Chapter 13 Pyrimidines

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13.1 Introduction

Pyrimidine is a six-membered heterocyclic ring with a structure similar to benzene except that two C–H units are replaced with nitrogen atoms. As a result, its bond lengths and bond angles differ from benzene as shown below. For example, the benzene ring bond length is 1.40 Å with a bond angle of 120 °. The pyrimidine ring is virtually flat, however, the electron distribution is no longer distributed equally at each atom. There is considerable depletion of electron density at the 2-, 4-, and 6-positions; a moderate depletion at the 5-position, and significantly increased electron density at the nitrogen atoms. Pyrimidine is a much weaker base (pK_a 1.31) than pyridine (pK_a 5.2) because the second ring-nitrogen shares the available π-electrons with the first nitrogen. The dipole moment of pyrimidine is measured to be in the range of 2.10 to 2.40 D. Proton NMR and ^{13}C NMR are shown below.