

departure of the N-C* bond from the C-C'O-N plane is allowed; (3) no distances between non-bonded atoms are unreasonably short; and (4) the configuration around each alpha carbon atom is *levo*, with the Fischer convention correct.⁶

These assumptions are insufficient to determine the coordinates uniquely, the values obtained depending on the postulates made with regard to the hydrogen bond length and the minimum permissible distance between the β carbon atom and neighboring oxygen atoms. Nevertheless, the following set of coordinates is presented, with certain other pertinent magnitudes derived from them.

| | x, Å. | y, Å. | z, Å. | ρ , Å. | ϕ , deg. |
|---|-------|--------|-------|-------------|---------------|
| Axis | 0 | 0 | 0 | | |
| C | 0.00 | -2.245 | 0.00 | 2.245 | 0.0 |
| C' | 1.21 | -1.30 | 0.00 | 1.78 | 42.9 |
| O | 1.70 | -0.90 | -1.06 | 1.92 | 62.1 |
| N | 1.69 | -0.95 | 1.18 | 1.94 | 60.7 |
| C* | 2.21 | 0.39 | 1.47 | 2.245 | 100.0 |
| C β | 0.28 | -3.48 | -0.88 | 3.51 | 4.2 |
| H _N | 1.18 | -1.36 | 1.96 | 1.80 | 41.0 |
| Hydrogen bond distance | | | | | 2.88Å. |
| Angle between N-C* and C-C'O-N plane | | | | | 30° |
| Angle H-N...O between N-H bond and hydrogen bond axis | | | | | 5° |
| Angle C'=O...N between C'=O bond and hydrogen bond axis | | | | | 140° |
| Angle between C=O and helical axis | | | | | 31° |
| Angle between N-H and helical axis | | | | | 39° |
| Angle N-C-C β | | | | | 116° |
| Angle C'-C-C β | | | | | 112° |

To obtain the coordinates of the hydrogen atom of the NH group, it was assumed that the N-H bond has a length of 1.014Å., that it lies in the C-C'O-N plane, and that it makes equal angles (113°) with the N-C' and N-C* bonds. In computing the C β coordinates, this atom was assumed to be 2.97Å. from each of the two neighboring carbonyl oxygen atoms. This leads to the slightly large value given for the N-C-C β angle.

Reasonable minor changes in the assumptions would lead to some variations from the coordinates given. They would not, however, reduce the angle between the N-C* bond and the C-C'O-N plane significantly, nor would they change greatly the angles of tilt of the C=O and N-H bonds.

The coordinates listed are for a right-handed spiral, since (assuming the Fischer convention correct) a left-handed spiral would lead to much too small a distance between the β carbon atom and a carbonyl oxygen atom in the next turn of the helix. It may be noted that Pauling and Corey's second alternative set of C β coordinates for the 13-atom ring structure, which are the ones to use (according to the Fischer convention) for *levo* polypeptides in their left-handed spiral, give a C β ...O distance of only 2.64Å. I conclude that *levo* polypeptides form right-handed spirals and *dextro* polypeptides left-handed spirals, whichever of these two types of structure is correct.

Some of the conclusions to be drawn from the re-

(6) A. F. Peerdeman, A. J. Van Bommel and J. M. Bijvoet, *Proc. Acad. Sci. Amsterdam*, **B44**, 3 (1951).

sults of these calculations are discussed briefly in another communication.¹

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THE PLANARITY OF THE AMIDE GROUP IN POLYPEPTIDES

Sir:

Dr. M. L. Huggins has kindly sent us copies of his Letters,^{1,2} in which he has proposed a helical configuration of polypeptide chains as an alternative to the α helix described in our earlier publications.^{3,4,5} In his configuration the amide group is not planar. The deformation of the amide group from the planar configuration can be described as a rotation of 17.5° of the NHC* plane about the C'-N axis plus a bending of 15° of the N-C* bond and the N-H bond out of the rotated plane, to the same side. The part of the strain energy due to the rotation of the π orbital of the nitrogen atom can be calculated by the formula^{6,7} $A \sin^2 \delta$ with $A = 30$ kcal. mole⁻¹ and $\delta = 17.5^\circ$; this calculation gives 2.7 kcal. mole⁻¹. The strain energy of deformation of the N-C* bond and the N-H bond can be calculated by the assumption that the bond energy is proportional to the strength of the bond orbital of the nitrogen atom in the bond direction, which is for these bonds 15° from the direction of maximum strength. With use of the bond energies of the bonds (48.6 and 83.7 kcal. mole⁻¹, respectively), this calculation leads to 3.3 kcal. mole⁻¹ for the bending energy of the two bonds. The total strain energy for the distorted amide group is thus found to be 6 kcal. mole⁻¹. This strain energy, which in the structure proposed by Huggins applies to every residue, is so great as to make the structure unacceptable in comparison with the α helix, which is just as satisfactory in every other respect, so far as we are aware, and which involves planar amide groups.

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

(2) M. L. Huggins, *ibid.*, **74**, 3963 (1952).

(3) L. Pauling and R. B. Corey, *ibid.*, **72**, 5349 (1950).

(4) L. Pauling, R. B. Corey and H. R. Branson, *Proc. Nat. Acad. Sci.*, **37**, 205 (1951).

(5) L. Pauling and R. B. Corey, *ibid.*, **37**, 235 (1951).

(6) L. Pauling and R. B. Corey, *ibid.*, **37**, 251 (1951).

(7) R. B. Corey and L. Pauling, *Proc. Roy. Soc. (London)*, to be published; presented at the Discussion Conference of the Royal Society of London, May 1, 1952.

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LIPOTHIAMIDE PYROPHOSPHATE: COENZYME FOR OXIDATIVE DECARBOXYLATION OF α -KETO ACIDS

Sir:

It has been reported¹ recently that lipothiamide (LT), the amide of α -lipoic acid (α -LA) and thiamin, is required for oxidation of pyruvate and α -ketoglutarate by resting cell suspensions of an *Escherichia coli* mutant. The organism lacks the

(1) L. J. Reed and B. G. DeBuck, *THIS JOURNAL*, **74**, 3457 (1952).