	Trans-cyclooctene () R	
Pyrolysis of 180 °C-cholesteric A Trimethylcyclooctyl 130 °C-cholesteric B	Yield 46% 52%	e.e. 3.6% 7.1%
162 °C-isotropic phase C	57%	0%
180 °C-cholesteric A	53%	1.9%
185 °C-cholesteric D	61%	1.4%
185 °C-cholesteric E	64%	0%
-Cyclooctene 180 °C-isotropic phase F	62%	0%
	Hexahelicene (+) P	
	Yield	e.e.
27 °C-cholesteric G	75%	0.66% [5]
42 °C-compensated nematic H	75%	0.7%
57 °C-isotropic phase G	75%	0.2%
	 180 °C-cholesteric A 130 °C-cholesteric B 162 °C-isotropic phase C 180 °C-cholesteric A 185 °C-cholesteric E 180 °C-isotropic phase F 27 °C-cholesteric G 42 °C-compensated nematic H 57 °C-isotropic phase G 	Trans-cycloo180 °C-cholesteric A46%130 °C-cholesteric B52%162 °C-isotropic phase C57%180 °C-cholesteric A53%185 °C-cholesteric D61%185 °C-cholesteric E64%180 °C-isotropic phase F62%Hexahelicene27 °C-cholesteric G75%42 °C-compensated nematic H75%57 °C-isotropic phase G75%

A: 3-(p-anisyl)3,5-cholestadiene. B: a mixture of 44.5% of A, 40.2% of C and 15.3% of p-azoxyanisole. C: 3-phenyl-3,5-cholestadiene. D: 3-(p-tolyl)3,5-cholestadiene. E: cholesteryl p-nitrobenzoate. F: compound A diluted by decaline. G: mixture of cholesteryl nonanoate and chloride in the ratio 3/2. H: mixture of cholesteryl chloride and myristate in the ratio 1.75/1.

Empirical Models of Hydration of Small Peptides

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In the course of a general study of peptides hydration, different aspects of solute-solvent interactions have been examined for a cyclic dipeptide C--(L-Thr-L-His). This dipeptide belongs to a series of model peptides containing polar side chains which have been investigated elsewhere.

A qualitative study based on the concept of 'static accessibility' to water, allows to analyse the various processes of hydration. The maximum solvation criterium involves large destabilization of the conformations governed by intramolecular interactions. The amphiphilic character of the solute molecule seems to determine conformations which are in better agreement with those found experimentally. A quantitative study based on energy calculations has been carried out. The stabilities of the hydration sites of the cyclic dipeptide have been evaluated by two empirical potential treatments: the Caillet--Claverie's potential and a simplified method (EMPWI) [1] using a suitable charge distribution. The agreement between the results obtained by the two methods allows to use the simplest model for calculations of more complex molecules.

The conformations of cyclic dipeptides *in vacuo* [2] have been calculated elsewhere and investigated in the solid state by crystallography [3] and in solution by NMR experiments [4]. A general comparison between all these different approaches allows to propose a semi-quantitative picture of the hydration of a small peptide.

References

- 1 F. Vovelle and M. Ptak, Int. J. Peptide Protein Res., 13, 435 (1979).
- 2 M. Genest and M. Ptak, Int. J. Peptide Protein Res., 11, 194 (1978).
- 3 M. Cotrait, M. Ptak, M. Busetta and A. Heitz, J. Am. Chem. Soc., 98, 1073 (1976).
- 4 M. Ptak, M. Dreux and A. Heitz, Biopolymers, 1129 (1978).