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Nicholson

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[54] **MODELS REPRESENTING MOLECULAR STRUCTURE**

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Related U.S. Application Data

[63] Continuation-in-part of Ser. No. 31,200, April 23, 1970, abandoned.

[52] **U.S. Cl.** ..... **35/18 A**

[51] **Int. Cl.** **G09b 23/26**

[58] **Field of Search** ..... 35/18 R, 18 A

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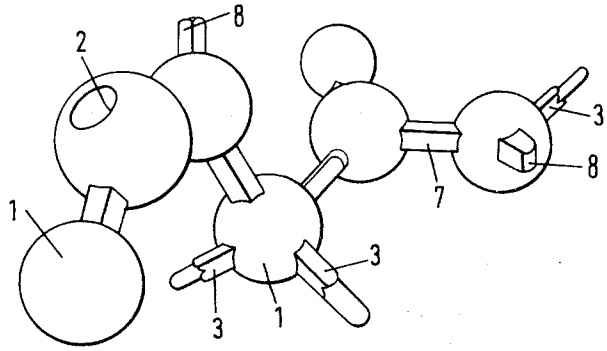
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[57] **ABSTRACT**

In a model representing a molecular structure comprising atoms and interatomic bonds, a unit representing a multivalent atom comprises a spherical body having a plurality of integral arms radiating from the body and a single socket comprising a cylindrical hole of circular cross section extending diametrically of the body to a depth greater than the radius of the body and less than the diameter. The number of arms is one less than the valence number of the atom represented. Each of the arms has a portion of polygonal cross section adjacent the spherical body and a circular cylindrical end portion of a diameter to fit tightly into the socket of another unit. The cylindrical end portion of the arm is at least as long as the depth of the socket and has a radiused end portion engaging a like inner end of the socket so as to determine the extent to which the arm is inserted in the socket and thereby determine accurately the interatomic distance between adjacent units.

9 Claims, 6 Drawing Figures



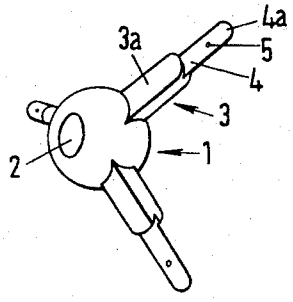


FIG. 1.

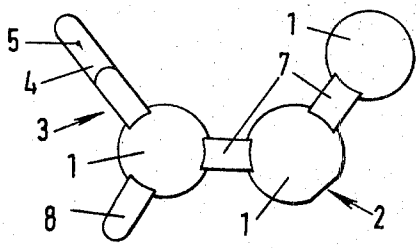


FIG. 2.

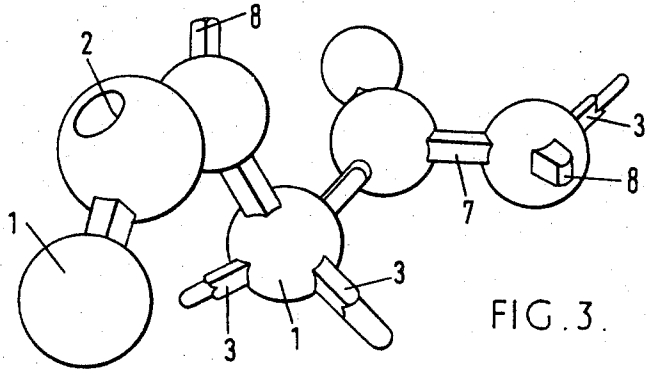


FIG. 3.

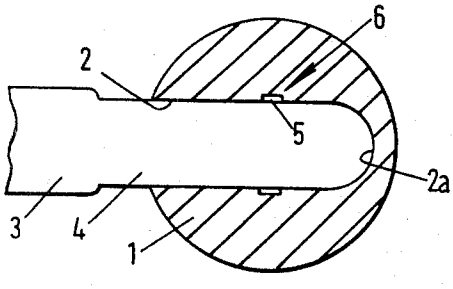


FIG. 4.

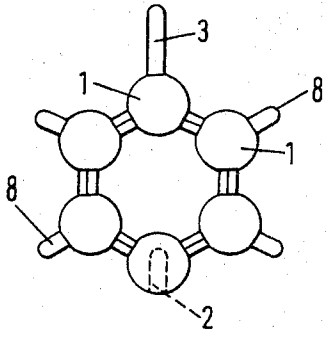


FIG. 5.

