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Scale models of polypeptide chains with permanent connections between 'backbone' atoms.*

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An earlier communication (Corey & Casler, 1958) described the recent use of small permanent magnets for hydrogen bonds in molecular models constructed of colored, rubber-like vinyl plastic. These models were originally developed (Corey & Pauling, 1953) several years ago for use in studies of the structures of amino acids, peptides, and related compounds. In many respects they resemble the Stuart-type models now commercially available, adjacent bonded atoms being held together by means of snap fasteners and double-ended brass studs. When used for constructing very large molecules, the weight of the models and the local strains that develop when they are handled sometimes cause the snap fasteners connecting bonded atoms to pull apart. This occurrence is especially frequent with representations of molecules of polypeptides and similar compounds that consist essentially of long chains of atoms. For such molecules it is highly desirable that the 'backbone' of the chain be constructed so that its adjacent atoms will not separate, even when subjected to considerable manipulative stress. This note describes models for representing a polypeptide or a linear carbon chain embodying this feature.

The device employed for joining adjacent atoms in the chain is shown in Fig. 1. It consists of a double-ended aluminum stud S that can be locked into an aluminum insert A around which the plastic atom is cast. The stud S is locked into A by means of a round brass or steel rod R that passes through a hole in A so as to fit into a circular keyway in the stud. The assembly includes a backing plate B which serves to anchor the insert A firmly in the plastic atom.

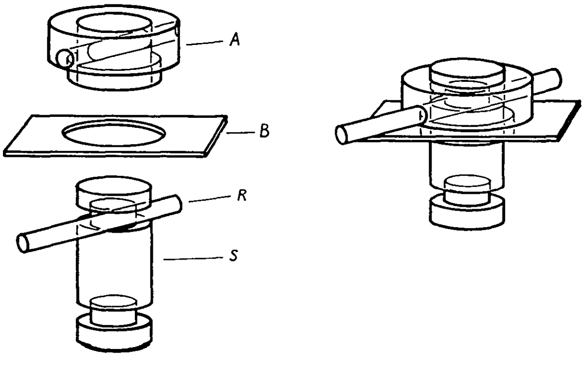

Fig. 1. An exploded view of the locking device for joining adjacent atoms of a chain. S is a double-ended stud that can be locked to the atom insert A by the insertion of a rod R. B is a backing plate that serves to anchor A firmly in the plastic atom.

Fig. 2 is a phantom drawing of a typical α-carbon atom. Two of the bonds—those connecting to adjacent amide groups in the chain—are made by means of the new stud fasteners; the other two—those connecting to a hydrogen atom and a side chain—are the usual snap fasteners. For the sake of clarity of the drawing, only one snap fastener, that on the front of the model, is shown.

Fig. 3 is an assembly drawing of a portion of a polypeptide chain showing the positions of the stud fasteners in the amide groups and the α-carbon atoms. The two snap fasteners on the α-carbon atoms are not shown.

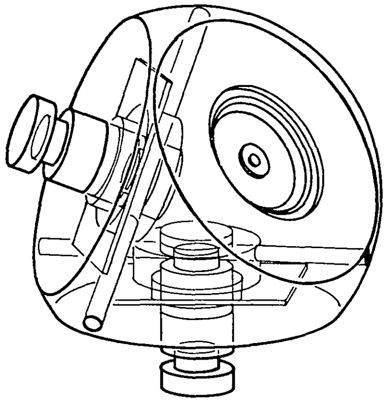

Fig. 2. A phantom drawing of a typical α-carbon atom, showing the two inserts and stud connectors that form the intra-chain bonds. One of the two snap fasteners is not shown in this drawing for the sake of clarity.

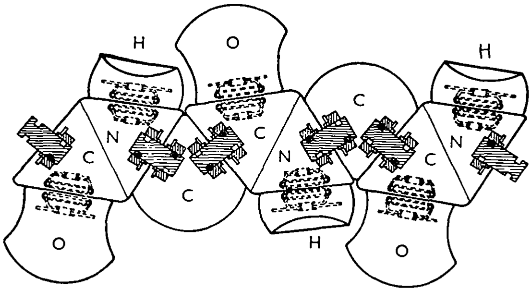

Fig. 3. An assembly drawing of a portion of a polypeptide chain showing the positions of the locked stud fasteners in the amide groups and the α-carbon atoms.

