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A SIMPLE CENTERING JIG AND GONIOMETER FOR PUNCHING OR DRILLING SPHERES FOR STRUCTURE MODELS

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INTRODUCTION

In most crystal or molecular structure models using spheres to represent atoms,* the bond directions must be rather accurately located. Some crystal structures have atoms whose coordination polyhedra are regular. For these atoms the bond directions are easily located by punching or drilling jigs such as those described by Dore (1926), Evans (1948), Wooster (1945), and Gibb and Bassow (1957). The jigs of Wooster and of Evans allow 26 holes to be drilled along the symmetry axes of the cubic system and thus can be used to drill several different regular coordinations; however, a different jig is necessary for each size of sphere.

For irregular coordinations, more elaborate devices are necessary to position the bond directions accurately. Several drilling goniometers described by Buerger (1935), Terpstra (1939), Haywood (1949), and Decker and Asp (1955) are based on a system using spherical coordinates to locate the bond directions. These coordinates are rarely published. This paper describes a new goniometer which is versatile enough for use in drilling any irregular coordination yet requires only a knowledge of the bond angles.

GENERAL DESCRIPTION

Two devices are used in drilling the spheres in any desired coordination. The centering jig is used to drill the first hole through the center of the sphere. Then the goniometer locates a second hole related to the first by a known bond angle. For all succeeding holes, the goniometer essentially guides the drill or punch along that radius of the sphere which makes the desired angles with two previously located radii.

* A detailed review of structure model types is given in a separate article (Smith, 1960).

Centering Jig

The centering jig, shown in Fig. 1, may be constructed using metal or cardboard supports and metal tubes for guides. The author has found that a cardboard jig made of 1/16 inch thick poster board is strong enough to be used as a drilling guide as well as a punching guide. Figure 2 gives the dimensions of a jig suitable for balls up to $1\frac{1}{2}$ inch in diameter and for use with commercially available drills. If tubing of $\frac{1}{8}$ inch inside diameter is used for the guide tubes, bushings with 3/32 inch and 1/16

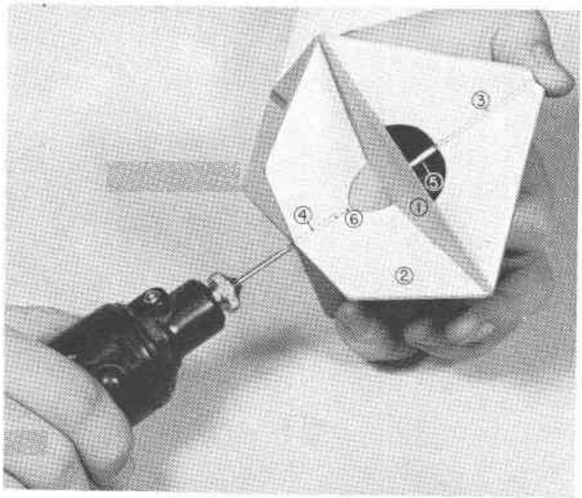

FIG. 1. The centering jig showing the drilling operation. Numbers refer to parts in Fig. 2.

inch inside diameters and $\frac{1}{8}$ inch outside diameters may be used to make the jig universal for $\frac{1}{8}$, 3/32, and 1/16-inch rods. The bushings not only provide for a variety of hole sizes, but also prevent wandering of the drill or punch and protect the guide tubes from wear.

This jig may be used either for drilling holes in wood or punching holes in Styrofoam. To use it, the bushing is inserted in the lower guide and the ball is placed in the conical cavity. The upper bushing is pushed through the upper guide against the ball. To drill a wooden ball, the upper bushing is held against the ball by means of the finger, and the hole is drilled through the lower bushing using a small hand grinder motor and a drill of appropriate diameter. The depth of the drilled hole may be controlled by adjusting the length of the drill that protrudes from the chuck.