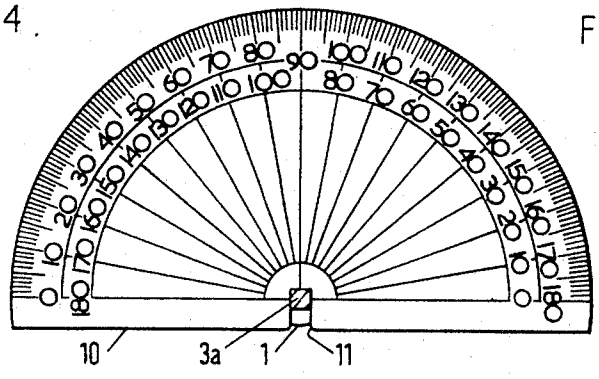


FIG. 6.

MODELS REPRESENTING MOLECULAR STRUCTURE

This application is a continuation-in-part of my copending application Ser. No. 31,200, filed Apr. 23, 1970, now abandoned.

The present invention relates to molecular models of the type in which spherical bodies representing atoms are interconnected by bars or rods representing interatomic bonds. The center of each sphere represents the center of an atom. While the bodies representing atoms are preferably spherical and for convenience are herein referred to as being spherical it will be understood that they can if desired be other shapes for example polyhedral.

A number of systems for building models of molecules have been proposed in which units or devices each representing an atom are detachably joined by separate rods representing interatomic bonds. A disadvantage with this system is the time and effort involved in assembling similar chemical structures. While this may not be important when the final model is small it is a considerable inconvenience in the case of models of compounds of high molecular weight such as nucleic acids and proteins. Moreover, large models constructed of bodies representing atoms and separate rods representing interatomic bonds lack the structural strength and rigidity to maintain their intended form and conformation. Such models accordingly require numerous supports which detract from their appearance.

It is an object of the present invention to provide a method of construction of rigid molecular models which requires no separate bond elements. In accordance with the present invention a unit representing a multivalent atom comprises a spherical body having a plurality of integral arms radiating from the body and a single socket comprising a cylindrical hole of circular cross section extending diametrically into the body with a depth greater than the radius of the body and less than the diameter. The number of arms is one less than the valence number of the atom represented and the arms and socket are oriented angularly relative to one another at substantially the correct valency angles of the atom. Each of the arms has a portion of polygonal cross section adjacent the body to permit proper angular orientation of the units and a circular cylindrical end portion of a diameter to fit tightly in the socket of another unit. The length of the cylindrical end portion is at least as great as the depth of the socket so that the distance the arm is inserted into the socket and hence the interatomic distances between the units is precisely determined by engagement of the end of the arm with the bottom of the socket. Recurring invariant groups of atoms are molded as one unit with interconnecting bonds between the atoms and with the atomic centers accurately positioned. With the construction in accordance with the present invention it is possible easily and quickly to construct models of large molecules which despite their size are rigid and stable.

The invention will be more fully understood from the following description in conjunction with the accompanying drawings which illustrate by way of example typical atom units and groups for construction of a model in accordance with the invention.

IN THE DRAWINGS

FIG. **1** is a perspective view of a unit representing a carbon atom;

FIG. **2** is a perspective view illustrating a planar peptide group;

FIG. **3** is a perspective view of a part of a polypeptide assembled with the units illustrated in FIGS. **1** and **2**;

FIG. **4** is an enlarged sectional view of an arm of one unit fitted into the socket of another;

FIG. **5** is a view of a unit representing a phenyl (phenylene) group, and

FIG. **6** is a view illustrating schematically how a protractor is utilized in establishing the correct angular relationship between connected units.

In accordance with the present invention a molded unit may represent either an individual atom or a group of atoms. When the atoms of a group in the chemical compound to be molded are joined together and lie in or near the same plane they are conveniently molded as a single unit comprising a plurality of spherical bodies interconnected by integral portions representing bonds between the atoms. The centers of the spherical bodies accordingly lie in or near a common plane and are spatially separated from one another in scale proportion to the true interatomic distances. The joining portions are preferably of square or other polygonal cross section. Hydrogen is not represented as a sphere but the position of the center of a hydrogen atom is given by the end of an arm of a length equal to the scale interatomic bond distance.

