

**Table referenced as "Conformations of polypeptides (Blout et al 1961)"**

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# THE DEPENDENCE OF THE CONFORMATIONS OF SYNTHETIC POLYPEPTIDES ON AMINO ACID COMPOSITION<sup>1,2</sup>

Sir:

Several years ago the  $\alpha$  helix<sup>3</sup> was demonstrated by X-ray diffraction in a few synthetic polypeptides<sup>4,5,6</sup> and recently has been shown to be a basic structural unit of certain proteins.<sup>7</sup> Infrared dichroism also has been used to identify the  $\alpha$ -helical conformation<sup>8</sup> and to distinguish between it and  $\beta$  structures. The

data are shown in the table. It should be noted that the conformation does not appear to depend on the molecular weight in the samples examined, since some high molecular weight polypeptides are  $\alpha$ -helical while others of the same or higher degree of polymerization show only  $\beta$  or random conformations in the solid state.

On the basis of the results presented here we believe that there are two classes of polypeptides, those which form  $\alpha$  structures and those which form  $\beta$  structures. The

MOLECULAR AND INFRARED SPECTRAL PROPERTIES OF VARIOUS SYNTHETIC POLYPEPTIDES

Polypeptide	$\eta_{sp}/c^a$	Estimated <sup>b</sup>		Amide I <sup>c</sup>		Amide II <sup>c</sup>		Structure <sup>e</sup>
		DP <sub>n</sub>	MW <sub>n</sub>	Frequency (cm. <sup>-1</sup> )	Dichroism	Frequency (cm. <sup>-1</sup> )	Dichroism	
Poly-L-valine	0.29	190	19,000	1638	⊥	1545		$\beta$
Poly-L-leucine	.11	35	3,900	1650		1543	⊥	$\alpha$
Poly-S-methyl-L-cysteine	.24	140	16,000	1632	⊥	1540, 1525		$\beta$
Poly-S-benzyl-L-cysteine	.49	365	77,000	1632	⊥	1524		$\beta$
Poly-L-methionine	.22	135	18,000	1648		1540	⊥	$\alpha$
Poly-O-acetyl-L-serine	.14	130	16,800	1637	⊥	1520		$\beta$
Poly-L-serine	.10 <sup>d</sup>	130	11,300	1653	..	1525-1535	..	Random
Poly- $\beta$ -benzyl-L-aspartate	.30	190	39,000	1668		1563	⊥	$\alpha$
Poly- $\gamma$ -benzyl-L-glutamate	.15	100	22,000	1645		1542	⊥	$\alpha$

<sup>a</sup> The reduced specific viscosities were determined at a concentration of 0.2% in either dichloroacetic acid or trifluoroacetic acid to assure that the polypeptides were in the random form. <sup>b</sup> The weight average degrees of polymerization (DP<sub>w</sub>) and the weight average molecular weights (MW<sub>w</sub>) were estimated from the correlation of the viscosities of the random form of poly- $\gamma$ -benzyl-L-glutamate with light scattering and sedimentation measurements (see P. Doty, J. H. Bradbury and A. M. Holtzer, THIS JOURNAL, 78, 947 (1956); J. C. Mitchell, A. E. Woodward and P. Doty, *ibid.*, 79, 3955 (1957)). <sup>c</sup> Of oriented films. <sup>d</sup> Intrinsic viscosity in water.

Polaroid Corporation, Cambridge 39, Massachusetts.

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(9) In this paper we do not distinguish between the various extended conformations.

tides is exemplified by those derived from L-cysteine and L-serine. From the data in the table it is apparent that these polypeptides in the oriented solid state exist in the  $\beta$  conformation. In these cases it is not possible to attribute the lack of formation of a helical structure to steric factors. It appears that with these materials the  $\beta$  form is the thermodynamically stable state. It is interesting that the next higher homolog of poly-S-methyl-L-cysteine, namely, poly-L-methionine, does form an  $\alpha$  structure. As has been noted previously,<sup>11</sup> both the esters of poly- $\alpha$ -L-glutamic acid and the esters of its des-methylene homolog, poly- $\alpha$ -L-aspartic acid, form  $\alpha$  structures.

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