Punches made from brass rod of appropriate diameter with one end pointed are used to punch holes in Styrofoam balls. The punch should be

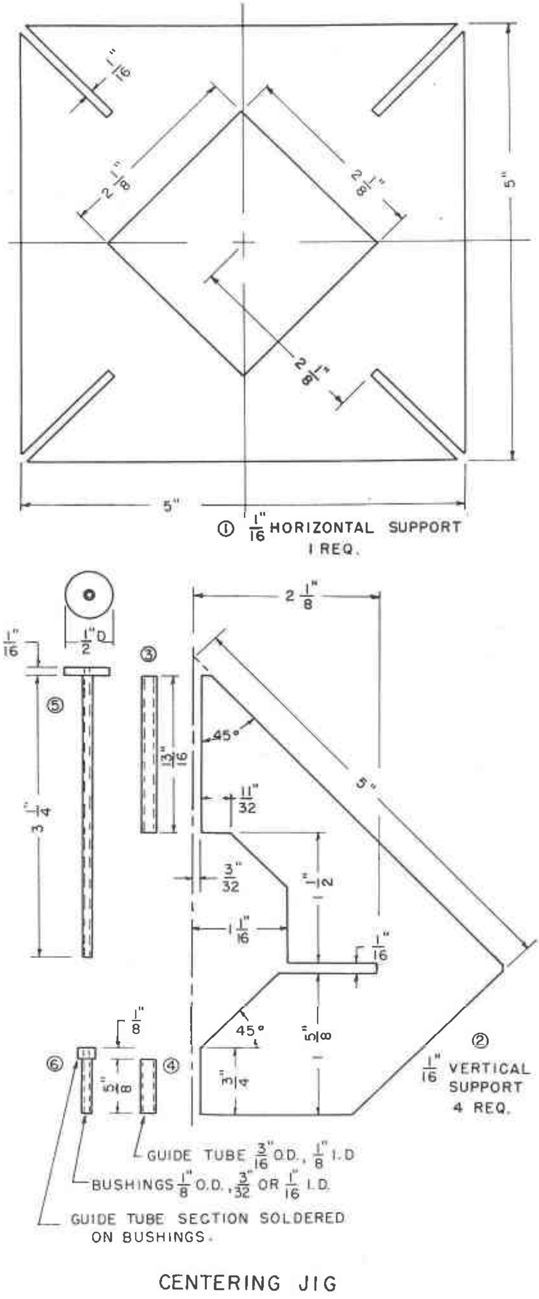

FIG. 2. Working drawing of the centering jig.

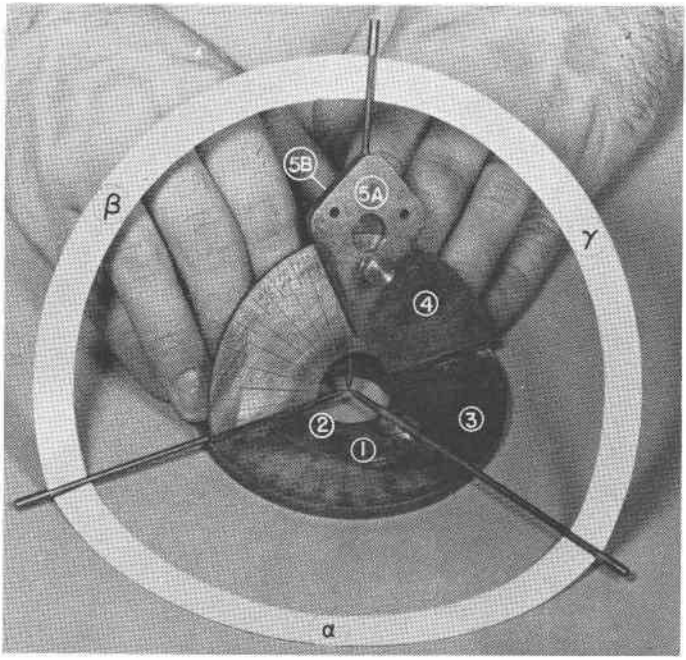

FIG. 3. The goniometer jig showing the three principal angles. Numbers refer to parts in Fig. 4.

fitted with a cap about $\frac{1}{4}$ inch in diameter for the finger to push against. The punch is inserted through the upper bushing, passes through the ball, and enters the lower bushing.

