowledge of the drilling coordinates and space group. It is advisable, however, to have a sketch or drawing of the structure to facilitate construction.

Ball sizes are suggested based upon the scale used by the writers, $1'' = 2\text{\AA}$. Since the publication of the earlier paper, wooden balls have become available from the same source in diameter intervals of $1/16''$. Better representation of atomic sizes is now attained due to the availability of the intermediate sizes.

Where an easy construction scheme has been found for a model it is briefly described.

³ Ewald, P. P., and Hermann, C., *Strukturbericht: 1913-1928*, Leipzig (1931).

⁴ Hermann, C., Lohrmann, O., and Philipp, H.: *Strukturbericht*, Band II, 1928-1932, Leipzig (1937).

⁵ Gottfried, C., and Schossberger, F.: *Strukturbericht*, Band III, 1933-1935, Leipzig (1937).

⁶ Gottfried, C.: *Strukturbericht*, Band IV, 1936, Leipzig (1938).

⁷ Wyckoff, Ralph W. G., *The structure of crystals*, 2nd ed., New York, 1931.

⁸ Wyckoff, Ralph W. G., *The structure of crystals; Supplement for 1931-1934 to the 2nd ed.*, New York, 1935.

⁹ Bragg, W. L., *Atomic structure of minerals*. Ithaca, 1937.

Models for all known mineral structural types in the composition range included in this paper are available with the following exceptions: sulfur, millerite, brookite, cotunnite, calaverite, baddeleyite and krennerite. For the benefit of any wishing to add to the available models, the following list gives all structural types within the composition range included in this paper, for which model calculations have not yet been made:

A	FORMULA TYPE		AB ₂
	AB		
A-6 In	D-31	calomel	C-11 MoSi ₂
A-10 Hg	B-13	millerite	C-12 CaSi ₂
A-11 Ga	B-14	FeAs	
A-12 α - Mn	B-15}	FeB	C-13 HgI ₂
	B-27}		
A-13 β -Mn			C-14 MgZn ₂
A-15 β -W	B-16	GeS	C-15 MgCu ₂
A-16 orthorhombic-S	B-19	AuCd	C-16 CuAl ₂
A-17 black-P	B-20}	FeSi	C-19 CdCl ₂
A-18 Cl	B-28}		
A-19 Po	B-21	CO	C-21 brookite
	B-22	K(SH)	C-22 Fe ₂ P
	B-23	α -AgI	C-23 cotunnite
	B-24	TlF	C-24 HgBr ₂
	B-25	γ -NH ₄ Br	C-26 NO ₂
	B-29	SnS	C-27 CdI ₂
	B-30	MnZn	C-28 HgCl ₂
	B-31	MnP	C-29 SrH ₂
	B-32	NaTl	C-31 Zn(OH) ₂
	B-33	TlI	C-32 AlB ₂
			C-34 calaverite
			C-36 MgNi ₂
			C-37 Co ₂ Si
			C-38 Cu ₂ Sb
			C-39 ZrW ₂
			C-40 CrSi ₂
			C-41 Fe ₂ W
			C-43 baddeleyite
			C-44 GeS ₂
			C-46 krennerite

THE STRUCTURES OF THE ELEMENTS

A-1, Copper,¹⁰ $Fm\bar{3}m$ (O_h^5)

Copper illustrates the structure of several of the common face-centered cubic metals. After drilling, the first hole is not utilized, and the initial holes of all balls are pointed in the direction of the same axis. The closest interatomic distance, $d = 2.55\text{\AA}$, has been altered to 2.50\AA to

¹⁰ S₁, pp. 13-14; W., pp. 200; B., pp. 48-50.

meet the requirements of available ball sizes. The model is assembled most easily by constructing (100) sheets and pinning them together, omitting certain of the pins between the adjacent planes.

A-2, α -Iron,¹¹ $Im3m$ (O_h^9)

α -iron illustrates the structure of the body-centered cubic metals. Although it is possible to utilize drilling coordinates in which the initial hole may be pegged, the coordinates listed give a more symmetrical model, especially if more than one cell is constructed. It is desirable to point the first holes of all balls in the model in the direction of the same a -axis. The closest interatomic distance, $d = 2.477\text{\AA}$, has been represented as 2.500\AA in the model. The structure is assembled by constructing (110) sheets and later fastening them together.

A-3, Magnesium,¹² $C6/mmc$ (D_{6h}^4)

Magnesium is a representative example of hexagonal closest packing with axial ratio $c:a = 1.625:1$. The distances between atoms, 3.20\AA in the (0001) plane and 3.19 between adjacent (0001) planes, have both been changed in the model to 3.25\AA . The initial holes are not used and point in the direction of the c -axis. The model is best assembled by constructing (0001) sheets and pinning them together. The structure is so tight that no weakness results if certain pins are omitted to facilitate construction.

A-4, Diamond,¹³ $Fd3m$ (O_h^7)

Diamond illustrates the simple tetrahedral structure. The interatomic distance, 1.542\AA , has been slightly changed in the model, where it is represented as 1.500\AA . The model is most readily assembled by constructing (111) sheets and pinning one completed sheet to the next. The initial hole is utilized.

A-5, White Tin,¹⁴ $I4/amd$ (D_{4h}^{19})

White tin has a distorted tetrahedral structure which can be considered as a diamond structure collapsed along one of the three cubic axes. The simplest cell is a body-centered one derived by a reorientation of the (100) and (010) planes of the face-centered diamond into (110) and ($\bar{1}10$) planes of white tin. The interatomic distance, 3.02\AA , has been represented in the model as 3.00\AA . The first hole of each ball is not used and points in the direction of the c -axis. The model is assembled most easily by pinning together separate (001) sheets.

¹¹ Sr., pp. 15-16; W., p. 202; B., pp. 48-50.

¹² Sr., pp. 16-19; W., pp. 200-201.

¹³ Sr., pp. 19-21; W., p. 202; B., pp. 51-53.

¹⁴ Sr., pp. 21-23; W., p. 211.

A-7, *Bismuth*,¹⁵ $R\bar{3}m$ (D_{3d}^5)

Bismuth may be regarded as having a distorted simple cubic structure. Actually, it is composed of separate basal sheets. The closest interatomic distance, $d=3.10\text{\AA}$, is represented in the model as 3.125\AA . Each atom is bonded to three close neighbors in contact at distance d and in the same basal sheet, and to two others vertically one sheet above and two sheets below by means of spacing bars whose lengths are respectively 1.97 and 2.31 inches. These bar lengths are calculated on the basis that depth of holes drilled in the balls is exactly $\frac{3}{8}$ inch. The longer spacing bar is utilized between initial holes (which point towards each other in the structure) and the shorter bar between $\rho=180^\circ$ holes. The bars are aligned in the direction of the principal axis of the resulting rhombohedron which is also the direction in which initial holes are pointed.

A-8, *Selenium*,¹⁶ $C3_12$, $C3_22$ (D_3^4 , D_3^6)

The closest interatomic distance between selenium atoms, $d=2.32\text{\AA}$, is adjusted to 2.375\AA in the model. The structure consists of strings of selenium atoms spiralling about three-fold screw axes through the lattice points, with contact between atoms in an individual string, and with strings separated from one another at non-packing distances.

This model is conveniently made by constructing (0001) sheets of balls separated by spacing bars. The balls are translation equivalents arranged at points of a hexagonal plane lattice. The basal planes are fastened together by pinning atoms in contact so that the strings are arranged along vertical screw axes.

Spacing bars are cut 1.78 inches long for use in holes of $\frac{3}{8}$ " depth. The initial holes point in the direction of the c -axis and are not bonded.

A-9, *Graphite*,¹⁷ $C6mc$ (C_{6v}^4)

Graphite consists of planes composed of rings of carbon atoms with individual planes separated by greater than packing distances. The interatomic distance, 1.42\AA , is represented as 1.375\AA . There are two kinds of carbon atoms in the structure which alternate with each other in any of the hexagonal rings composing an individual (0001) plane. The difference is indicated by the diagram in the reference: above and below one kind, C_1 , lies a similar atom, C_1 , in adjacent planes at $\pm c/2$ distance; whereas the other kind, C_2 , lies in planes at $\pm c/2$ above and below the open center of a hexagonal ring. Two separate drillings are required, one for C_1 , the other for C_2 . All initial holes point in the direction of the

¹⁵ S_I., pp. 25-27; W., pp. 202-203; B., pp. 50-51.

¹⁶ S_I., pp. 27-28; W., p. 203.

¹⁷ S_I., pp. 28-30; W., p. 208; B., pp. 52-54.

c-axis. Spacing bars 1.51 inches long hold the (0001) planes apart at distance $c/2$. All holes are $\frac{1}{4}$ " deep and tie pins are $\frac{3}{8}$ " long.

