

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Folding an infinitely long polypeptide into a helical conformation

JOEL IRETA, MATTHIAS SCHEFFLER, Fritz-Haber Institut der Max-Planck-Gesellschaft, Berlin, Germany — The potential-energy surface and harmonic vibrational analysis of an infinitely long polypeptide are studied using density-functional theory in the Perdew, Burke, and Ernzerhof approximation to the exchange-correlation functional. We find that the π -helix, α -helix, and 3_{10} -helix are stable respect to the fully extended structure (FES) at 0 K, both in right- and left-handed conformations. Accounting for the temperature effects it is found that the left-handed helices are energetically degenerated respect to FES and the right-handed helices slightly more stable than FES, at room temperature. The minimum-energy pathway along the potential-energy surface shows that the barrier to fold a FES into a left-handed helix is at least three times larger than the barrier to fold it into a right-handed helix. This suggests that the very low occurrence of left-handed helices in protein structures is due to both thermodynamic and kinetic effects.

Joel Ireta
Fritz-Haber Institut der Max-Planck-Gesellschaft, Berlin, Germany

Date submitted: 29 Nov 2005

Electronic form version 1.4