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Proteins —Volume III

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INFRARED SPECTRA OF PROTEINS

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The following tables summarize the frequencies and, for ordered solids, the polarization characteristics of conformation-sensitive infrared absorption bands of polypeptides and proteins. In the commonly used rock salt region of the spectra there are two such bands, one at 1650 ± 40 cm^{-1} and a second one at 1530 ± 30 cm^{-1}. The precise frequency and polarization (for ordered solids) of these bands depends on the secondary structure (conformation) of the sample. Table 1 lists the calculated frequencies for unordered solids and for five different ordered conformations in the solid state. Note that each conformation gives rise to more than one component of each band, but some of these predicted components are very weak. The polarization is parallel (∥) or perpendicular (⊥) with respect to the direction of chain propagation.

Table 2 lists the prominent components of absorption bands for the unordered form and five different conformations. In practice conformational information is usually deduced from the frequencies and polarization characteristics of these prominent components.

Table 3 gives comparative data for proteins and polypeptides in the solid state, in H_2O solution, and in D_2O solution. The data are limited to the amide I band because in aqueous solution the amide II band is extremely difficult to observe. Spectra are much easier to obtain in D_2O solution than in H_2O solution because H_2O is less transparent in this region of the infrared spectrum.

Table 1
TABLE OF CALCULATED CHARACTERISTIC POLYPEPTIDE FREQUENCIES,[a] cm^{-1}

Conformation	Amide I[b]	Amide II	Polarization
Unordered	1658	1520	–
Antiparallel-chain	1685 w	1530 s	∥
pleated sheet	1632 s	1510 w	⊥
	1668 vw	1550 w	⊥
Parallel-chain	1648 w	1530 s	∥
pleated sheet	1632 s	1550 w	⊥
Parallel-chain	1648 s	1550 s	⊥, ∥[c]
polar sheet	1632 ww	1530 w	⊥
α-Helix	1650 s	1516 w	∥
	1646 w	1546 s	⊥
Triple helix	1624 vw	1558 s	∥
(polyglycine II)	1648 s	1531 w	⊥

Compiled by H. Susi.

[a]Based on Reference 1.
[b]s, strong; w, weak; vw very weak.
[c]Amide I, ⊥; amide II ⊥.

REFERENCE

1. Krimm, *J. Mol. Biol.*, 4, 528 (1962).

Table 2
TABLE OF PROMINENT AMIDE I AND AMIDE II COMPONENTS,[a] cm^{-1} (SOLID STATE)

Conformation	Strongest amide I component	Strongest amide II component	Weak amide I component
Unordered	1658	1520	–
Antiparallel-chain pleated sheet	1632 ⊥	1530 ∥	1685 ∥
Parallel-chain pleated sheet	1632 ⊥	1530 ∥	–
Parallel-chain polar sheet	1648 ⊥	1550 ∥	–
α-Helix	1650 ∥	1546 ⊥	–
Triple helix (polyglycine II)	1648 ⊥	1558 ∥	–

Compiled by H. Susi.

[a]Based on Reference 1.

REFERENCE

1. Susi, in *Structure and Stability of Biological Macromolecules*, Timasheff and Fasman, Eds., Marcel Dekker, New York, 1969, chap. 7.

Table 3
OBSERVED AMIDE I FREQUENCIES OF PROTEINS IN SOLID STATE AND IN SOLUTION[a]

	D_2O solution	H_2O solution	Solid	Example
Antiparallel-chain pleated sheet	1632	1632	1632	β-Lactoglobulin
	–	–	1630–34	Fibrous proteins
	1675	1690	1690	β-Lactoglobulin
	–	–	1695	Fibrous proteins
α-Helix	1649	–	–	β-Lactoglobulin
	1650	1652	1652	Myoglobin
	–	–	1652	Fibrous proteins
Unordered	1643	1656	–	β-Lactoglobulin (denatured)
	1643	1656	–	α_s-Casein
	–	–	1664	Fibrous proteins

Compiled by H. Susi.

[a]Based on Reference 1.

REFERENCE

1. Susi, in *Structure and Stability of Biological Macromolecules*, Timashoff and Fasman, Eds., Marcel Dekker, New York, 1969, chap. 7.