NBS MONOGRAPH 14

Bibliography on Molecular and Crystal Structure Models

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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National Bureau of Standards Monograph 14

Issued May 20, 1960

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington 25, D.C. - Price 15 cents

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Bibliography on Molecular and Crystal Structure Models

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A bibliography on molecular and crystal structure models is presented. The references are classified into those discussing models in general, static models, dynamic models, or construction devices. The static models are further classified in molecular (Fisher-Hirschfelder-Taylor type), closed packing, open molecular, open crystal structure, open with parallel rods, polyhedral, and miscellaneous models. A short annotation is given which describes the model types and indicates the more significant articles pertaining to them.

1. Introduction

The mounting volume of literature on molecular and crystal structure models reflects their increasing importance in modern scientific research. The original use of models for depicting atomic arrangements is obscure, but it may date back to Kepler (1611) in his *Strena seu de nive sexangula*. As early as 1690 Huygens, in his *Treatise on Optics*, considered the calcite structure to be composed of a three-dimensional array of flattened spheroids. Haüy (1784) in his *Essai d'une theorie sur la structure des crystaux appliquée à plusieurs generes de substances crystallisées* pictured the calcite structure as consisting of a three-dimensional array of unit rhombohedra and showed the relation of these units to the usual scalenohedral habit of crystallized calcite. Frankenheim (1842) and Bravais (1848) show a ball-and-spoke representation of the 14 space lattices. However, it was Pasteur (1848), van't Hoff (1874), and Le Bel (1874) who used the first truly molecular representations in their work on optically active compounds. Barlow (1884, 1897), Kelvin (1889), and Barlow and Pope (1906, 1907, 1908, 1910) used packing models incorporating spheres to explain hexagonal and cubic close packing and some simple crystal structure types.

Since 1912, when the use of X-rays for determining crystal structures had its beginning, models have played an even more common role as an important research tool. Besides being used as an instructional aid in classrooms, many types of structure models are used extensively in research laboratories throughout the world. Even researchers who can "think in three dimensions" find that the time spent in constructing a model is usually justified because the mutual relations of the atoms are much more apparent in the model. The model is often an aid to the chemist for interpreting the results of structure analyses. Chemical reactions and the physical properties of crystalline material, such as optical, elastic, electrical, magnetic, and thermal properties can be qualitatively correlated with the crystal structure most easily when a model is available. Models are now being used as research tools by physicists, chemists, geologists, metallurgists, and biologists.

Special models have been developed to interpret many properties of cleavage, stacking disorder, deformation under mechanical stress, isomerism, and steric hindrance. Further developments in the field of specialized models are the dynamic or working models. These models represent atomic and molecular movements and interactions which take place during chemical and physical processes. Such effects as thermal motion, phase changes, and dislocations or disruption of ordered arrays by foreign ions have been well illustrated by working models.

2. Organization of the Bibliography

Because of the ever-increasing use of structure models in scientific research and the widely scattered literature on them, it was felt that a bibliography covering the various types and uses, conventions as to scale and other characteristics, and construction techniques would be useful, especially for anyone planning to construct a model for the first time. This bibliography includes most of the readily available papers, but some references in less accessible journals have probably been missed. Also missing are references to many variations in models developed for special purposes that unfortunately have never appeared in print.

The references in this bibliography have been grouped into four broad categories: Models in general; static models; dynamic models; and construction devices. Only the static models have been further subdivided, because they are the most common and show a great divergence of types. Many of the static models are actually combinations of two or more basic types. Thus a clear-cut subdivision is quite difficult. Four subgroups have been used: closed models, open models, polyhedral models, and miscellaneous. Each reference has been classified as far as possible according to the dominant features of the model described.

3. Models in General

Because of the wide variety of structure model types, very few papers were classified as general in content. Only the discussion by Nicholson (1952) is really a survey paper. He describes several types of crystal models seen in various laboratories, some of which are not described elsewhere in the literature. These previously undescribed types are an indication that many types of models developed for specific uses have never been described in the literature. Gibb and Winnerman (1958) discuss the applications of crystal models,

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particularly packing models, for understanding salt reactions. Bragg and Bragg (1929) have compiled a set of stereophotographs of crystal structure models of several types.

Other general papers contain the color and size standards established by the British Institute of Physics (1947) which is generally followed in the United States. This same code is reproduced by Lipson and Cochran (1953). A few variations from this code do occur; for example, white is as commonly used for silicon as is the black listed in the specifications. In some of the more complex mineral structures which contain several different metal atoms, the color code has been altered. Also in the Fisher-Hirschfelder-Taylor model sets, blue is used for oxygen instead of red. Thus anyone inspecting any model for the first time must check the identification of the atoms.