A-14, *Iodine*,¹⁸ $Ccma$ (D_{2h}^{18})

The closest interatomic distance between iodine atoms, 2.70Å, is represented in the model as 2.75Å. The entire structure is proportionally enlarged in the model. Revised cell constants are:

$$\begin{aligned} a &= 4.9\text{Å} \\ b &= 7.4\text{Å} \\ c &= 9.95\text{Å} \end{aligned}$$

As each atom is in close packing contact with but one neighbor, the model must be constructed on a wooden baseboard representing the (010) plane as shown in figure 1. Holes are drilled in the baseboard at the indicated positions. Long brass rods are inserted in these holes, and paired atoms are suspended on the brass rods. After the usual drilling of the balls, the initial hole is redrilled completely through the ball.

The centers of the pairs along the same set of pins are spaced at intervals corresponding to the unit length on *b*, 3.7 inches. Pairs along adjacent sets of pins are spaced similarly but their centers are located at $b/2$ positions.

A-17, *Black Phosphorus*,¹⁹ $Bmab$ (D_{2h}^{18})

Black phosphorus has a layer structure. Each phosphorus atom is in packing contact with three other atoms in its own layer and equidistant from two others on the same symmetry plane in a neighboring layer. The layers are physically supported in the model with the aid of space bars 1.612 inches long, extending in the last-mentioned directions.

In the actual structure the distances between phosphorus atoms in the same layer are 2.17Å and 2.20Å. In the model, the parameter has been changed from .090 to .0863 to equalize all interatomic distances between immediate neighbors in the same layer to 2.19Å. This distance has been represented in the model as 2.25Å, and all dimensions of the model scaled up in this same ratio.

STRUCTURES OF THE AB TYPE

B-1, *Halite*,²⁰ $Fm\bar{3}m$ (O_h^5)

Halite can be very closely represented by altering the Na-Cl interatomic distance, $d=2.814\text{Å}$, so that the scale distance in the model is 2.8125Å. The structure is readily assembled by constructing (100) planes and pinning them together. It is best to have the initial holes of all balls pointing in the direction of the same *a*-axis.

¹⁸ W., pp. 209-210; S_{II} p. 5.

¹⁹ S_{III}, p. 6.

²⁰ S_I, pp. 72-74; W., p. 215; B., pp. 57-60.

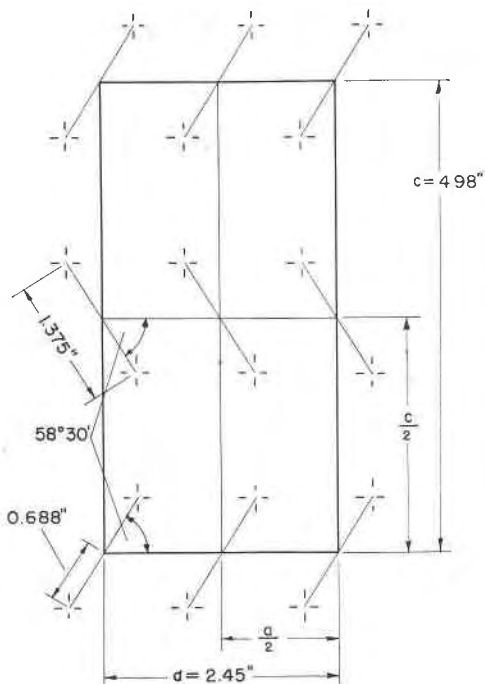


FIG. 1. Layout of baseboard for the construction of the iodine model. The edges of the board are not shown. The heavy rectangle outlines the unit cell and the crosses locate the positions for holes into which supporting rods are to be set.

B-2, *Caesium Chloride*,²¹ $Pm\bar{3}m$ (O_h^1)

Caesium chloride, although not occurring in nature, is an important representative of a type of AB structures which includes several alloys. The model is a scale representation of the structure in that there is no change in the interatomic distances. The initial holes are not used and point in the direction of one of the axes. A model of more than one cell can be constructed most readily by fastening together adjacent (110) planes as in alpha-iron.

B-3, *Sphalerite*,²² $F\bar{4}3m$ (T_d^2)

Sphalerite is a simple tetrahedral array of alternating zinc and sulphur atoms based on the diamond pattern. The interatomic distance, $d = 2.35\text{\AA}$, is represented in the structure as 2.375\AA . The model is most readily assembled by first constructing (111) sheets, which are composed of puckered hexagonal rings of alternating zinc and sulphur, and then

²¹ S_1 , pp. 74-77; W., p. 214.

²² S_1 , pp. 76-77; W., pp. 215-216; B., pp. 62-65.

pinning these together. Care must be taken that the wurtzite structure does not result. Sphalerite differs from wurtzite in that its face-centered lattice requires the atoms of successive (111) sheets to occupy positions screening the holes of the next underlying sheet when viewed from the direction of a trigonal axis. Initial holes should all point in the direction of the same trigonal axis.

B-4, *Wurtzite*,²³ $C6mc$ (C_{6v}^4)

The interatomic distance, $d = 2.36\text{\AA}$, is slightly magnified in this model, as in sphalerite. The same drilling coordinates hold for both wurtzite and sphalerite. Wurtzite is constructed by pinning together adjacent (0001) sheets, each of which is similar to a (111) sheet of sphalerite. In the wurtzite structure, atoms in one sheet do *not* screen the holes in the adjacent (0001) sheet as they do in the case of octahedral sheets in sphalerite. This results in channels parallel to the c -axis. The initial holes should point in the c -axis direction.

B-5, B-6, B-7, *Carborundum*,²⁴ III, II, and I

There are five modifications of SiC, all of which are tetrahedral structures showing various kinds of alternations between sphalerite and wurtzite packing. The interatomic distance $S-C$, 1.89\AA , is represented in the models as 1.875\AA . The model constructor is referred to the *Strukturbericht* reference for details of stacking sequence (especially S_I p. 84) and for decision as to the appropriate number of balls necessary to give a representative picture of the unit cell.

B-8, *Niccolite*,²⁵ $C6mc$ (C_{6v}^4)

The closest packing distance between Ni and As atoms, 2.43\AA , is represented as 2.4375\AA . The Ni-Ni interatomic distance, 2.52\AA , is represented as 2.50\AA . Nickel atoms lie in packing contact with each other along columns in the c -axis direction. Initial holes of all balls should point in the c -axis direction.

B-8, *Pyrrhotite*,²⁶ $C6mc$ (C_{6v}^4)

The arrangement of atoms in pyrrhotite is similar to that in niccolite, but the cell is more expanded in the direction of the c -axis. As a result of this, the metals do not touch, as they do in the niccolite structure. The metal atoms have a perfectly regular octahedral sulfur coordination. The Fe-S distance is actually 2.47\AA in the structure; it is represented as 2.50\AA in the model, and all dimensions are expanded by this amount.

²³ S_I , pp. 78-79; $W.$, pp. 216-217; $B.$, pp. 64-65.

²⁴ S_I , pp. 80-84; $W.$, pp. 222-223.

²⁵ S_I , pp. 84-87; $W.$, p. 217; $B.$, pp. 65-68.

²⁶ S_I , pp. 84-87; $W.$, pp. 217-218; $B.$, pp. 65-68.

In calculating this structure, the original drilling coordinates have been transformed by rotation so that the first hole is utilized for bonding.

B-9, *Cinnabar*,²⁷ $C3_12, C3_22$ (D_3^4, D_3^6)

The interatomic distance between Hg and S, $d = 2.52\text{\AA}$, is altered to 2.50\AA in the model. It is stated that uncertainty exists as to which of the two parametric values holds for cinnabar:²⁸ $u = 0.33, v = 0.21$ or $u = 0.72, v = 0.55$. Inasmuch as they lead to different structures, the coordinates for both are listed. With the exception of different drilling coordinates, generalizations pertain to both examples. The lengths of the a -axis and c -axis are truly represented (Buckley's values).

The model is assembled by constructing sheets consisting of Hg balls at points of a hexagonal plane lattice and held apart at non-packing distances by spacing bars. Alternate sheets of Hg atoms are united by intermediate layers of S atoms; each S atom is bonded to two Hg atoms, one in the sheet above and one below. Initial holes of both types of balls are not used, and point in the same direction along the c -axis. Spacing bars between Hg atoms are cut 1.39 inches long, for seating in holes $\frac{3}{8}$ " in depth. Atoms contained in the same basal plane are translation equivalents and must be oriented accordingly.

B-11 *Lead Oxide*,²⁹ (tetragonal), $P4/nmm$ (D_{4h}^7)

This is a layer structure composed of identical (001) sheets held together by space bars. The interatomic distance between Pb and O, 2.33\AA , is represented in the model by a scale distance of 2.3125\AA . An imperceptible contraction of the a -axis occurs in the model but, as spacing bars are used between (001) sheets, their lengths are adjusted so that c is truly represented. Initial holes in Pb are utilized for spacing bars and point in the direction of the tetragonal axis. Easiest assembly is by constructing 100 strings of Pb-O-Pb-O-Pb, etc., attaching these to form (001) sheets, and then fastening the sheets together with space bars $1\frac{5}{8}$ " long.