For the initial drilling of wooden spheres on a drill press, a simpler jig may be used. Any block with a right circular conical depression is clamped with the axis of the cone along the axis of the drill press. Balls with only small departures from sphericity will be reasonably centered by this method.

Principle of the Goniometer

After the first hole is drilled with the centering jig, the goniometer is used to drill holes along all other bond directions. This device is based on the three-circle goniometer (Fig. 3). One pair of drilling guides is attached to a fixed annular ring about which another annular ring with another pair of guides is free to move. A scale on the movable circle indicates the angle, α, of this rotation. A graduated semicircle is hinged on the movable circle and another drilling guide can be adjusted to the desired angle, β, on this scale. The angle, γ, through which the hinged semicircle is rotated

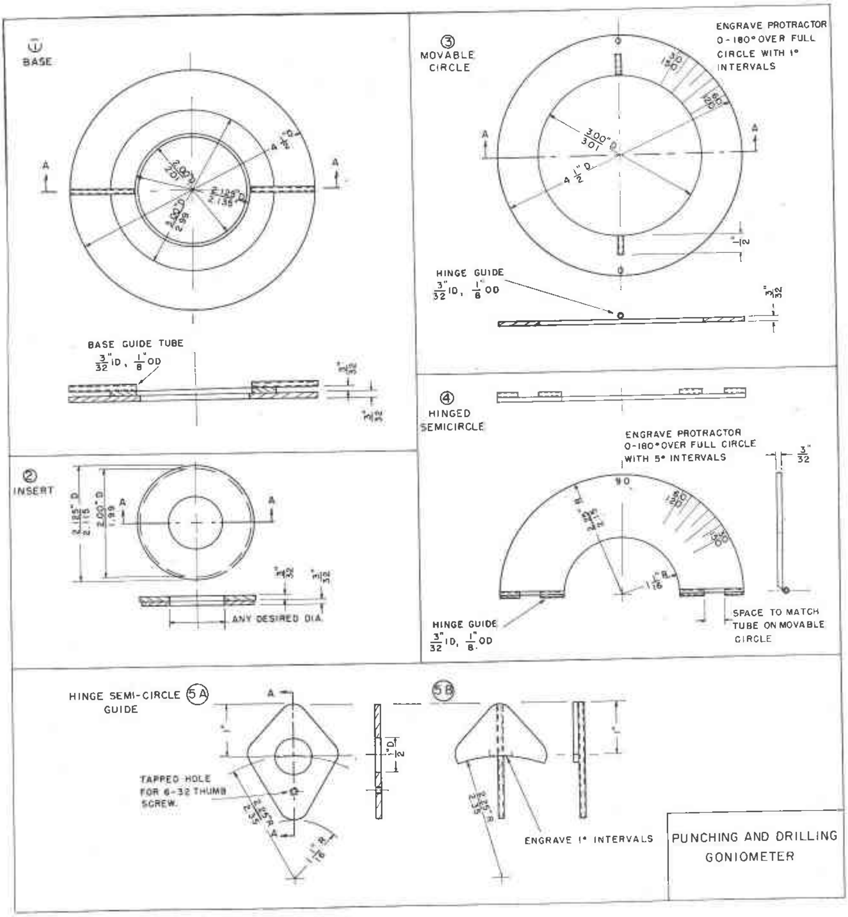

FIG. 4. Working drawing of the goniometer.

cannot be set directly on the goniometer, but in use this angle is defined by previously drilled holes.