The units whether they contain one sphere or a plurality of spheres are joined with one another by a connection consisting of an integral arm of one of the units fitting tightly into a socket provided in another unit. Each socket is situated in a sphere representing an atom and is circular in cross section and of a depth greater than the radius of the sphere and slightly less than the diameter. Each of the connecting arms is integral with a sphere and has a polygonal cross section adjacent the sphere and an end portion of circular cross section with a diameter that is slightly greater than the diameter of the socket into which it is to be fitted so as to provide a tight frictional fit. The circular portion of the arm has a length at least equal to the depth of the socket so that the end of the arm engages the bottom of the socket and thereby accurately establishes the distance the arm is inserted into the socket and thus the correct interatomic distance between the two connected bodies. It is convenient to make the point at which the cross section changes from polygonal to circular to coincide with the point at which the center of a hydrogen atom would be located if the atom represented by the spherical body were linked to a hydrogen atom. Thus, by cutting off the circular portion of an arm the correct scale interatomic bond distance of the atom to a hydrogen atom is obtained.

The connection between two units is made by inserting the integral arm of one unit into the single socket of another unit. The arm is inserted all the way into the socket so as to engage the bottom of the socket. Two units can be rotated angularly relative to one another if sufficient force is applied but the circular portion of the arm fits sufficiently tightly in the socket as to prevent other than intentional and forcible movement. Slight differences in interatomic bond distances be-

tween different pairs of atoms is allowed for by having different depths of socket in different spheres. However, the depth of the socket after allowing for this slight variation is as deep as possible and in any event is greater than the radius of the spherical body. The depth of the socket and the corresponding interfitting length of the arm prevents relative movement of the socket and the arm and thus assures rigidity of the assembled model. The fact that the arm is integral with one of the bodies contributes further to the rigidity of the assembly. Further the depth of the socket gives a large area of frictional contact with the arm thereby increasing the rotational friction so that the units stay in their correct relative orientation. As described below resistance to disengagement of an arm from a socket may be further increased by providing a nodule or collar on the arm fitting into an annular groove provided in the socket. However, the depth of insertion of the arm into the socket is determined not by such collar or nodule but by engagement of the end of the arm with the bottom of the socket.

Units representing a single atom and its interatomic bonds comprise a spherical body having a single socket and a number of radiating arms equal to one less than the number of valencies of the atom represented. The longitudinal axes of the socket and the arms pass through the center of the sphere and are angularly disposed at substantially the same angles as the known directed valencies of the represented atom. Each molded unit representing a group of atoms has at least one socket and may or may not have one or more arms. If the unit is part of a repeating pattern then at least one arm is required.

The van der Waal's radius of the atoms is conveniently illustrated by arranging the radius of the spheres to be one quarter to one half and preferably one third of the true van der Waal's radius of the atoms expressed in the same scale as the interatomic distances. The van der Waal's radius is given by the outermost point of a second sphere of identical radius placed or imagined in contact with the first.

The polygonal cross section of the arm adjacent the spherical body facilitates molding the units in a two-piece mold and further facilitates model building with the use of a protractor to measure the rotational angles between connected units so as to conform with the molecular structure.

Referring now to the units shown by way of example in the drawings, FIG. **1** illustrates a unit representing a carbon atom having a valency of four. The unit is shown as comprising a spherical body **1** having a single radially extending socket **2** and three radially projecting integral arms **3.** Each of the arms has a portion **3***a* of square cross section adjacent the spherical body and a circular cylindrical end portion **4** with a rounded end **4***a*. The socket **2** and the arms **3** are arranged in a tetrahedral relationship at an angle of approximately 108° or 109.5° to each other. The point of transition from a square cross section to a circular cross section of the arms **3** is at a distance from the center of the sphere equal to the carbon-hydrogen interatomic bond distance. As illustrated in FIG. **4,** the socket **2** extends through and beyond the center of the sphere and ends in a curved bottom **2a** which is engaged by the curved end of an arm **3** of an adjacent unit so as to establish in a definite and positive manner the depth of insertion of the arm in the socket and thereby the interatomic distance between the two atoms. The end portion **4** of the arm **3** has a diameter slightly greater than the diameter of the socket **2** so as to fit tightly into the socket with a tight fit so as to maintain the units in assembled relation and in correct spacial and angular relation relative to one another. The socket **2** and the interfitting end portion **4** of the arm **3** are cylindrical rather than tapered so that the distance of insertion of the arm in the socket is determined by the depth of the socket and not by the interengagement of two tapered portions.

