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Dimerization of Pyrrole

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Abstract: Accurate ab-inito quantum mechanical calculations of pyrrole dimers are reported. The thermodynamical stabilities of dimers with α - α, α - β, and β - β type linkages are compared in order to predict the possibilities of branching in polypyrroles. Calculations employing large basis sets and including electron correlation effects predict the α - α dimers as the most stable form. However, an α - β type bonding requires only 1.5-2.0 kcal/mol, and the energy necessary to introduce a β - β type bond is 3.6-4.0 kcal/mol. These values show that a high degree of branching is possible even at room temperatures.

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