Synthesis and Solid-State Structures of Alkyl-Substituted 3-Cyano-2-pyridones

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A series of 3-cyano-pyridones carrying a variety of alkyl substituents at C-5 and C-6 has been synthesized and their solid-state structures have been studied. Hydrogen bonding interactions between individual pyridone molecules lead either to the formation of symmetric dimers of the $R_2^2(8)$ type or to helical chains of the C(4) type. Based on known and calculated structures for the 2-pyridone parent system, the solid-state structures can be divided in two groups representing cases with little external influence on the hydrogen bonding array (group A) and those with a larger external influence (group B).

Key words: Hydrogen Bonds, Dimerization, Solid State Structure, Aggregation, Alkylation