Construction of the Goniometer

Figure 4 is a working drawing of the components of a goniometer for drilling balls up to two inches in diameter. The positions of the section of tubing which act as the drilling guides are shown in the drawing, on the part to which they are permanently attached. Their inside diameter should be the same as the outside diameter of the rods to be used as "spokes" in the model, or, if desired, tubing of $\frac{1}{8}$ inch inside diameter may be used with bushings as used for the centering jig. The pieces of rod used as pins for holding the balls in place as shown in Fig. 3 are similar to those rods used for the centering jig.

The base and insert are most easily made from two annular rings of brass which are soldered together. The movable circle is put in position on the base and the base guide tubes are soldered *on the base only*. These guide tubes may be kept aligned by slipping them over an aluminum rod and then clamping them in position. Stationery binder clips make good clamps. When this operation has been completed, the movable circle must rotate freely with respect to the base.

After the base is assembled, the hinge guides for the hinged semicircle are set in position. First, the two pieces of tubing are soldered on the movable circle, again using the aluminum rod for alignment. Then the four tubes are soldered on the hinged semicircle using the aluminum rod and the two tube segments on the movable circle as guides. Care must be taken to align the zero position of the hinged semicircle with the center line of the hinge guide tubes. Finally, the hinged semicircle guide can be assembled by soldering the guide tube and Part A to opposite sides of Part B so that the vernier on Part B is visible through the hole in Part A. The goniometer is then ready for use.

For Styrofoam spheres, a more suitable version may be constructed by using 1/16 inch poster cardboard for all pieces except the guides.

Use of the Goniometer

In using the goniometer to position holes along bond directions, the ball is put in the center of the goniometer with a pin through its center hole and the base guides of the jig. An insert disc, with a hole just large enough for the ball, is used to keep the ball centered on the base guide pin but just free to rotate. The first bond angle is measured on the movable circle, and the hole is drilled through the appropriate hinge guide. Then the second bond angle is set on the movable circle and the third bond angle is set on the hinged semicircle. The ball is rotated until the hole just drilled and the hinged semicircle guide are aligned, and a pin is passed through the semicircle guide into the ball. The third hole is then drilled through the hinge guide. This sequence of operations is repeated as many times as necessary, taking care each time that the three bond angles are measured in the correct order. For bond directions more than 120° from the original center hole, it is usually advisable to shift one of the closer bond directions to the base guide position.

The holes may be drilled using a hand hobby grinder motor and the appropriate drill. The depth of the drilled hole is controlled by the length of the drill protruding from the chuck. The depth is best set at about $\frac{1}{4}$ inch less than the radius of the ball. All the holes except the initial center hole will have the same depth, and the "spokes" may be cut uniformly $\frac{1}{2}$ inch

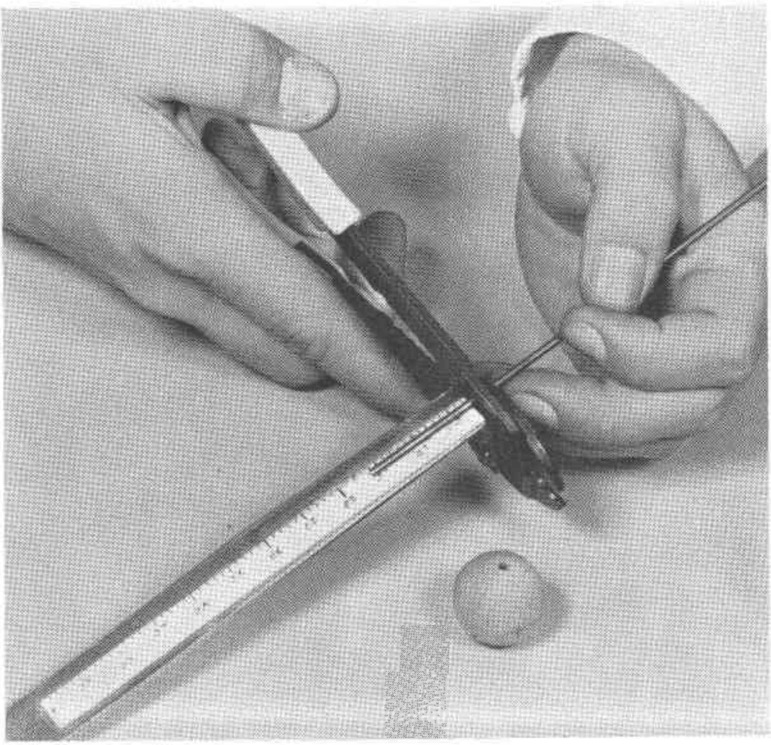

Fig. 5. The modified electrician's crimping tool for cutting "bonds."

