drostene-17a-ol-3,11,17-trione, m.p. 238–242°; $[\alpha]^{23}D$ +121° (*c*, 0.48 in $CHCl_3$) and the known Δ^4-pregnene-17α-ol-3,11,20-trione,[10] m.p. 232–235°; $[\alpha]^{24}D$ +186° (*c*, 0.33 in $CHCl_3$). The conversion of VII into VI under conditions reported[11] to effect the expansion of ring D in 17α-hydroxyprogesterone served to establish the structure of VI.

(10) L. H. Sarett, THIS JOURNAL, **70**, 1454 (1948); T. H. Kritchevsky, D. L. Garmaise and T. F. Gallagher, *ibid.*, **74**, 483 (1952).

(11) J. van Euw and T. Reichstein, *Helv. Chim. Acta*, **24**, 879 (1941).

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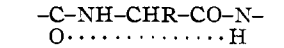
POLYPEPTIDE HELICES IN PROTEINS

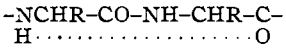
Sir:

About fifteen years ago[1] I discussed the principles underlying protein structure and proposed that the polypeptide chains in proteins, when not nearly fully extended, have folded or helical structures, with adjacent folds or turns of the helix connected by N–H···O hydrogen bonds. Considerable evidence has since accumulated in favor of these proposals and they are now generally accepted.

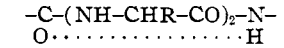
As the simplest examples illustrating these principles, I discussed a folded structure containing 7-atom rings



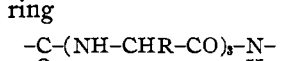
and helices containing 8-atom rings



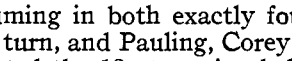
and 10-atom rings



Bragg, Kendrew and Perutz[2] have recently considered similar 11-atom ring



and 13-atom ring



helices, assuming in both exactly four amino-acid residues per turn, and Pauling, Corey and Branson[3] have advocated the 13-atom ring helix with about 3.7 residues per turn. They pointed out, as I had done in the case of the 10-atom ring structure, that it is not necessary that this number be integral. (At the recent Chemical Conclave I mistakenly believed and stated that their model was merely a refinement of my 10-atom ring structure.)

(1) M. L. Huggins, Abstracts, Rochester Meeting, American Chemical Society, B10 (1937); see also Abstracts, Memphis Meeting, A.C.S., P4 (1942); *Annual Review of Biochemistry*, **11**, 27 (1942); *Chem. Revs.*, **32**, 195 (1943).

(2) W. L. Bragg, J. C. Kendrew and M. F. Perutz, *Proc. Roy. Soc. (London)*, **A203**, 321 (1950).

(3) L. Pauling and R. B. Corey, THIS JOURNAL, **72**, 5349 (1950); *Proc. Nat. Acad. Sci.*, **37**, 235, 241, 256, 261, 282 (1951); L. Pauling, R. B. Corey and H. R. Branson, *ibid.*, **37**, 205 (1951).

An 11-atom ring structure is possible,[4] consistent with the published X-ray data and with all of Pauling and Corey's postulates regarding bond angles and distances, except that the N–C* bond is not in the C–C'O–NH plane, but makes an angle of about 30° with it. This is not unreasonable, on the basis of their estimate of about equal contributions of structures containing coplanar nitrogen and tetrahedral nitrogen. On the other hand, approximate coplanarity has been found in glycylglycine[5] and acetylglycine[6] crystals; this would seem to favor the 13-atom ring structure, which permits such coplanarity. However, since the energy difference associated with the difference in bond orientation is probably small and may be counteracted by environmental differences, this evidence is not very strong.

In neither the 11-atom ring structure nor the 13-atom ring structure is the C=O bond tilted with respect to the axis of the helix more than the N–H bond, unless the assumptions made are considerably in error. Hence, the infrared spectrum differences, tentatively and cautiously attributed by Bamford and co-workers[7] to such a difference in angle of tilt, should probably be interpreted in some other way.

In agreement with Bamford and his colleagues, I believe that, pending further experimental data, both of these structures should be considered possible for the alpha synthetic polypeptides, the alpha fibrous proteins and corpuscular proteins. Perhaps both types are sometimes present together, in fibrous natural proteins for example. All other types of structure seem to be definitely eliminated, at least for the alpha synthetic polypeptides, by the X-ray data.[7–9]

(4) M. L. Huggins, THIS JOURNAL, **74**, 3963 (1952).

(5) E. W. Hughes and W. J. Moore, *ibid.*, **71**, 2618 (1949).

(6) G. B. Carpenter and J. Donohue, *ibid.*, **72**, 2315 (1950).

(7) C. H. Bamford, L. Brown, A. Elliott, W. E. Hanby and I. F. Trotter, *Nature*, **169**, 357 (1952).

(8) M. F. Perutz, *ibid.*, **167**, 1053 (1951); **168**, 653 (1951); H. E. Huxley and M. F. Perutz, *ibid.*, **167**, 1054 (1951).

(9) W. Cochran and F. H. C. Crick, *ibid.*, **169**, 234 (1952).

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COÖRDINATES OF THE 11-ATOM RING POLYPEPTIDE HELIX

Sir:

In order to facilitate comparison of the 11-atom ring helical polypeptide structure[1,2] with other structures and with experimental data, I have calculated atomic coördinates, on the following assumptions: (1) the translational and rotational shifts per amino-acid residue are 1.47Å. and 100°, as observed[2–4] in poly-(methyl glutamate); (2) the bond distances and bond angles are those assumed by Pauling and Corey,[5] except that some

(1) M. L. Huggins, THIS JOURNAL, **74**, 3963 (1952).

(2) C. H. Bamford, L. Brown, A. Elliott, W. E. Hanby and I. F. Trotter, *Nature*, **169**, 357 (1952).

(3) L. Pauling and R. B. Corey, *Proc. Nat. Acad. Sci.*, **37**, 241 (1951); *Nature*, **169**, 494 (1952).

(4) M. F. Perutz, *ibid.*, **167**, 1053 (1951).

(5) L. Pauling and R. B. Corey, *Proc. Nat. Acad. Sci.*, **37**, 235 (1951).