A compilation of bond angles and interatomic distances in molecules and ions, which is useful to model builders, has been edited by Sutton (1958). It includes data obtained by spectroscopy and X-ray, electron, and neutron diffraction up to and including the year 1955. Another source for this information is the Groth Institute at the Pennsylvania State University.

4. Static Models

Static models, in contrast to the dynamic models, are very widely used at the present time. They are primarily employed to depict accurately the relative atom positions and bond angles in either molecules or crystals. Two main types of these models exist. In the first, the atoms are represented by spheres scaled to the effective atomic radii, and the model consists of these spheres placed in contact in their respective positions. The internal portions of these models are not usually visible, and this type of model will be termed closed. The second type, which will be termed open, consists of units representing atoms, usually spheres of wood or plastic, linked by rods representing the bonds. These open models show valency angles, interatomic distances, and symmetry more clearly than do the closed models. However, only rarely is any attempt made to represent atomic radii with the size of the spheres, and this type of model is not so easily used to study spatial relations and steric hindrance as the closed type. The wire models may be considered open models in which the balls representing atoms have shrunk to the vanishing point.

A few additional types of static models exist which cannot be placed in these two main classifications. Of these, only the models made with coordination polyhedra warrant separate mention. The polyhedral model was developed primarily as a money and time saving structural representation which generally depicts the arrangement of anions about each cation or the closest neighbors around a carbon atom.

5. Closed Models

5.1. Closed Molecular Models

The closed models may be subdivided into two types, which, however, are not completely distinct. The first type, commonly called the Fisher-Hirschfelder-Taylor models (abbreviated henceforth as F.H.T.), are usually attributed to Stuart (1934). Discussions on the theoretical aspects of these models are given by Wepster (1946, 1951), Taylor (1941), Briegleb (1950 a, b), and Hartley and Robinson (1952). The F.H.T. models consist of plastic or wooden spheres whose radii are proportional to the Van der Waals radii, and whose colors (with some exceptions) correspond to the British code. These spheres are flattened by cutting along planes normal to expected bond directions by an amount corresponding to the difference between the Van der Waals radii and the single, double, or triple covalent bond radii. Thus for a given element several different atom models may be necessary; for example, five different models of the carbon atom are used to represent the five most common combinations of single, double, and triple bonds in which it occurs.

In the early models of the F.H.T. type, the atoms were bonded with wooden pegs which permitted rotation of atoms around single bonds but yielded a model with poor tensile strength. Consequently, several types of snap fasteners have been developed, notably by Taylor (1941, 1943) and Hartley and Robinson (1952). Casler and Corey (1958) describe a magnetic coupling used primarily for hydrogen bonds.

The F.H.T. models incorporate several desirable features. (1) The models are quickly constructed, and most molecules can be made or at least approximated. (2) The size of the model closely represents a scaled-up molecule. (3) The space-filling characteristics are easily observable. (4) Steric hindrance may be observed by using rotatable bonds. Briegleb (1950) and Hartley and Robinson (1952) list several shortcomings of the standard F.H.T. model and suggest modifications which will allow the bond angles to be distorted up to 12° and give the model some flexibility. Both the F.H.T. models and the Courtauld (Hartley and Robinson) models are commercially available through chemical supply companies. Recently Godfrey (1959) has described a slightly modified F.H.T. model which is also commercially available.

The recent availability of spheres of several colors and sizes made from foamed polystyrene has led several people, notably Lambert (1953), to construct their own Stuart models. The spheres are given flattened surfaces normal to bond directions as in the F.H.T. models. They can be bonded temporarily by metal rods or pipe cleaners or permanently by glues.

5.2. Closed Packing Models

The second type of closed model is the packing model. The main distinction between this model and F.H.T. type is that the atoms are assumed to be spherical, and the radii of the spheres are made proportional to ionic, metallic, or covalent radii of the represented atoms. Spheres of wood, cork, foamed polystyrene, and plastics have been used in these models. Whereas the F.H.T. models are most applicable to organic models, the packing model is more suitable for representing inorganic crystal structures, especially those with metallic and ionic bonding.

Packing models are constructed by marking on the surface of each sphere all the bond directions and gluing or pinning the spheres at the appropriate points of contact. Plastic balls may be glued by placing a drop of solvent at their point of contact. Buerger and Butler (1936) have described the process fairly completely. Davidson (1952) describes the use of cork balls, and Hatch, Comeforo, and Pace (1952) and Ordway (1952) describe models made with hollow, transparent plastic spheres. The use of foamed polystyrene spheres is discussed in the paper on a punching jig by Gibb and Bassow (1957).