shorter than the actual scaled length. If desired, even the center hole may be this fixed depth. However, a second shallow hole 180° away may still prove desirable to permit the added support of a second base guide pin.

The same sequence of operations is used for punching Styrofoam spheres with the goniometer. The punch has less tendency to wander if it is rotated as it is pushed into the ball. The center hole must be pushed completely through the ball when using Styrofoam because the full support of the base pin is necessary in the goniometer punching operations.

Cutting the Rods

The bonding rods may be cut accurately and rapidly by an electrician's crimping tool with threaded holes for shearing screws, modified as shown in Fig. 5. A hole of the same diameter as the rods is drilled through the pliers with their jaws open. A bracket, readily mounted in the threaded holes of the pliers, supports a scale as shown in Fig. 5. This scale, which reads directly in Angstroms, is shifted on the bracket to allow for the fact that the rods do not extend to the centers of the spheres. Rods cut with this device have square ends with no annoying burrs.

General Constructional Aids

The most efficient procedure for constructing models with these devices is to drill all the balls for equivalent atoms at one time, remembering that in structures with inversion axes of symmetry one half of the atoms have bond patterns which are a mirror image of the other half. If the first three holes drilled are systematically marked by spinning three different colored wax pencils in the holes, the orientation of each ball may be quickly ascertained when the model is being assembled later.

Models made with wooden balls generally require no glue if the holes are drilled slightly undersized, but Styrofoam, because of its inherent weakness, must be glued. The use of Styrofoam has been primarily restricted to packing models; but, if a polyvinyl emulsion glue is used, the open models also are strong enough to withstand moderate handling. For the strength of the model it is best to have each Styrofoam sphere supported by three or more non-coplanar rods.

Appendix

If the necessary data on bond angles are not available they may be calculated from the atomic coordinates.

For triclinic structures the bond angle may be calculated using the following formula:

$$\cos\theta = \frac{\mathbf{V}_1\cdot\mathbf{V}_2}{|\mathbf{V}_1||\mathbf{V}_2|}$$

where $\mathbf{V}_1$ and $\mathbf{V}_2$ are vectors from one atom to two adjacent atoms.

$$\mathbf{V}_1 = (x_1 - x)\mathbf{a} + (y_1 - y)\mathbf{b} + (z_1 - z)\mathbf{c}$$
$$\mathbf{V}_2 = (x_2 - x)\mathbf{a} + (y_2 - y)\mathbf{b} + (z_2 - z)\mathbf{c}$$

where x, y, z; x_1, y_1, z_1; and x_2, y_2, z_2 are the atomic coordinates of the first atom and the other two respectively, and **a**, **b**, and **c** are the unit cell vectors.

$$\begin{aligned}\mathbf{V}_1\cdot\mathbf{V}_2 = {} & (x_1 - x)(x_2 - x)a^2 + (y_1 - y)(y_2 - y)b^2 + (z_1 - z)(z_2 - z)c^2 \\ & + [(x_1 - x)(y_2 - y) + (x_2 - x)(y_1 - y)]ab\cos\gamma \\ & + [(x_1 - x)(z_2 - z) + (x_2 - x)(z_1 - z)]ac\cos\beta \\ & + [(y_1 - y)(z_2 - z) + (y_2 - y)(z_1 - z)]bc\cos\alpha, \\ |\mathbf{V}_1| = {} & [\mathbf{V}_1\cdot\mathbf{V}_1]^{1/2} = [(x_1 - x)^2a^2 + (y_1 - y)^2b^2 \\ & + (z_1 - z)^2c^2 + 2(x_1 - x)(y_1 - y)ab\cos\gamma \\ & + 2(x_1 - x)(z_1 - z)ac\cos\beta + 2(y_1 - y)(z_1 - z)bc\cos\alpha]^{1/2}\end{aligned}$$