D-31, *Calomel*,³⁰ $I 4/mmm$ (D_{4h}^{17})

Ball sizes have been chosen on the assumption that the opposing chlorine atoms of neighboring layers are in contact. The Hg-Cl interatomic distance, 2.52\AA is represented in the model as 2.50\AA . The entire structure is correspondingly shrunk by less than 1%. The c -axis, in addition, loses $.1\text{\AA}$ by the ball sizes chosen, but this can be compensated,

²⁷ S_I, pp. 87-89; W., pp. 221-222; B., pp. 68-69.

²⁸ W., p. 222.

²⁹ S_I, pp. 89-95; W., pp. 218-219.

³⁰ S_I, pp. 237-239.

if desired, by the use of a spacing bar of .80" length between opposing chlorines ($\rho=0^\circ$) set in holes $\frac{3}{8}$ " deep.

B-12, *Boron nitride*,³¹ $C6mc$ (C_{6v}^4)

The boron nitride structure is the same as the graphite structure in which B takes the place of C_2 and N takes the place of C_1 . The interatomic packing distance in the (0001) sheets, $d=1.45\text{\AA}$, is represented in the models by 1.4475\AA . Spacing bars are 1.48 inches long and hold the (0001) planes apart at distance $c/2$. All holes are $\frac{1}{4}$ " deep and tie pins are $\frac{3}{8}$ " long.

B-18, *Covellite*,³² $C6/mmc$ (D_{6h}^4)

The covellite structure consists of hexagonal basal sheets, each composed of copper and sulfur atoms. There are two kinds of copper atoms and two kinds of sulfur, each restricted to a unique type of coordination within the structure. Starting with a sheet composed of S_{II} and Cu_{II} (see Fig. 2), the next sheet is a true plane of S_I and Cu_I in alternating

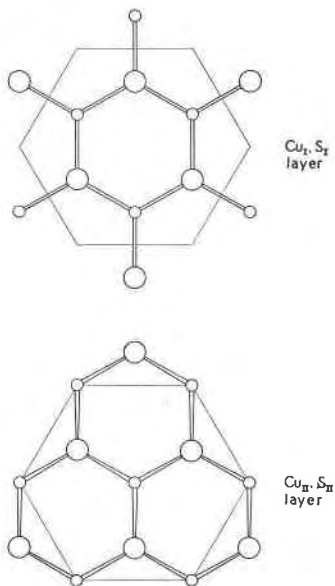


FIG. 2. Plans of the two different kinds of (0001) layers in the covellite structure, showing bonding within the layers. The hexagon drawn in fine lines outlines the hexagonal cell (containing three primitive translation units). The large circles represent Cu atoms, the small circles, S atoms.

³¹ S_I , p. 95; W., p. 208.

³² S_{II} , pp. 10-11; B, p. 77.

hexagonal array and at level $c/4$. There is a reflection plane of symmetry contained in all planes composed of Cu_I and S_I , so the next sheet is a duplicate of the first. This completes half the cell. A duplicate sequence is next constructed, rotated 180° from the first, and attached to it, bonding S_{II} of the lower unit to S_{II} to the upper one. All initial holes point in the c -axis direction.

The following tabulation indicates the liberties which have been taken with the actual structure.

	Structure	Model
Cell constants: a	3.80Å	3.77Å
c	16.46Å	16.50Å
Interatomic distances		
S_{II} - S_{II}	2.05Å	2.00Å
S_{II} - Cu_{II}	2.32Å	2.3125Å
S_I - Cu_I	2.20Å	2.1875Å
Cu_{II} - S_I	2.34Å	2.375Å

It is possible to adjust the structure in other directions, but the adjustments outlined above cause little deviation from the actual structure. The bond angles for S_I and Cu_I , 109° , are very close to the tetrahedral angle, $109^\circ 28'$.

B-17, *Cooperite*,³³ $P4/mmc$ (D_{4h}^2)

The interatomic distance between Pt and S atoms, 2.32Å, is represented in the model as 2.3125Å. Initial holes of Pt are not used and point in the same [100] direction within any (001) plane; initial holes of Pt in the adjacent planes point in the [010] direction. Initial holes of S point in the [001] direction and are not bonded. Easiest assembly is accomplished by pinning together separate (011) planes. A primitive cell gives a very poor representation of the structure; it is best to construct a C -centered one, which, incidentally, is then directly comparable with the tenorite structure.

B-26, *Tenorite*,³⁴ $C2/c$ (C_{2h}^6)

This is a slightly collapsed cooperite structure. In order to construct it, it is highly desirable to have a C -centered cooperite structure already made, as a guide. Figure 1 of Tunell, Posnjak and Ksanda's article³⁵ should first be altered as follows: draw colored lines between Cu and O atoms to show approximately square Cu bonds and approximately tetrahedral O bonds. Then label all oxygens on the $\frac{c}{4}$ level "L" (left) and all those on the $\frac{3c}{4}$ level "R" (right).

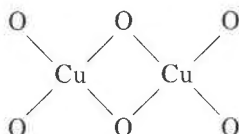
³³ S_{II} ., pp. 9-10; B., pp. 69-70.

³⁴ B., pp. 92-93; S_{III} , pp. 11-12.

³⁵ *Zeits. Krist.*, (A) vol. 90, p. 134, 1935.

The mark between holes in the oxygens gives the direction of the 2-fold axis on which these lie, and fixes the orientation. The mark between holes in the coppers identifies the acute angle of the almost square bonds. This acute bisector should lie in the (001) plane.

The assembly in this model is best made (if the model is one cell plus environs as included in the table) by constructing the lower [101] ribbons of the type



and adding crossing $[10\bar{1}]$ ribbons thereto. For larger models, the cooperative type of construction should be followed, i.e., by fitting together (111) sheets. This construction method is exceedingly difficult because of the many orientation requirements involved.

STRUCTURES OF THE AB_2 TYPE

Many of these structures are closely represented by the models on the scale adopted. Those in which the atoms lie in special positions have had ball sizes so chosen as to represent most closely the interatomic distances. The departures from true representation are therefore but slight magnifications or contractions of interatomic distance and cell edges.

More serious distortions have to be compensated in structure where the atoms lie in positions with variable parameters as in the case of marcasite. In general, these difficulties are overcome as in marcasite by the method discussed in the earlier paper.¹

Special problems for successful construction of models are presented by the silica minerals; the final section of this paper will illustrate the type of adjustment utilized in calculating the drilling coordinates for these structures.

C-1, Fluorite,³⁶ $Fm\bar{3}m$ (O_h^5)

The interatomic distance between Ca and F, $d = 2.362\text{\AA}$, is represented in the model as 2.375\AA . Initial holes are not used, and point in the direction of the same cubic axis. Notwithstanding the simplicity of the structure, the model is difficult to construct because of its exceedingly close packing. If more than a unit cell is built, it is easiest to construct separate (110) planes and pin them together, omitting all but necessary pins.

³⁶ Sr., pp. 148-150; W., p. 230; B., p. 57.

C-2, *Pyrite*,³⁷ $Pa3 (T_h^6)$

The interatomic distance between S atoms, $d=2.10\text{\AA}$, is represented in the model as 2.125\AA . The Fe-S distance, $e=2.26\text{\AA}$, is represented as 2.25\AA . The cell edge in the model is represented as 5.38\AA as compared with 5.40\AA in the actual structure.

This structure is so complex that it is necessary to understand the space group before attempting construction. Initial holes of balls representing Fe atoms are not used and must point in the direction of a 3-fold axis in the space group. The initial hole of S is everywhere bonded to the initial hole of the other S constituting the sulfur pair. Easiest construction is realized by pinning together individual strings made up of Fe-S-S-Fe or S-S-Fe-S-S which are elongated in the direction of a cubic axis. The strings are then joined to form (100) sheets, which are subsequently pinned together.

C-3, *Cuprite*,³⁸ $Pn3m (C_h^4)$

The cuprite structure consists of two identical space networks which thread through one another's interstices but in no place come in contact. Because of this unusual situation, in the model representation of the structure one network must be suspended from the other by space bars of arbitrary location. The individual networks have an arrangement identical with that of cristobalite in which the cristobalite silicon has been replaced by the cuprite oxygen and the cristobalite oxygen has been replaced by the cuprite copper.

