Enthalpies of hydrogen-bonds in α-helical peptides. An ONIOM DFT/AM1 study.

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Streszczenie

We report the enthalpy differences between α-helical and extended β-strand conformations of acetyl(Ala)$_n$NH$_2$, for n = 8, 10, 12−17, calculated using molecular (MO) orbital theory from complete vibrational analyses of the optimized species. The calculations used the ONIOM method with B3LYP/D95(d.p) as the high and AM1 as the low levels. The incremental change in enthalpy upon addition of one Ala to a growing β-strand defined using the hypothetical polycondensation reaction, n Ala + CH_3COOH + NH_3 → acetyl(Ala)$_n$NH$_2$ + n H_2O, reaches its asymptotic limit of −1.4 kcal/mol at n = 10, while that for the α-helix continues to increase in magnitude at n = 17. The asymptotic limit of the enthalpic preference of the α-helix over β-strand is estimated to be about 3 kcal/mol, while that for n = 17 is 11.99 kcal/mol or about 0.8 kcal/mol/H-bond, which is similar to measured values for polyalanines of this size in aqueous solution.

Słowa kluczowe

Chemical structure, Energy, Enthalpy, Peptides and proteins

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