6. Open Models

In the open models the balls representing the atoms do not touch; instead they are usually connected by rods representing the bonds. The balls may or may not be scaled in diameter. In these models the atoms within can be seen as well as those on the surface, and thus this representation is more suitable for complex structures and for photographic illustration. The symmetry and bond patterns are more easily visible, but the packing characteristics of the atoms are not so apparent. In general, it is easier to construct an open model of a distorted molecule than a closed one if the departures from regular arrangement are large.

The open models have been divided into three groups. The first group contains molecular models which are primarily organic in nature, and the second group contains the more general structure models. The models of both these groups have sometimes been called the "ball and spoke" type. The third group consists of vertical rods mounted at certain positions on a base plate and supporting balls at specific heights.

6.1. Open Molecular Models

The open molecular models are commonly called the Brode-Hurd-Boord models (Brode and Boord 1932). Sets of balls of uniform size, with holes drilled to a uniform depth in expected bond directions, are commercially available for building these models. The balls are joined by rigid rods whose lengths are proportional to the bond lengths. Present sets also contain flexible rods or helical springs for making double and triple bonds and allowing some distortion. With these sets most molecules can be constructed. Pouleur (1932) devised a slightly different set of models which had two or three parallel holes in directions of double and triple bonds. Wooster (1944) and Wooster, McGowan, and Moore (1949) suggest using balls with 26 holes corresponding to the symmetry directions in the cubic system. Brenner (1948) suggests using rubber balls instead of rigid balls which, coupled with flexible rods, will allow the construction of more distorted models. Sets based on all these different systems are commercially available.

6.2. Open Structure Models

The open structure models are closely related to the open molecular models in both origin and construction; the main difference is that these models show the atomic positions as related to the unit cell and thus show the crystal symmetry and the repeat unit. In general, when making these models, much greater care must be taken in positioning the atoms and their bond directions than in the moecular models. Models of this type representing many known structure are available from several commercial sources.

These models are usually made with wooden balls, although plastics, cork, and recently foamed polystyrene have been used. Holes are drilled in these balls in bond directions, and the balls are joined with rods of Monel, brass, or aluminum. As these models are usually built with permanency as an objective, iron rods are avoided because they rust. A good general description is given by Seymour (1938). Several devices for drilling the holes are available and will be described under constructional devices. Only one commercially available set, described by Noyce (1951), is primarily designed for constructing these models. It is quite limited in use because most crystal structures are somewhat irregular, and thus each compound presents a special construction problem.

Several attempts to simplify the construction of the open models have been made. Gruner (1932) builds the wire frame first and then adds the atoms, using Plastic Wood. Perkins (1951) uses clay to form the atoms and, after the construction is complete, fires the entire model to make it permanent. The other attempts at simplification are seen in the many devices for positioning the holes in the correct bond directions.

6.3. Open Models with Parallel Rods

Another type of open model, first described by Sohncke (1879), consists of spheres supported on parallel rods which are usually vertical. The rods are rigidly mounted in a block of wood, clay, paraffin, or foamed polystyrene, or held in place by a wire mesh. The position of the rod in the base corresponds to the coordinates of the atom

in the projection of the structure on that plane. The sphere representing the atom may be adjusted on the rod to make its height correspond with the third coordinate. The vertical rods have no significance in the finished model. This type of model is very useful to crystallographers who are studying projected electron density maps.

7. Polyhedral Models

The polyhedral model consists of polyhedra, usually of cardboard or paper, which depict the coordination of anions around a central cation or of bonded atoms around a central covalent atom. The corners of the polyhedra correspond to the positions of the surrounding atoms. The model is built up by joining appropriate corners and edges of the polyhedra. These models have an advantage in being inexpensive to build for a class project, although they do not show the relationships inside a completed model too well, and they do not show the positions of the central atoms. Schneer (1952) describes their construction fairly completely. Pauling (1939) has used these models extensively for illustration. Quite often polyhedra have been used for certain radicals such as SiO_4 and SO_4 in models of the vertical rod type. They have also been used combined with molecular models to show complex ions (Wendlandt, 1957).

The versatility of these models was emphasized by Ashley (1930) who constructed them with irregular as well as regular coordination polyhedra. Elaborate models with irregular polyhedra are rarely constructed, however, because the precise knowledge of the coordination together with the work of deriving the shapes of the cardboard pieces usually justifies a model representing the individual atomic positions.