The closest interatomic distance between Cu and O, $d=1.84\text{\AA}$, is represented in the model as 1.875\AA . Spacing bars 1.67 inches long extend vertically from the O of one network to the O of the other. Holes in O are drilled $\frac{3}{8}$ " deep, in Cu $\frac{1}{4}$ ". Tie pins must be $\frac{1}{2}$ " long instead of the usual $\frac{5}{8}$ " length. The spacing bars are all located in the direction of the vertical axis. The model is constructed by pinning together, *via* the Cu balls, separate (110) planes containing both Cu and O.

C-4, *Rutile*,³⁹ $P4/mnm (D_{4h}^{14})$

Interatomic distances, $d=2.01\text{\AA}$, between Ti and O, and $e=2.46\text{\AA}$, between O and O, are represented in the model by 2.00\AA and 2.50\AA , respectively. The model is most easily constructed by assembling separate (110) planes.

C-5, *Anatase*,⁴⁰ $I4/amd (D_{4h}^{19})$

The interatomic distances in the anatase structure have been ad-

³⁷ Sr., pp. 150-153; W., p. 234; B., pp. 71-73.

³⁸ Sr., pp. 153-155; W., p. 241; B., pp. 90-91.

³⁹ Sr., pp. 155-158; W., pp. 230-231; B., pp. 102-103.

⁴⁰ Sr., pp. 158-161; W., pp. 249-250; B., p. 104.

justed in the model in order to correspond with the ball sizes adopted for rutile. The model is constructed by assembling (001) sheets of Ti and O balls. The initial holes of all balls point in the c -axis direction. The alterations are as follows:

	Structure	Model
(d) Ti-O	1.95Å	2.00
(d') Ti-O	1.91Å	2.00
(e') O-O	2.43Å	2.50

C-6, *Tin Disulphide*,⁴¹ $C3m$ (D_{3d}^3)

Tin disulphide has been taken as a convenient representative of the "cadmium iodide structure." It can be represented either as an ionic bond structure or as a covalent bond structure, data for both being given in the tables. The Sn-S distances are 2.55Å in the actual structure; they are represented as 2.50Å in the models. The closest S-S distances are 3.59Å and 3.62Å in the actual structure; they are all idealized to 3.562Å in the models.

If ionic bonding is assumed, the structure can be represented by hexagonal close-packed S ions in contact (construction the same as the magnesium model) with Sn ions stuffed into the interstices between sulfur octahedra. For this model, a single hole is drilled in the Sn ion to attach it to one of its six neighboring sulfur ions.

If covalent bonding is assumed, the structure becomes a series of identical, separated sheets. The sheets are kept together by means of space bars, 2.175 inches long and parallel to the c axis, extending between tin atoms.

C-7, *Molybdenite*,⁴² $C6/mmc$ (D_{6h}^4)

This is a layer structure, composed of separate hexagonal MoS_2 layers. The layers are separated from one another at greater than packing distances, arranged for in the model by means of spacing bars. The interatomic distance, $d=2.35\text{Å}$, is altered to 2.375Å in the structure. The lengths of the a -axis and c -axis in the model truly represent the structural axes. All initial holes point in the direction of the c -axis but it is not necessary to place a spacing bar in every position available. Spacing bars are cut 1.87" long for holes $\frac{3}{8}$ " in depth.

C-18, *Marcasite*,⁴³ $Pnmm$ (D_{2h}^{12})

The adjustment of the marcasite structure has been discussed in the earlier paper.⁴⁴ Several other compounds, löllingite, FeP_2 , $FeSb_2$, and

⁴¹ Sr., pp. 161-163; W., pp. 232-233.

⁴² Sr., pp. 164-166; W., p. 233; B., p. 77.

⁴³ Sr., pp. 495-497; Sr., p. 272; WS., pp. 23-26; B., pp. 73-75.

⁴⁴ Reference 1, pp. 160-167.

CaCl_2 , whose structures are of the marcasite-type have been adjusted and calculated in a similar manner. Their coördinates are listed without comment.

In structures where balls are drilled with holes at nearly equal ρ angles as in marcasite, it is well to mark certain holes with a scratch or prick of the drill bit on the ball surface in order to facilitate identification of this hole and thus easy orientation when assembling. Holes thus marked are noted with an "m" in the tabulation.

C-18, *Löllingite*,⁴⁵ $Pnmm$ (D_{2h}^{12})

See under *marcasite*, above.

C-18, *Iron di-phosphide*,⁴⁶ $Pnmm$ (D_{2h}^{12})

See under *marcasite*, above.

C-18, *Iron di-antimonide*,⁴⁷ $Pnmm$ (D_{2h}^{12})

See under *marcasite*, above.

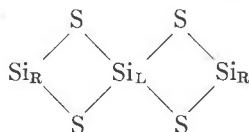
C-18 (C-35), *Hydrophilite*,⁴⁸ $Pnmm$ (D_{2h}^{12})

See under *marcasite*, above. Hydrophilite has a marcasite-like structure, but the Cl atoms are not so obviously paired.

C-42, *Silicon di-sulfide*,⁴⁹ $Icma$ (D_{2h}^{26})

The structure consists of individual strings of SiS_2 along sets of B-centered b -axes. A wooden baseboard has a rectangle laid off on it to represent the unit cell in the (010) plane, $a=2.8$ inches and $c=4.8$ inches. At the corners and the center of this rectangle, holes are drilled and long brass rods inserted into them. The balls representing Si have their initial holes drilled all the way through and these are impaled on the rods and held apart by balls representing S. The strings are of two configurations, right and left.

To construct a single cell, make four strings as follows:



and place these at the cell corners. Make up one string as follows:

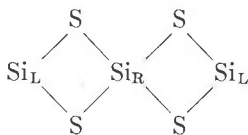
⁴⁵ S_{II}, pp. 273-274; B., pp. 73-75; WS, pp. 23-26.

⁴⁶ WS, p. 24; S_{III}, p. 310.

⁴⁷ S_I, p. 497.

⁴⁸ S_{III}, pp. 30-31, p. 278.

⁴⁹ S_{III}, pp. 37-38, 286.



and place it at the cell center.

C-9, *High Cristobalite*⁵⁰ (Ideal, after Wyckoff), $Fd\bar{3}m$ (O_h^7)

The interatomic O—O distance, $d = 2.52\text{\AA}$, is adjusted to 2.50\AA . Silicon ions are represented by small glass beads or lead pellets. They are not pinned, for the size chosen fits exactly into the interstitial space within the four oxygen members of a tetrahedron. Buckshot, 0.30" in diameter are satisfactory (No. 1 Buckshot, eastern size; no. 5 or 6 buckshot, western size).

The model is most readily assembled by constructing individual rows of tetrahedra in the [110] direction and pinning them together. The initial holes point towards the unpinned Si pellet.

C-30, *Low Cristobalite*,⁵¹ $P4_12_1$, $P4_32_1$ (D_4^4, D_4^8)

The adjustment of the low cristobalite structure for the derivation of drilling coördinates of the model is given in the appendix. Several of the silica structures have undergone somewhat similar adjustments. The principal adjustment of the actual structures is an idealization of slightly distorted SiO_4 tetrahedra. The actual O—O distances, which vary from $2.58\text{--}2.63\text{\AA}$, are represented in the model as 2.625\AA .

The initial hole of O is not used, and points in the direction of the c -axis. The model is most easily constructed by assembling individual tetrahedra, pinning them into rows, and uniting the rows.

C-10, *High Tridymite*,⁵² $C6/mmc$ (D_{6h}^4)

The interatomic O—O distance, 2.52\AA , is represented in the model as 2.50\AA . The structure is composed of hexagonal rings of O_{I} atoms in the (0001) plane, united to the adjacent (0001) plane by O_{II} atoms which are mutually shared by upper and lower tetrahedra. The initial holes of O_{I} point towards a Si but are not used, and the unused initial holes of O_{II} point towards Si, which direction is also the c -axis direction. The model is assembled by uniting (0001) planes.

C-8, *High Quartz*,⁵³ $C6_22$, $C6_42$ (D_6^4, D_6^5)

The interatomic O—O distance, 2.59\AA , is represented in the model as 2.625\AA . Initial holes are not used and point towards an unbonded Si

⁵⁰ Si., pp. 169–171; B., pp. 88–90; WS., pp. 28–29.

⁵¹ Si_{III}, pp. 25–26.

⁵² Si., pp. 171–174; B., p. 88; W., pp. 248–249.

⁵³ Si., pp. 166–169; W., pp. 246–247; B., pp. 84–85.

pellet. The model is best assembled by assembling separate (0001) planes of tetrahedra.

“C-8,” *Low Quartz*,⁵⁴ $C3_12$, $C3_22$, (D_3^4 , D_3^6)

Although each oxygen atom actually has four different coördination distances to other oxygens varying from 2.62Å–2.57Å, the structure has been idealized by representing all O-O spacings as 2.625Å. Initial holes are not used and point in the c -axis direction. The model is best assembled by constructing individual rows of tetrahedra, and uniting to form (0001) planes. The adjustment of this structure to drilling coördinates was made in a similar way to that of low cristobalite described in the appendix.