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Bonds within the chain are formed by inserting one end of a stud into an atom, locking the stud in place by inserting a locking rod as shown in Fig. 2, then inserting the other end of the stud in the second atom, pressing the two atoms firmly together so as to bring the keyway in the stud in line with the hole in the second atom, and finally by pushing in the second locking rod. The distance between the two keyways is designed so as to require a slight compression of the atoms at the interface when the bond is made. The resulting friction between the surfaces of adjacent atoms prevents too much freedom of rotation around the bonds, so that the chain will tend to retain desired configurations. Bonds in the chain can be broken by poking the locking rods out of the atoms with a separate rod of the same diameter or with an appropriate tool.

It may be noted that the carbon atom described here for constructing a peptide chain can also be used for building a linear carbon–carbon chain.

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The lattice constant of strontium nitrate, $Sr(NO_3)_2$.

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An accurate determination of the lattice constant of strontium nitrate has been made, following an observation by one of the authors (Deshpande, 1955) that the value reported in literature is too high. The value reported by Vegard (1922) is 7·81 Å and that reported by Jaeger & Van Melle (1928) is 7·80 Å. Deshpande (1955) gives a value of 7·7794±0·0003 Å at 20° C. in terms of Cu $K\alpha_2 = 1{\cdot}54434$ Å and Cu $K\alpha_1 = 1{\cdot}54050$ Å.

In the present investigation the lattice parameter was determined from powder photographs, obtained with a Debye–Scherrer camera of 11·46 cm. diameter. The photographs gave eight sharp and well resolved $\alpha_1\alpha_2$ doublets in the high-angle region. Filtered copper radiation was used and the values of the wavelengths were the same as given above. Pure salt supplied by Merck was recrystallized and used for the preparation of the specimens. Photographs were taken with different samples and measurements were made independently by the authors. The values of the lattice parameter obtained from the various reflections on a film were extrapolated to $\theta = 90°$, using Nelson & Riley's (1945) error function. The best straight line was fitted by the least-squares method.

Since, with the particular camera used, it was not possible to measure the specimen temperature directly, the lattice constant of NaCl was used as an indicator of temperature.

Powder photographs of sodium chloride were taken under identical conditions and the temperature of the specimen was estimated from the results so obtained. As the temperature of the specimens varied from film to film, the values of the lattice parameter were reduced to 20 °C., the value of the coefficient of thermal expansion used being 30×10^{-6} °C.$^{-1}$ (Deshpande, 1955). The mean of the values thus obtained is 7·7798 Å. The maximum deviation of the individual values from the mean is 0·0002 Å. This value is found to be in good agreement with the one obtained by Deshpande (1955). The data for some of the films are given in Table 1.

Table 1. *Lattice constant of* $Sr(NO_3)_2$

Film No.	Temperature (°C.)	Extrapolated *a*	*a* at 20 °C.
8	36	7·7833 Å	7·7796 Å
9	36	7·7835	7·7798
23	32	7·7828	7·7800
27	33	7·7830	7·7800
40	31	7·7825	7·7799

Mean of several values of *a* 7·7798±0·0002 Å.

The density of the substance was also calculated from the relation $\varrho = Mn/(NV)$, where M is the molecular weight, n is the number of molecules in the unit cell, N is Avagadro's number and V is the volume of the unit cell. Taking $M = 211{\cdot}65$ and $N = 6{\cdot}02385 \times 10^{23}$, after Straumanis (1949), the present value of a gives the density as 2·985. The experimental value reported in *International Critical Tables* is 2·986 g.cm.$^{-3}$ at 20 °C. Vegard reports the calculated density as 2·930 g.cm.$^{-3}$. It is obvious from these figures that the present value of a is more accurate than that of Vegard.

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