8. Miscellaneous Types

Many miscellaneous model types have been developed. One type closely related to the open models is the wire model. Hughes and Taylor (1949) describe a jig for making rigid wire molecular representations for projection onto an electron density map. Tilton (1958b) uses rigid wire tetrahedra coupled with cylindrical clamps to depict network structures in silica glass. The Dreiding wire models described by Fieser and Fieser (1959) are commercially available. Models based on several parallel sheets of Lucite or glass have been used by Brown (1951), Gordon (1938), Welch (1953), Westbrook (1957), and Wyckoff and Ksanda (1926). The atoms are mounted on the transparent sheets as either plastic balls, corks, electric lamps, or painted circles. Contoured three-dimensional Fourier electron density maps have been assembled in this manner. Whalen (1957) has drawn a chain of atoms on a strip of paper which he then twisted to form an α-helix (polypeptide chain) configuration. Lambert (1957) has used foamed polystyrene to represent molecular orbitals. Undoubtedly many other types of models have never been described in the literature or are discussed only in connection with a specific problem.

9. Dynamic Models

Dynamic models have been developed primarily to study the effect of thermal motion on atomic arrangements. One of the early dynamic models, described by Kettering, Shutts, and Anderson (1930) and consisting of balls connected with helical springs, is still commonly used in classrooms today. Models for showing molecular vibrations have been described by Childs and Jahn (1937) and Trenkler (1935). Several models for stimulating the effect of thermal motion on ordered lattices of spheres have been devised. Pohl (1952) and Hilsch (1954) have used magnets, Woolley and McLachlan (1949, 1950) have used lead shots between plates, and Bragg and Nye (1947) have used soap bubbles. Magnetic balls floating on water have been employed by Dietzel (1956) to represent the effects of thermal motion, simulated by blowing across the surface of the tank. There is little doubt that the development of dynamic models is just beginning.

10. Construction Devices

Drilling jigs may be separated into two groups: those which will drill holes only in certain special directions, and those which will drill holes in any desired position. In the first group fall the jigs of Wooster (1945) and Evans (1948) which will position twenty-six holes along the symmetry directions of the cubic system, that of Gibb and Bassow (1957) which will punch tetrahedral and octahedral holes in foamed polystyrene spheres, and that of Anker (1959) which drills marked holes in rubber spheres. More elaborate devices for positioning holes in any desired direction have been developed by Buerger (1935), Decker and Asp (1955), and Haywood (1949), using a spherical coordinate system to locate the bond direction, and by Smith (1960) using bond angles.

For wire models, Hughes and Taylor (1958) made a device for bending wire to conform with bond directions.

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11.2. Static Models

a. Closed Molecular (Stuart Type)

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Washington, D.C., December 15, 1959.

U.S. GOVERNMENT PRINTING OFFICE: 1960

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Electricity and Electronics. Resistance and Reactance. Electron Devices. Electrical Instruments. Magnetic Measurements. Dielectrics. Engineering Electronics. Electronic Instrumentation. Electrochemistry.

Optics and Metrology. Photometry and Colorimetry. Optical Instruments. Photographic Technology. Length. Engineering Metrology.

Heat. Temperature Physics. Thermodynamics. Cryogenic Physics. Rheology. Molecular Kinetics. Free Radicals Research.

Atomic Physics. Spectroscopy. Radiometry. Mass Spectrometry. Solid State Physics. Electron Physics. Atomic Physics.

Radiation Physics. Neutron Physics. Radiation Theory. Radioactivity. X-ray. High Energy Radiation. Nucleonic Instrumentation. Radiological Equipment.

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Mechanics. Sound. Mechanical Instruments. Fluid Mechanics. Engineering Mechanics. Mass and Scale. Capacity, Density, and Fluid Meters. Combustion Controls.

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Mineral Products. Engineering Ceramics. Glass. Refractories. Enameled Metals. Constitution and Microstructure.

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Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics.

Data Processing Systems. SEAC Engineering Group. Components and Techniques. Digital Circuitry. Digital Systems. Analog Systems. Applications Engineering.

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Cryogenic Engineering. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Gas Liquefaction.

Radio Propagation Physics. Upper Atmosphere Research. Ionosphere Research. Regular Prediction Services. Sun-Earth Relationships. VHF Research. Radio Warning Services. Airglow and Aurora. Radio Astronomy and Arctic Propagation.

Radio Propagation Engineering. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Propagation-Terrain Effects. Radio-Meteorology. Lower Atmosphere Physics.

Radio Standards. High-Frequency Electrical Standards. Radio Broadcast Service. Radio and Microwave Materials. Atomic Frequency and Time Standards. Electronic Calibration Center. Microwave Circuit Standards.

Radio Communication and Systems. Low Frequency and Very Low Frequency Research. High Frequency and Very High Frequency Research. Modulation Systems. Antenna Research. Navigation Systems. Systems Analysis Field Operations.