APPENDIX

COORDINATE CALCULATIONS IN CASES OF LOW BOND SYMMETRY.

General Procedure.—Many of the structures which have been discussed have been characterized by atoms situated in positions of considerable symmetry. In such cases the distribution of nearest neighbors and, therefore, the distribution of mechanical bonds in the model have been symmetrical. In structures containing atoms in positions of little or no symmetry, the methods of calculating drilling coördinates which have been discussed are ordinarily ones of very great difficulty. The more general cases are readily treated by the following simple general principles:

The necessary adjustments are first accomplished and new coördinates of the atoms calculated for the adjusted structure. If the crystal is not isometric, *these coördinates must be transformed into new ones referred to isometric, orthogonal axes.* This is ordinarily easily accomplished except for triclinic crystals, where the transformation is tedious. An example of the transformation for monoclinic crystals is given beyond. Let the new coördinates of two atoms be $[[x_1y_1z_1]]$ and $[[x_2y_2z_2]]$. The drilling coördinates of the bond from atom 1 to atom 2, referred to the new Z axis as origin direction, can be seen from figure 3 to be:

$$\rho = 90^\circ - \tan^{-1} \left(\frac{z_2 - z_1}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}} \right) \quad (1)$$

$$\text{or} \quad \rho = 90^\circ - \sin^{-1} \left(\frac{z_2 - z_1}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}} \right) \quad (2)$$

where $\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}$ is the interatomic distance.

$$\phi = \tan^{-1} \left(\frac{y_2 - y_1}{x_2 - x_1} \right). \quad (3)$$

⁵⁴ WS., p. 26; B., p. 85; S_{III}, p. 21.

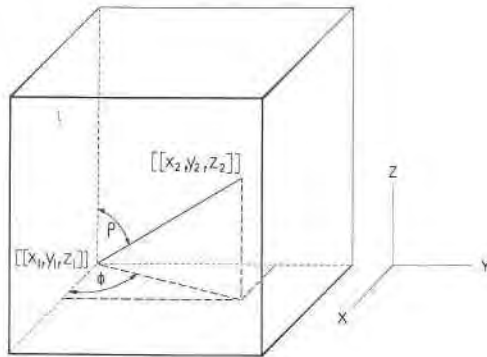


FIG. 3. The derivation of the drilling coordinates, ρ and ϕ , for a bond extending from a ball with coordinates $[[x_1, y_1, z_1]]$, to a ball with coordinates $[[x_2, y_2, z_2]]$. The origin direction for drilling coordinate ρ is Z .

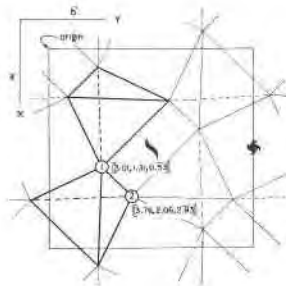
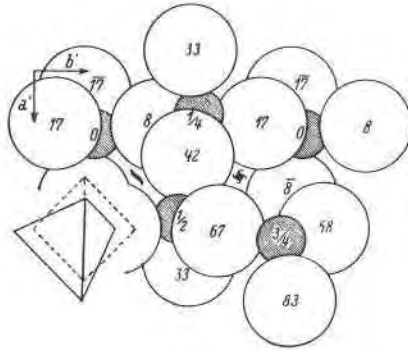


FIG. 4A. Nieuwenkamp's illustration of the structure of low cristobalite projected on $(00\bar{1})$.

FIG. 4B. Diagrammatic representation of the adjusted low cristobalite structure corresponding with part of Fig. 4A, and illustrating the derivation of the drilling coordinates for the bond extending from oxygen atom 1 to oxygen atom 2.

The origin direction, Z , which becomes the first, unused, hole, may be any of the coördinate directions which it is convenient to use. The only restriction on the choice of the direction, Z , is that it should not have a bond nearer to it than about $\rho = 30^\circ$, for such holes are mechanically impossible to drill.

Application to low-cristobalite drilling coördinates.—The low-cristobalite structure⁵⁵ furnishes an illustration of the usefulness of this general method. The bonds are between oxygen atoms occupying the general position of a structure of low symmetry. Low cristobalite is tetragonal $P4_12_1(D_4^2)$ and has a structure projected on (001) as shown in Fig. 4A.

The adjustments need not be discussed in detail. They include regularizing the slightly irregular SiO_4 tetrahedron and shrinking the actual cell dimensions slightly to permit the use of commercial ball sizes. The new coördinates of two atoms, referred to an isometric coördinate system are shown in Fig. 4B. Utilizing the relations given above, the drilling coördinates of the bond from atom (1) to atom (2) are:

$$\begin{aligned}\rho &= 90^\circ - \tan^{-1} \left(\frac{2.93 - .53}{\sqrt{(3.76 - 3.01)^2 + (2.06 - 1.31)^2}} \right) \\ &= 90^\circ - (-66^\circ) = 156^\circ \\ \phi &= \tan^{-1} \left(\frac{2.06 - 1.31}{3.76 - 3.01} \right) \\ &= 45^\circ.\end{aligned}$$

Application to tenorite drilling coördinates.—A simple example in which generalized crystal coördinates must first be transformed into isometric orthogonal coördinates, is afforded by the structure of tenorite.⁵⁶ Tenorite is monoclinic, and has a structure which can be described as a somewhat collapsed cooperite structure. Each copper atom is surrounded by four oxygen atoms at the corners of an almost square rectangle, and each oxygen atom is surrounded by four copper atoms at corners of an irregular tetrahedron of symmetry C_2 . The collapse and consequent irregularity of the coördinations give rise to the monoclinic nature of the structure.

All Cu-O distances between immediate neighbors are given by the investigators as 1.95Å. This can be represented in commercially available ball sizes by 1.9375Å (1 15/16"). Since no adjustments except the change of scale are required, the structure of tenorite can be exactly represented in a model by allowing an all-around linear shrinkage of about $\frac{1}{2}\%$.

⁵⁵ Nieuwenkamp, W., Die Kristallstruktur des Tief-Cristobalits SiO_2 . *Zeits. Krist.*, Vol. 92, pp. 82-88, 1935.

⁵⁶ Tunell, G., Posnjak, E., and Ksanda, C. J., Geometrical and optical properties, and crystal structure of tenorite: *Zeits. Krist.*, vol. 90, pp. 120-142, 1935.

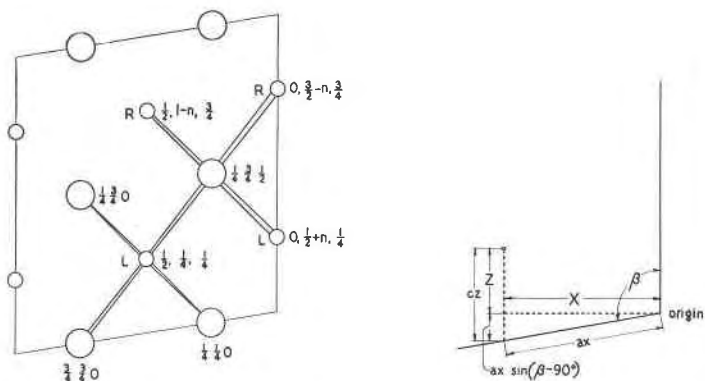


FIG. 5A. Projection of the structure of tenorite on $(0\bar{1}0)$, showing the bonding between atoms having the coordinates indicated. Large circles are copper atom positions, small circles are oxygen atom positions. The designations "L" and "R" indicate atoms whose environments and drilling coordinates are related to one another as left and right, respectively. The fine lines outline the unit cell.

FIG. 5B. The derivation of isometric orthogonal coordinates, X , Y , and Z from the monoclinic coordinates, x , y , and z . The direction Y is to become the origin direction for drilling coordinates ρ .

Figure 5A shows a duplicate of Tunell, Posnjak and Ksanda's Fig. 2c, which is a projection of tenorite on $(0\bar{1}0)$, but slightly modified to bring out the bonding. The relation between the monoclinic coordinates and isometric coordinates taken parallel and perpendicular to the monoclinic c -axis, is shown in Fig. 5B. The new isometric coordinates, XYZ , are evidently derivable from the monoclinic coordinates xyz with the aid of the following transformation:

$$\begin{aligned} X &= ax \cos (\beta-90) \\ Y &= b y \\ Z &= c z - ax \sin (\beta-90) \end{aligned}$$

Carrying out these transformations for the eight atoms linked by bonds as in Fig. 5A, yields the isometric orthogonal coordinates listed in Table I.