and

$$\begin{aligned}|\mathbf{V}_2| = {} & [\mathbf{V}_2\cdot\mathbf{V}_2]^{1/2} = [(x_2 - x)^2a^2 + (y_2 - y)^2b^2 + (z_2 - z)^2c^2 \\ & + 2(x_2 - x)(y_2 - y)ab\cos\gamma \\ & + 2(x_2 - x)(z_2 - z)ac\cos\beta + 2(y_2 - y)(z_2 - z)bc\cos\alpha]^{1/2}.\end{aligned}$$

Substituting these relations in the equation for cos θ gives the complete formula. For the monoclinic system with the b axis unique the formula is:

$$\mathbf{V}_1 \cdot \mathbf{V}_2 = (x_1 - x)(x_2 - x)a^2 + (y_1 - y)(y_2 - y)b^2 + (z_1 - z)(z_2 - z)c^2 + [(x_1 - x)(z_2 - z) + (x_2 - x)(z_1 - z)]ac\cos\beta,$$

$$|\mathbf{V}_1| = [(x_1 - x)^2a^2 + (y_1 - y)^2b^2 + (z_1 - z)^2c^2 + 2(x_1 - x)(z_1 - z)ac\cos\beta]^{1/2},$$

and

$$|\mathbf{V}_2| = [(x_2 - x)^2a^2 + (y_2 - y)^2b^2 + (z_2 - z)^2c^2 + 2(x_2 - x)(z_2 - z)ac\cos\beta]^{1/2}.$$

For the hexagonal system:

$$\mathbf{V}_1 \cdot \mathbf{V}_2 = [(x_1 - x)(x_2 - x) + (y_1 - y)(y_2 - y)]a^2 + (z_1 - z)(z_2 - z)c^2 - \tfrac{1}{2}[(x_1 - x)(y_2 - y) + (x_2 - x)(y_1 - y)]a^2,$$

$$|\mathbf{V}_1| = [\{(x_1 - x)^2 + (y_1 - y)^2 - (x_1 - x)(y_1 - y)\}a^2 + (z_1 - z)^2c^2]^{1/2},$$

and

$$|\mathbf{V}_2| = [\{(x_2 - x)^2 + (y_2 - y)^2 - (x_2 - x)(y_2 - y)\}a^2 + (z_2 - z)^2c^2]^{1/2}.$$

For the orthorhombic system:

$$\cos\theta = \frac{(x_1-x)(x_2-x)a^2+(y_1-y)(y_2-y)b^2+(z_1-z)(z_2-z)c^2}{[(x_1-x)^2a^2+(y_1-y)^2b^2+(z_1-z)^2c^2]^{1/2}[(x_2-x)^2a^2+(y_2-y)^2b^2+(z_2-z)^2c^2]^{1/2}}.$$

For the tetragonal system:

$$\cos\theta = \frac{[(x_1-x)(x_2-x)+(y_1-y)(y_2-y)]a^2+(z_1-z)(z_2-z)c^2}{[\{(x_1-x)^2+(y_1-y)^2\}a^2+(z_1-z)^2c^2]^{1/2}[\{(x_2-x)^2+(y_2-y)^2\}a^2+(z_2-z)^2c^2]^{1/2}}.$$

For the cubic system:

$$\cos\theta = \frac{(x_1-x)(x_2-x)+(y_1-y)(y_2-y)+(z_1-z)(z_2-z)}{[(x_1-x)^2+(y_1-y)^2+(z_1-z)^2]^{1/2}[(x_2-x)^2+(y_2-y)^2+(z_2-z)^2]^{1/2}}.$$

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