William G. Hoover
and **Duward Shriver**
University of Michigan
Ann Arbor

Inexpensive Stuart-type Molecular Models

The great usefulness of molecular models as a teaching aid and guide to research workers has prompted the design of many types of models.[1] One of the most popular types was originated by Stuart[2]; these models depict both the covalent and the Van der Waals radii. Although excellent Stuart model sets are available commercially[3] such sets usually contain only a fraction of the kinds of atoms necessary to depict many interesting inorganic systems. The synthetic ingenuity of modern organic and inorganic chemists continually widens this gap. To meet the need for a wider variety of atoms at reasonable cost (of the order of a few cents per atom) we have developed a procedure for the inexpensive duplication, in plastic, of original atomic prototypes. Prototypes of new atoms may be made from wood and duplicated in plastic (Fig. 1).

The general design of a Stuart-type model involves a sphere proportional to the Van der Waals radius of the atom. Faces are cut on the sphere, at proper angles, corresponding to the covalent radii.[2,4] Inspection of the data on interatomic distances shows that covalent radii of constituent atoms are not always strictly additive.[4] Van der Waals radii are also variable. Thus, while the Van der Waals radii of most atoms are very close to their ionic radii, we find in the case of hydrogen an ionic radius of about 1.5 Å and a van der Waals radius of 1.2 Å in hydrocarbons.[5,4] In glycine the apparent radius of hydrogen varies from 1.06 to 1.34 Å.[4] If steric interactions are of interest it is clearly necessary to have several sizes of hydrogen available.

From the standpoint of convenience and versatility, pegs are the best devices for connecting atomic models. The use of pegs permits some variation in bond length when appropriate washers are inserted between atoms. Short lengths of polyethylene tubing serve well as connecting pegs. When about 0.25 in. o.d. tubing is used and the models are made to the scale 1 cm = 1 Å the models are compatible with Catalin models.[3a] It is thus possible to supplement standard Catalin sets.

Materials necessary for the construction of these models are relatively inexpensive. Liquid rubber (latex), which is needed for the molds, is available at most hobby shops (a quart, sufficient for roughly 100 molds, costs about $4). Silicone rubber lacks the strength necessary for molds which are to be used repeatedly. Resins (either polyester or epoxy) can be obtained from boat shops as well as the sources listed below.[6] Epoxy resin costs about $15 per gallon, a quantity sufficient for approximately 500 atoms; polyester resin costs about $6 per gallon. Although both types of resin are satisfactory for model making we found polyester superior in handling properties as well as in price.

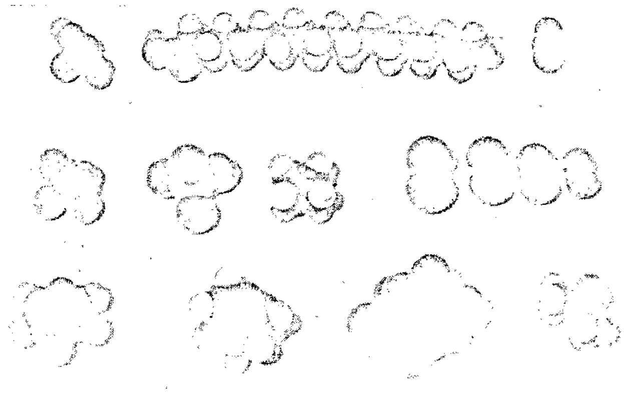

Figure 1. A collection of molecular models which have been produced by the procedure described in the text. From left to right, top row: sulfuric acid, stearic acid, carbon dioxide; second row: phosphorus pentafluoride, gallium tetrachloride anion, cyclobutane, the halogens; bottom row: pyridine, cyclooctatetraene, *n*-perchlorobutane, the $H_2B(NH_3)_2^+$ cation.

Resin may be colored with mineral pigments (available at paint stores), or oil-soluble, *p*H insensitive pharmaceutical dyes, etc. This method of coloring is superior to painting after casting, both in time consumed and in finished appearance. Polyethylene tubing is available from scientific supply houses (about 15¢ per foot).

Model Making Procedure

Before making molds, all holes in selected prototypes must be filled with modeling clay to leave flat faces which will release easily from the molds. Holes for bonds may be drilled in the models after casting. The molds are best poured on a sheet of glass. This permits examination of the undersurface for undesirable bubbles (which may be destroyed by a pinprick while the rubber

[1] (*a*) Campbell, J. A., this Journal, 25, 200 (1948); (*b*) Sublusky, L. A., this Journal, 35, 26 (1958); (*c*) Sattler, L., this Journal, 15, 444 (1938).

[2] Stuart, H. A., *Z. physik. Chem.* (Leipzig) B27, 350 (1934).

[3] (*a*) Catalin Limited, Waltham Abbey, Essex, England; (*b*) Fisher Scientific Co., 109 Fisher Bldg., Pittsburgh 19, Penna.; (*c*) Anglo-American Scientific, 195 Devonshire St., Boston, Mass.; (*d*) Arthur F. Smith Co., 311 Alexander St., Rochester, N. Y.; (*e*) Arthur S. LaPine & Co., 6001 South Knox Ave., Chicago 29, Ill.