The drilling coordinates may now be calculated by substituting the isometric orthogonal coordinates in relations like (1) and (3) but such as to make \bar{Y} the origin of ρ . For example, in calculating the drilling coordinates for the copper at $[\frac{1}{4} \frac{3}{4} \frac{1}{2}]$, the coordinates for the hole to the oxygen at $[0, 3/2 - n, \frac{3}{4}]$ are,

$$\begin{aligned} \rho &= 90^\circ - \tan^{-1} \left(\frac{3.831 - 2.362}{\sqrt{(0 - 1.147)^2 + (3.124 - 2.558)^2}} \right) \\ &= 90^\circ - 48.9^\circ \\ &= 41.1^\circ \end{aligned}$$

$$\phi = \tan^{-1} \left(\frac{3.124 - 2.558}{0 - 1.147} \right)$$

$$= -26.2^\circ = +333.8^\circ.$$

A full calculation of the drilling coordinates to either the oxygen at $[[0, \frac{1}{2} + n, \frac{1}{4}]]$ or the oxygen at $[[\frac{1}{2}, 1 - n, \frac{3}{4}]]$, is also needed. All other drilling coordinates may be obtained by symmetry from these two sets of coordinates because the copper is located on an inversion center and the oxygen on a two-fold rotation axis normal to the plane of the projection. Note that the symmetry of the location of the oxygens requires both *right* and *left* oxygens to be drilled.

It is desirable to transform the drilling coordinates once more so that holes of low ρ reading are avoided. For this purpose, the copper and oxygen coordinates are separately plotted on a rotating stereographic net, and the points rotated until the copper coordination rectangle is normal to the first hole (giving the bond holes all ρ coordinates of 90°) and until the first hole of the oxygen is one of the bond holes (giving the other bond holes ρ coordinates in roughly the same region). The resulting drilling data are found in the tabulation.

TABLE 1

Monoclinic and isometric orthogonal coordinates of tenorite. Atoms are listed in counter-clockwise rotary order (as seen in Fig. 5A) about central atoms of other species, namely Cu about O at $[[\frac{1}{2}, n, \frac{1}{4}]]$, and O about Cu at $[[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]]$.

Atom	Monoclinic coordinates			Isometric orthogonal coordinates (Ångstrom units)		
	<i>x</i>	<i>y</i>	<i>z</i>	<i>X</i>	<i>Y</i>	<i>Z</i>
Cu	$\frac{1}{4}$	$\frac{1}{4}$	0	1.147	0.853	-0.192
Cu	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{1}{2}$	1.147	2.558	2.362
Cu	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{2}$	3.441	0.853	1.978
Cu	$\frac{3}{4}$	$\frac{3}{4}$	0	3.441	2.558	-0.576
O	$\frac{1}{2}$	<i>n</i>	$\frac{1}{4}$	2.294	1.991	0.893
O	0	$\frac{1}{2} + n$	$\frac{1}{4}$	0	3.695	1.277
O	0	$\frac{3}{2} - n$	$\frac{3}{4}$	0	3.124	3.831
O	$\frac{1}{2}$	$1 - n$	$\frac{3}{4}$	2.294	5.401	3.447
		<i>a</i> = 4.653		β = $99^\circ 29'$		
		<i>b</i> = 3.410		<i>n</i> = .584		
		<i>c</i> = 5.108				

A technique for the construction of models illustrating the arrangement and packing of atoms in crystals. M. J. Buerger and R. D. Butler. *The American Mineralogist*, vol. 21, pp. 150-172, 1936.

Errata: p. 161, lines 5 and 6

$$u_b = .203 \pm .01$$

$$v_c = .375 \pm .01$$

p. 165, line 6

$$AH = \sqrt{\left(\frac{a}{2} - 0\right)^2 + \left(\left[\frac{b}{2} - y_b\right] - y_b\right)^2 + \left(\left[\frac{c}{2} + z_c\right] - z_c\right)^2} = 3.16 \text{ \AA.}$$

p. 167, Table 1, second last line in column:

$$270^\circ - \angle ADm = 229^\circ$$

p. 168, line 14,

$$V:S = 2.186 \text{ \AA}$$

A-1, Copper

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Cu	1 $\frac{1}{4}$ "	14	0	0	unused	
			45	0	Cu	$\rho = 135$
			45	90	Cu	
			45	180	Cu	
			45	270	Cu	
			90	45	Cu	$\rho = 90$
			90	135	Cu	
			90	225	Cu	
			90	315	Cu	
			135	0	Cu	$\rho = 45$
			135	90	Cu	
			135	180	Cu	
			135	270	Cu	

A-2, α -Iron

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{1}{4}''$	9	0	0	unused	
			55	0	Fe	$\rho = 125$
			55	90	Fe	
			55	180	Fe	
			55	270	Fe	
			125	0	Fe	$\rho = 55$
			125	90	Fe	
			125	180	Fe	
			125	270	Fe	

A-3, Magnesium

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Mg	$1\frac{5}{8}''$	17 hex	0	0	unused	
			35	0	Mg	$\rho = 145$
			35	120	Mg	
			35	240	Mg	
			90	30	Mg	$\rho = 90$
			90	90	Mg	
			90	150	Mg	
			90	210	Mg	
			90	270	Mg	
			90	330	Mg	
			145	0	Mg	$\rho = 35$
			145	120	Mg	
			145	240	Mg	

A-4, *Diamond*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
C	$\frac{3}{4}$ "	26	0	0	C	$\rho=0$
			109½	0	C	$\rho=109\frac{1}{2}$
			109½	120	C	
			109½	240	C	

A-5, *White Tin*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Sn	$1\frac{1}{2}$ "	13 P	0	0	unused	
		26 F	75	0	Sn	$\rho=75$
			75	180	Sn	
			115	90	Sn	$\rho=115$
			115	270	Sn	

A-7, *Bismuth*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Bi	$1\frac{9}{16}$ "	27	0	0	2.31" spacing bar to Bi	$\rho=0$
			180	0	1.97" spacing bar to Bi	$\rho=180$
			122	0	Bi	$\rho=122$
122	120	Bi				
122	240	Bi				

A-8, Selenium

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Se	$1\frac{3}{16}''$	16 28 hex	0	0	unused	
			45	90	Se	$\rho=135$
			90	0	spacing bar spacing bar spacing bar spacing bar spacing bar	$\rho=90$
			90	60		
			90	120		
			90	180		
			90	240		
90	300	spacing bar				
135	30	Se	$\rho=45$			

A-9, Graphite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
C ₁	$\frac{11}{16}''$	9 hex	0	0	spacing bar to C ₁	$\rho=180$
			90	0	C ₂ C ₂ C ₂	$\rho=90$
			90	120		
			90	240		
			180	0	spacing bar to C ₁	$\rho=0$
C ₂	$\frac{11}{16}''$	17 hex	0	0	unused	
			90	0	C ₁ C ₁ C ₁	$\rho=90$
			90	120		
			90	240		

A-14, Iodine

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
I	$1\frac{3}{8}''$	28	0	0*	spacing bar	$\rho=0$
			90	0	I	$\rho=90$

* This hole is drilled completely through the ball.

A-17, Black Phosphorus

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
P	$1\frac{1}{8}''$	36	0	0	space bar to P	$\rho=69$
			69	180	space bar to P	$\rho=0$
			112	$125\frac{1}{2}$	P	$\phi=125\frac{1}{2}$
			112	$234\frac{1}{2}$	P	$\phi=234\frac{1}{2}$
			$125\frac{1}{2}$	0	P	$\rho=125\frac{1}{2}$

B-1, Halite

Na	$1''$	14	0	0	Cl	$\rho=180$
			90	0	Cl	$\rho=90$
			90	90	Cl	
			90	180	Cl	
			90	270	Cl	
			180	0	Cl	$\rho=0$
Cl	$1\frac{1}{16}''$	13	0	0	Na	$\rho=180$
			90	0	Na	$\rho=90$
			90	90	Na	
			90	180	Na	
			90	270	Na	
			180	0	Na	$\rho=0$

B-2, Caesium Chloride

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Cs	$1\frac{3}{4}''$	8	0	0	unused	
			55	0	Cl	$\rho = 125$
			55	90	Cl	
			55	180	Cl	
			55	270	Cl	
			125	0	Cl	$\rho = 55$
			125	90	Cl	
			125	180	Cl	
125	270	Cl				
Cl	$1\frac{13}{16}''$	1	0	0	unused	
			55	0	Cs	$\rho = 125$
			55	90	Cs	
			55	180	Cs	
			55	270	Cs	
			125	0	Cs	$\rho = 55$
			125	90	Cs	
			125	180	Cs	
125	270	Cs				

B-3, B-4, Sphalerite and Wurtzite

Zn	$1\frac{5}{16}''$	14* 11† 20†hex	0	0	S	$\rho = 0$
			109½	0	S	$\rho = 109\frac{1}{2}$
			109½	120	S	
			109½	240	S	
S	$1\frac{1}{16}''$	12* 10† 19†hex	0	0	Zn	$\rho = 0$
			109½	0	Zn	$\rho = 109\frac{1}{2}$
			109½	120	Zn	
			109½	240	Zn	

* Sphalerite.