The square cross sectional shape of the portions **3a** of the arms **3** adjacent the spherical body **1** facilitate molding the unit in a two-part mold. By reason of the angular relation of the radial arms **3** to one another and to the socket **2** the intersections between the surface of the spherical body **1** and the faces of the arms nearest the opening of the socket **2** lie approximately in a diametrical plane perpendicular to the axis of the socket. The molds are accordingly arranged to part of this plane. Moreover, as will be explained below the square cross section of the portions of the arms adjacent the spherical body **1** facilitates establishing correct angular orientation of the units relative to one another.

The depth of the socket **2** is greater than the radius of the spherical body **1** and preferably almost equal to the diameter of the spherical body. However, the socket does not extend all the way through the spherical body as this would not provide a socket bottom for limiting the distance of insertion of the arm **3** of a connecting unit. Preferably the depth of the socket is at least 75 percent of the diameter of the spherical body. This provides a long bearing surface for the arm **3.** Since the arm extends beyond the center of the sphere **1** it will be apparent that only one socket can be provided. The diameter of the socket is preferably between 10 and 50 percent of the diameter of the sphere **1.** If the diameter of the socket is made greater than 50 percent of the diameter of the sphere, the strength of the remaining material of the sphere may not be sufficient to withstand the expansion forces resulting from forcing an arm **3** into the socket. If the socket is made too small the correspondingly small diameter of the portion of the arm inserted in the socket may not provide sufficient strength and rigidity. Preferably the diameter of the socket **2** is approximately 40 percent of the diameter of the sphere. For example if the sphere has a diameter of one centimeter the diameter of the socket is approximately 4 mm. The diameter of the cylindrical portion of the arm is a few thousandths greater than the diameter of the socket in order to provide a tight fit. The polygonal portion **3***a* of the arm preferably has the same cross sectional dimension as the cylindrical portion.

While the tight fit of the arm in the socket is ordinarily sufficient to prevent unintentional disengagement of the units from one another the arm may, if desired, be provided with a small collar or nodule **5** which is received in an annular groove **6** in the socket to provide a snap fit. The leading face of the nodule is preferably gradually inclined so that the nodule is pressed inwardly and not sheared off when the arm is inserted into the socket. The entrance edge of the socket may if desired be slightly rounded or bevelled to avoid shearing off the nodule on the arm.

The peptide group shown by way of example in FIG. **2** comprises three spherical bodies, integrally interconnected with one another by bond portions **7.** The por-

tions 7 are preferably of square cross section but may if desired be of other polygonal shape or round. One of the spherical bodies is provided with a radially projecting arm 3 having a cylindrical end portion 4. Another of the cylindrical bodies has a socket 2 corresponding to the socket shown in FIGS. 1 and 4. There is also provided a shorter arm 8 projecting radially from one of the spherical bodies as shown. The arm 8 is not intended for connection to another unit but represents a hydrogen atom. The group shown in FIG. 2 is molded as a single unit. As the centers of the atoms and the axes of the socket and arm all lie in the same plane such unit can be molded conveniently in a two-part mold.

FIG. 3 illustrates a model of a molecular structure assembled from one of the units of FIG. 1 and two of the units of FIG. 2. The correct distances for the carbon-carbon and carbon-nitrogen bonds are immediately established on joining the devices by the arm and socket dimensions. Rotation of the carbon unit relative to the peptide bond unit to give the correct dihedral angle completely specifies the position in space of each represented atom. Orientation of the units relative to one another is facilitated by use of a protractor 10 as illustrated in FIG. 6. The protractor has a notch 11 of a shape to fit snugly on the square portion 3a of the arm 3 of a unit so as to orient the protractor with respect to that unit. It will be understood that if the arm has other polygonal shape the notch in the protractor is made to conform so as to fix the angular relation of the protractor relative to the unit on which it is placed.

In FIG. 5 there is shown a unit representing a phenyl or phenylene group consisting of six atoms with interconnecting bonds. The atoms are accordingly represented by six spheres 1, the centers of which all lie in a common plane. One of the spheres is provided with a radially projecting integral arm 3 while another (opposite) sphere is provided with a socket 2. The other spheres have short arms 8 representing hydrogen atoms.

