

E0023

Comparative Crystal Structures and Aromaticity Studies of a Diazetidine and a Benzodiazetidine.

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The compounds 1 and 2 (referred to as “diazetidine” and “benzodiazetidine”, respectively) were synthesized as part of an investigation in the nature of aromaticity of cyclic molecules bearing two nitrogen atoms and $4n+2$ electrons which could be in the π system. X-ray diffraction data sets were collected at 150 K using a Bruker *SMART* 1-K CCD single crystal diffractometer and Mo- K_{α} radiation. For 1, 14927 reflections were measured, the space group was found to be $P2_1/m$ with the following unit cell parameters: $a = 3.7770(1)$ Å, $b = 9.4807(2)$ Å, $c = 8.2024(2)$ Å, $\beta = 98.348(1)$, $Z = 2$. The refinement led to $R(F) = 0.0318$ for the strongest 1615 reflns [$F_o > 4\sigma(F_o)$]. For 2, 15598 reflections were measured, the space group was found to be $P2_12_12_1$ with the following unit cell parameters: $a = 7.3068(7)$ Å, $b = 9.8265(0)$ Å, $c = 15.0873(14)$ Å, $Z = 4$. The refinement led to $R(F) = 0.0435$ for the strongest 1329 reflns. The experimental structure of 2 suggests that there is some localization of the π system of the benzene portion of the molecule. However, NICS calculations (RHF/6-311+G**) show that the 4-member rings of both 1 and 2 are nonaromatic, and the aromaticity of the 6-member ring of 2 is virtually the same as in C_6H_6 .