† Wurtzite.

B-5, B-6, B-7, *Carborundum (all modifications)*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Si	$1\frac{1}{8}''$	—	0	0	C	$\rho=0$
			109 $\frac{1}{2}$	0	C	$\rho=109\frac{1}{2}$
			109 $\frac{1}{2}$	120	C	
			109 $\frac{1}{2}$	240	C	
C	$\frac{3}{4}''$	—	0	0	Si	$\rho=0$
			109 $\frac{1}{2}$	0	Si	$\rho=109\frac{1}{2}$
			109 $\frac{1}{2}$	120	Si	
			109 $\frac{1}{2}$	240	Si	

B-8, *Niccolite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom			
			ρ	ϕ					
Ni	$1\frac{1}{4}''$	21 hex	0	0	Ni	$\rho=180$			
			59	0	As	$\rho=121$			
			59	120	As				
			59	240	As				
			121	60	As	$\rho=59$			
			121	180	As				
			121	300	As				
			180	0	Ni	$\rho=0$			
			As	$1\frac{3}{16}''$	12 hex	0	0	unused	$\rho=121$
						59	0	Ni	
59	120	Ni							
59	240	Ni							
121	0	Ni				$\rho=59$			
121	120	Ni							
121	240	Ni							

B-8, *Pyrrhotite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	1 $\frac{1}{4}$ "	21 hex	0	0	S	
			90	0		
			90	90		
			90	180		
			90	270		
			180	0		
S	1 $\frac{1}{4}$ "	12 hex	0	0	Fe	
			70	0		
			90	135 $\frac{1}{2}$		
			90	224 $\frac{1}{2}$		
			132	72		
			132	288		

B-9, *Cinnabar* ($u=0.33, v=0.21$)

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Hg	1 $\frac{7}{16}$ "	16 28 hex	0	0	unused	
			50 $\frac{1}{2}$	22	S	$\rho = 129\frac{1}{2}$
			90	0	spacing bars to Hg	$\rho = 90$
			90	60		
			90	120		
			90	120		
			90	180		
			90	240		
90	300					
			129 $\frac{1}{2}$	338	S	$\rho = 50\frac{1}{2}$
S	1 $\frac{1}{16}$ "	12 21 hex	0	0	unused	
			50 $\frac{1}{2}$	38	Hg	$\rho = 129\frac{1}{2}$
			129 $\frac{1}{2}$	322	Hg	$\rho = 50\frac{1}{2}$

B-9, Cinnabar ($u=0.72, v=0.55$)

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Hg	$1\frac{7}{16}''$	16 28 hex	0	0	unused	
			$50\frac{1}{2}$	90	S	$\rho = 129\frac{1}{2}$
			90	0	spacing bars to Hg	$\rho = 90$
			90	60		
			90	120		
			90	180		
			90	240		
90	300					
			$129\frac{1}{2}$	270	S	$\rho = 50\frac{1}{2}$
S	$1\frac{1}{16}''$	12 21 hex	0	0	unused	
			$50\frac{1}{2}$	0	Hg	$\rho = 129\frac{1}{2}$
			$129\frac{1}{2}$	60	Hg	$\rho = 50\frac{1}{2}$

B-11, PbO

Pb	$1\frac{3}{8}''$	10	0	0	space bar to Pb	$\rho = 0$ $\phi = 180$
			121	0	O	
			121	90	O	
			121	180	O	
			121	270	O	
			180	0	space bar to Pb	$\rho = 0$ $\phi = 0$
O	—	8	0	0(m)	Pb up	$\rho = 121$
			$105\frac{1}{2}$	117	Pb down	$\rho = 121$
			$105\frac{1}{2}$	243	Pb down	$\rho = 121$
			118	0(m)	Pb up	$\rho = 121$

"D-31," Calomel

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Hg	$\frac{7}{8}$ "	27	0	0	Cl	$\rho=180$
			81	0	Cl	$\rho=81$
			81	90	Cl	
			81	180	Cl	
			81	270	Cl	
Cl	$1\frac{5}{8}$ "	27	0	0	Cl	$\rho=0$
			81	0	Hg	$\rho=81$
			81	90	Hg	
			81	180	Hg	
			81	270	Hg	
			180	0	Hg	$\rho=0$

B-12, Boron nitride

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
B	$\frac{3}{4}$ "	17 hex	0	0	unused	
			90	0	N	$\rho=90$
			90	120	N	
			90	240	N	
N	$\frac{11}{16}$ "	9 hex	0	0	spacing bar to N	$\rho=180$
			90	0	B	$\rho=90$
			90	120	B	
			90	240	B	
			180	0	spacing bar to N	$\rho=0$

B-18, *Covellite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coordinates		Bonded to	Key coordinate of neighboring atom
			ρ	ϕ		
Cu _I	1 $\frac{1}{8}$ "	12 hex	0	0	unused	
			90	0	S _I	$\rho=90$
			90	120	S _I	
90	240	S _I				
S _I	1 $\frac{1}{16}$ "	12 hex	0	0	Cu _{II}	$\rho=0$
			90	0	Cu _I	$\rho=90$
			90	120	Cu _I	
90	240	Cu _I				
S _{II}	1 $\frac{5}{16}$ "	24 hex	0	0	S _I	$\rho=0$ or $\rho=180$
			109	0	S _{II}	$\rho=109$
			109	120	S _{II}	
109	240	S _{II}				
S _{II}	1"	28 hex	0	0	S _{II}	$\rho=0$
			109	0	Cu _{II}	$\rho=109$
			109	120	Cu _{II}	
109	240	Cu _{II}				

B-17, *Cooperite*

Pt	1 $\frac{1}{4}$ "	14 C	0	0	unused	
			90	0	S	$\rho=131$
			90	98	S	
S	1 $\frac{1}{16}$ "	32 C	90	180	S	$\rho=49$
			90	278	S	
			0	0	unused	
S	1 $\frac{1}{16}$ "	32 C	49	0	Pt	$\rho=90$
			49	180	Pt	
			131	90	Pt	
			131	270	Pt	

B-26, Tenorite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Cu	1 $\frac{1}{4}$ "	14	0	0	unused	
			90	0	O	
			90	85	O	
			90	180(m)*	O	
			90	265(m)*	O	
O _R	1 $\frac{1}{16}$ "	16	0	0(m)*	Cu	
			96	107	Cu	
			104	260	Cu	
			108	0(m)*	Cu	
O _L	1 $\frac{1}{16}$ "	16	0	0(m)*	Cu	
			96	253	Cu	
			104	100	Cu	
			108	0(m)	Cu	

* Make one mark between these pairs of holes.

C-1, Fluorite

Ca	1"	14	0	0	unused	
			55	0	F	$\rho = 125$
			55	90	F	
			55	180	F	
			55	270	F	
			125	0	F	$\rho = 55$
			125	90	F	
			125	180	F	
125	270	F				
F	1 $\frac{3}{8}$ "	8	0	0	unused	
			55	0	Ca	$\rho = 125$
			55	180	Ca	
			125	90	Ca	$\rho = 55$
125	270	Ca				

C-2, Pyrite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{3}{16}''$	14	0	0	unused	
			58	0	S	$\rho = 102\frac{1}{2}$
			58	120	S	
			58	240	S	
			122	60	S	$\rho = 102\frac{1}{2}$
			122	180	S	
122	240	S				
S	$1\frac{1}{16}''$	26	0	0	S	$\rho = 0$
			102 $\frac{1}{2}$	0	Fe	$\rho = 58$ or $\rho = 122$
			102 $\frac{1}{2}$	120	Fe	
			102 $\frac{1}{2}$	240	Fe	

C-3, Cuprite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Cu	$\frac{5}{8}''$	4	0	0	O	$\rho = 125$
			180	0	O	$\rho = 55$
O	$1\frac{1}{4}''$	9	0	0	spacing bar to O	$\rho = 180$
			55	0	Cu	$\rho = 180$
			55	180	Cu	
			125	90	Cu	$\rho = 0$
125	270	Cu				
			180	0	spacing bar to O	$\rho = 0$

C-4, Rutile

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Ti	$\frac{3}{4}''$	9	0	0	O	$\rho=0$
			90	0	O	$\rho=128\frac{1}{2}$
			90	$77\frac{1}{2}$	O	
			90	180	O	
			90	$257\frac{1}{2}$	O	
180	0	O	$\rho=0$			
O	$1\frac{1}{4}''$	6	0	0	Ti	$\rho=0$
			$128\frac{1}{2}$	0	Ti	$\rho=90$
			$128\frac{1}{2}$	180	Ti	
180	0	O	$\rho=180$			