The units whether representing a single atom or a group are molded of plastic material which is sufficiently strong and rigid to provide a stable model even when a large number of units are assembled to represent a large molecule. A suitable material is polyethylene. For the backbone of the molecular structure it is desirable to use a high density polyethylene for example that known as "Rigidex" in order to provide greater rigidity. Side chain atoms may be made of a blend of low and medium density materials. The different atoms and different groups are preferably molded of plastic of different colors so as to permit color coding of the molecular structure.

With the construction in accordance with the present invention it is possible to assemble selected molded units to construct models even of large molecules which are stable and rigid. The diameter of the spherical bodies and the lengths of the arms are selected to conform to the molecular structure. The size of the spheres is selected so as to be a quarter to one half of the van der Waals radius and preferably one third the van der Waal's radius expressed on the same scale as the interatomic distances. An appropriate scale is 1 cm. = 1 A. By use of a protractor fitting on polygonal portions of the integral interconnecting arms as described above, it is possible to establish correct angular relationships between the connected units. Because of the high rotational friction about the connecting arms the units remain in the configuration in which they are assembled. Mechanisms of enzyme action including details of active sites and conformational changes replication and transcription of nucleic acids, the stereochemistry of bonding symmetry, reaction mechanisms transfer RNA recognition sites, proteinsynthesis, isomerism of sugars are some of the topics of study to which the model system in accordance with the invention lends itself. The use of different colors for different functional groups or moieties provides greater clarity for the interpretation of complex structures.

What I claim and desire to secure by Letters Patent is:

1. A scale model representing a molecular structure comprising atoms and interatomic bonds, comprising a plurality of units each representing a multivalent atom, each of said units comprising a spherical body having a single socket comprising a cylindrical hole of circular cross section extending diametrically of said body with a depth greater than the radius and less than the diameter of said body and a plurality of integral arms representing interatomic bonds radiating from said body, the number of arms being one less than the valence number of the atom represented, said single socket and said arms being oriented relative to one another at substantially the correct valency angles of said atom, each of said arms having at its free end a cylindrical portion of a diameter to fit tightly into a like socket of another unit of said model representing another atom, said cylindrical portion having a length at least as great as the depth of said socket, said cylindrical portion seating against the bottom of said socket to define accurately the depth of penetration of said cylindrical portion in the socket, the total length of said arm being substantially greater than the depth of said socket such that when the end of said cylindrical portion is seated on the bottom of the socket the length of the arm defines the interatomic distance between the atoms, whereby said units are assembled with an integral arm of one unit fitting tightly into the socket of another unit without play to form a substantially rigid structure.

2. A molecular model according to claim 1, in which said arms have portions of polygonal cross section adjacent said spherical body for orienting said units angularly relative to one another.

3. A molecular model according to claim 1, in which the radius of the spherical body is between one quarter and one half of the van der Waal's radius of the atom expressed in the same scale as the interatomic distance defined by said arms.

4. A molecular model according to claim 3, in which the scale is at least approximately 1 cm. = 1 A.

5. A molecular model according to claim 1, in which the diameter of said socket is between 10 and 50 percent of the diameter of said spherical body.

6. A molecular model according to claim 1, in which a unit representing a carbon atom has three said integral arms, the axes of said arms and socket intersecting at the center of said spherical body and being disposed at an angle of approximately 108° to one another.

7. A molecular model according to claim 2, in which the transition from said polygonal to said cylindrical portion of each said arm occurs at a distance from the center of the spherical body equal to the scale carbon-hydrogen interatomic bond distance.

8. A molecular model according to claim 1, further comprising a unit representing an invariant group com-

prising an integral structure including a plurality of spherical bodies spaced from one another and representing atoms, integral bar portions interconnecting said spherical bodies and representing interatomic bonds, the length of said arms representing interatomic distances, at least one of said spherical bodies having a single socket comprising a cylindrical hole of circular cross section extending diametrically of said body with a depth greater than the radius and less than the diameter of said body and at least one of said bodies having an integral arm representing an interatomic bond projecting radially from said body and having at its free end a cylindrical portion of a diameter to fit tightly into a like socket of another unit of said model and a length at least as great as the depth of said socket, whereby a plurality of units are assembled by fitting a said integral arm of one unit tightly into a socket of another unit to form a substantially rigid structure.

9. A molecular model according to claim **8,** in which at least one of said spherical bodies has an integral radially projecting arm which is shorter than said first mentioned arm and has a length representing a carbon-hydrogen interatomic bond distance.

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