[4] Pauling, L., "Nature of the Chemical Bond," 3rd. ed., Cornell Univ. Press, 1960, Chap. 7.

[5] Hurd, D. T., "Chemistry of the Hydrides," John Wiley & Sons, Inc., 1952, pp. 17, 25.

[6] (*a*) Defender Textile Corp., 380 Broadway, New York 13, N. Y.; (*b*) Adhesives Dept., Raybestos-Manhattan Inc., Bridgeport, Conn.

is still fluid) and observation of the color change taking place as the latex cures. After curing, the molds release easily from the smooth surface of the glass.

A small amount of liquid latex is brushed onto the glass, and the prototypes are placed on this rubber so that a thin coat (roughly 0.3 mm) will be beneath each prototype. This step is essential in order to obtain molds with well-formed faces. After all of the protypes have been placed on the sheet, liquid latex is brushed onto each to produce a coating roughly 0.5 mm thick. An even coating free from bubbles is desirable. For convenience in handling and storage it is suggested that several molds be connected together to form a sheet (Fig. 2). Such a sheet helps keep molds level while they are being filled with plastic. The cured molds may be identified by writing the relevant chemical symbols directly on the rubber with a ball point pen. Ordinarily about 24 hours should pass before applying a second coat. The number of coats required will depend chiefly on the model size. The larger the prototypes, the thicker must be the mold in order to insure its rigidity when filled with plastic. For example, models of 1 cm radius require only two coats, while those of 2 cm radius require four. When the rubber is well cured, the sheet of molds can be slowly pulled away from the glass.

Figure 2. The underside of some rubber molds.

Each prototype is then removed with the help of a razor blade, by carefully cutting away the thin rubber film that covers its face. Care must be taken to prevent this film (which may be tacky because of lack of contact with the air) from sticking to the interior of the mold. When all of the face coverings have been removed, the prototypes are carefully popped out through the relatively small opening. The molds are now ready for filling (Fig. 3).

If epoxy resin is used, such as that available from Raybestos-Manhattan, it is desirable to coat the inside of the mold with a small amount of Dow-Corning silicon stopcock grease. If a polyester resin is used such as that available from Defender Textile Co., no release agent is necessary.

The base and catalyst are mixed together in proportions suggested by the manufacturer, together with any desired coloring matter or filler. Epoxy resin is usually quite viscous and occludes bubbles on mixing; it is therefore desirable, in order to produce attractive models, to expose the resin to a vacuum before pouring. An ordinary vacuum desiccator attached to a water aspirator is convenient for this purpose. A small amount of acetone poured onto the surface of the plastic before exposing to vacuum aids in breaking the bubbles that form on the surface. A container two or three times the volume of the plastic is usually large enough to prevent overflow of the foam produced upon evacuation. It is frequently necessary to apply and release the vacuum several times to remove the bubbles. Using polyester resin there is no difficulty with bubble formation; the material flows freely and bubbles coming to the top may be pierced with a pin.

Figure 3. An empty mold, a filled mold, and a collection of boron atoms immediately after removal from a mold.

The molds are then filled with resin. Epoxy resin does not shrink on setting, so filling just to the top is sufficient. The molds may be squeezed gently from below to dislodge air bubbles forming at the surface of the molds. In contrast to epoxy resin, polyester shrinks noticeably so that an excess of plastic is needed at the top of the mold. Setting may be accelerated by placing the molds in a 50°C oven (a 100° oven damages the molds); acceleration is particularly desirable with epoxy models, which may take several days to set up. Polyester models will set in one hour, with the proper amount of catalyst. Larger amounts of catalyst shorten the setting time, but may produce enough heat to damage the molds or crack the models.

Beakers and other materials which have been used in the model-making process may be cleaned with acetone before the resin has set. Because of the long time interval before the epoxy resin sets up, it is practical to catalyze a large batch for storage at low temperature. We have been able to use epoxy which had been kept for over a month at the dry ice temperature.

After sufficient models have been cast and removed from the molds, the rough faces from the open sides of the molds are ground flush with sandpaper (a sanding disk in a table saw is convenient). Next, holes are drilled in the faces for bonds. Holes of $^{15}/_{64}$ in. diameter, about $^{6}/_{10}$ cm deep, are satisfactory. Pieces of polyethylene tubing, about $^{1}/_{2}$ in. o.d., $^{1}/_{8}$ in. i.d., and 1 cm in length, are a snug fit in such holes.

To drill the holes, the models may be clamped on a drill press stand or placed in a wooden jig. A simpler procedure, if the equipment is available, is to drill the models on a lathe. For this process most models can be held with a three jaw chuck, which makes centering of the holes particularly easy.

The drilled models may be slightly countersunk manually with a large ($^{1}/_{2}$ in.) drill to facilitate insertion of the bonds. If coloring matter was not added to the resin the models may then be painted.

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