C-5, Anatase

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Ti	$\frac{3}{4}''$	13	0	0	O	$\rho=0$
			78	0	O	$\rho=102$
			78	180	O	
			102	90	O	
			102	270	O	
180	0	O	$\rho=0$			
O	$1\frac{1}{4}''$	22	0	0	Ti	$\rho=0$ or $\rho=180$
			$50\frac{1}{2}$	0	O	$\rho=50\frac{1}{2}$
			$50\frac{1}{2}$	180	O	
102	0	Ti	$\rho=78$ or $\rho=102$			
102	180	Ti				

C-6, *Tin Disulfide* (covalent bond model)

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coordinates		Bonded to	Key coordinate of neighboring atom
			ρ	ϕ		
Sn	$1\frac{1}{2}''$	14	0	0	S	$\rho=0,90$
			$54\frac{3}{4}$	45	Sn	$\rho=54\frac{3}{4}$
			90	0	S	$\rho=0,90$
			90	90		
			90	180		
90	270					
180	0					
S	$1\frac{1}{16}''$	48	0	0	Sn	$\rho=0, 90, 180$
			90	0		
			90	90		

C-6, *Tin Disulfide* (ionic bond model)

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coordinates		Bonded to	Key coordinate of neighboring atom
			ρ	ϕ		
Sn	$1\frac{1}{6}''$	12	0	0	S	$\rho=54\frac{3}{4}^a$
S	$1\frac{3}{4}''$	24	0	0	not used	
			35	30	S	$\rho=145\frac{1}{4}$
			$54\frac{3}{4}$	90	Sn	$\rho=0$
			90	0	S	$\rho=90$
			90	60		
			90	120		
			90	180		
90	240					
90	300					
$145\frac{1}{4}$	90	S	$\rho=54\frac{3}{4}$			

C-7, Molybdenite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coordinates		Bonded to	Key coordinate of neighboring atom
			ρ	ϕ		
Mo	$1\frac{5}{16}''$	20 hex	0	0	spacing bar to S	$\rho=0$
			50	0	S	$\rho=130$
			50	120	S	
			50	240	S	
			130	0	S	
			130	120	S	
130	240	S				
S	$1\frac{1}{16}''$	38 hex	0	0	spacing bar to Mo	$\rho=0$
			130	0	Mo	$\rho=50$ or
			130	120	Mo	$\rho=130$
			130	240	Mo	

C-18, Marcasite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coordinates		Bonded to	Key coordinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{1}{8}''$	12	0	0	S	$\rho=103\frac{1}{2}$
			89	49(m)	S	$\rho=106\frac{1}{2}$
			89	311(m)	S	
			91	131	S	
			91	229	S	
			180	0	S	$\rho=103\frac{1}{2}$
S	$1\frac{1}{8}''$	12	0	0	S	$\rho=0$
			$103\frac{1}{2}$	0(m)	Fe	$\rho=0$ or $\rho=180$
			$106\frac{1}{2}$	$128\frac{1}{2}$	Fe	$\rho=89$ or
			$106\frac{1}{2}$	$231\frac{1}{2}$	Fe	$\rho=91$

C-18, *Löllingite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{1}{8}''$	9	0	0	As	$\rho=108$ $\phi=0$
			88	142(m)	As	$\rho=108$ $\phi=140, 220$
			88	218(m)	As	
			92	38	As	
92	312	As				
			180	0	As	$\rho=108$ $\phi=0$
As	$1\frac{1}{4}''$	12	0	0	As	$\rho=0$
			108	0(m)	Fe	$\rho=0$ or $\rho=180$
			108	140	Fe	$\rho=88$ or $\rho=92$
			108	220	Fe	

C-18, *Iron di-phosphide*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{1}{8}''$	9	0	0	P	$\rho=110\frac{1}{2}$
			88	145(m)	P	$\rho=107$
			88	215(m)	P	
			92	35	P	
92	325	P				
			180	0	P	$\rho=110\frac{1}{2}$
P	$1\frac{1}{8}''$	12	0	0	P	$\rho=0$
			$110\frac{1}{2}$	0(m)	Fe	$\rho=0$ or $\rho=180$
			107	143	Fe	$\rho=88$ or $\rho=92$
107	217	Fe				

C-18, *Iron di-antimonide*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Fe	$1\frac{1}{4}''$	9	0	0	Sb	$\rho=107$
			88	$142\frac{1}{2}(m)$	Sb	$\rho=108$
			88	$217\frac{1}{2}(m)$	Sb	
			92	$37\frac{1}{2}$	Sb	
			92	$322\frac{1}{2}$	Sb	
180	0	Sb	$\rho=107$			
Sb	$1\frac{3}{8}''$	12	0	0	Sb	$\rho=0$
			107	$0(m)$	Fe	$\rho=0$ or $\rho=180$
			108	140	Fe	$\rho=88$ or $\rho=92$
			108	220	Fe	

C-18 (C-35), *Hydrophilite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Ca	$1\frac{1}{4}''$	9	0	0	Cl	$\rho=0$
			90	$50(m)$	Cl	$\rho=128$
			90	$310(m)$	Cl	
			90	130	Cl	
			90	230	Cl	
180	0	Cl	$\rho=0$			
Cl	$1\frac{1}{2}''$	8	0	0	Ca	$\rho=0$
			128	80	Ca	$\rho=90$
			128	280	Ca	

C-42, Silicon di-sulphide

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
Si _R	1 $\frac{1}{8}$ "	9	0	0*	spacing bar	
			50 50	0 180	S S	$\rho=0$
			130 130	94 274	S S	$\rho=0$
Si _L	1 $\frac{1}{8}$ "	6	0	0*	spacing bar	
			50 50	0 180	S S	$\rho=80$
			130 130	86 266	S S	$\rho=80$
Si _R , Si _L	1 $\frac{1}{16}$ "	20	0 80	0 0	Si _R Si _L	$\rho=50$ or $\rho=130$

* Hole is drilled completely through the ball.

C-9, High Cristobalite

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
O	1 $\frac{1}{4}$ "	56	0	0	unused	
			35 35 35	0 120 240	O O O	$\rho=35$
			145 145 145	60 180 300	O O O	$\rho=145$
Si	.30"	18	—	—	—	

C-30, *Low Cristobalite*

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
O	$1\frac{5}{16}''$	56	0	0	unused	
			$48\frac{1}{2}$	$69\frac{1}{2}$	O	$\rho = 131\frac{1}{2}$
			66	0	O	$\rho = 66$
			$104\frac{1}{2}$	47	O	$\rho = 104\frac{1}{2}$ $\phi = 223$
			$104\frac{1}{2}$	223	O	$\rho = 104\frac{1}{2}$ $\phi = 47$
			$131\frac{1}{2}$	$160\frac{1}{2}$	O	$\rho = 48\frac{1}{2}$
			156	270	O	$\rho = 156$
Si	$.30''$	18	—	—	—	

C-10, *High Tridymite*

O _I	$1\frac{1}{4}''$	42 72 hex	0	0	unused				
			35	0	O _{II}	$\rho = 145$			
			35 35	120 240	O _I O _I	$\rho = 35$			
			145	60	O _I	$\rho = 145$			
			145	180	O _{II}	$\rho = 35$			
			145	300	O _I	$\rho = 145$			
O _{II}	$1\frac{1}{4}''$	14 24 hex	0	0	unused				
			35 35 35	0 120 240	O _I O _I O _I	$\rho = 145$			
			145 145 145	0 120 240	O _I O _I O _I	$\rho = 35$			
			Si	$.30''$	21 36 hex	—	—	—	

C-8, High Quartz

Atom	Ball Size	Number of balls required for one unit cell model	Drilling Coördinates		Bonded to	Key coördinate of neighboring atom
			ρ	ϕ		
O	$1\frac{5}{16}''$	38	0	0	unused	
			35	0	O	$\rho = 135$
			35	120	O	$\rho = 35$ $\phi = 120$
			35	240	O	$\rho = 124$
			124	305	O	$\rho = 35$ $\phi = 240$
			135	225	O	$\rho = 35$ $\phi = 0$
			165	45	O	$\rho = 165$
Si	.30"	12	—	—	—	

"C-8," Low Quartz

O	$1\frac{5}{16}''$	38	0	0	unused	
			48	$167\frac{1}{2}$	O	$\rho = 132$
			$63\frac{1}{2}$	240	O	$\rho = 63\frac{1}{2}$
			103	$46\frac{1}{2}$	O	$\rho = 103$ $\phi = 193\frac{1}{2}$
			103	$193\frac{1}{2}$	O	$\rho = 103$ $\phi = 46\frac{1}{2}$
			132	$107\frac{1}{2}$	O	$\rho = 48$
			$153\frac{1}{2}$	0	O	$\rho = 153\frac{1}{2}$
Si	.30"	12	—	—	—	