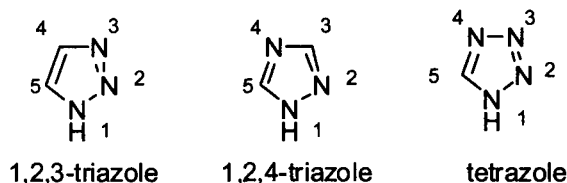


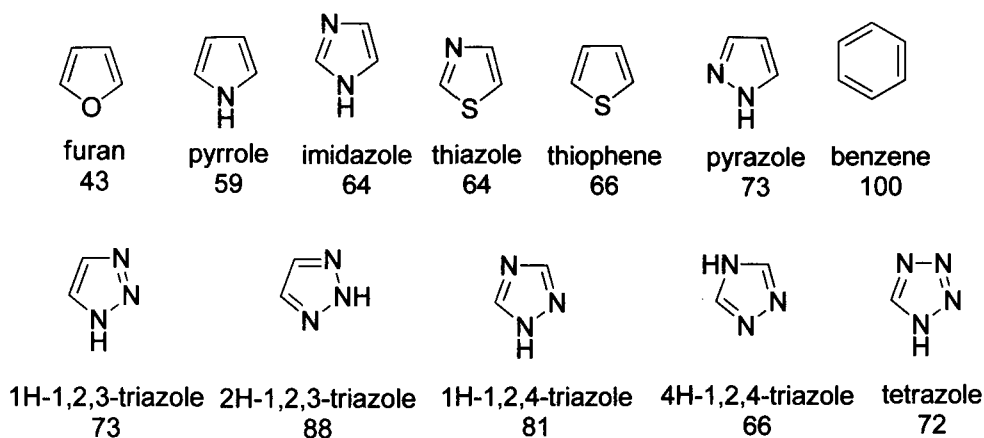
## Chapter 9 Triazoles and Tetrazoles

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### 9.1 Introduction



Triazole refers to either one of two isomeric five-membered ring compounds with molecular formula  $C_2H_3N_3$ . The 1,2,3-triazole is a colorless low melting solid with a melting point of 23–25 °C and a boiling point of 203 °C/752 mmHg, while the 1,2,4-triazole is a colorless crystalline solid with a melting point of 119–121 °C. Both compounds are corrosive and an irritant to both skin and eyes. Triazole is a five-membered aromatic heterocycle with three N heteroatoms. The aromaticity of triazole tautomers was assessed by the Bird indices: 2*H*-1,2,3-triazole (88) was found to be slightly more aromatic than its 1*H*-isomer (73).<sup>1</sup> The small difference in Bird indices supports only a weak influence of the aromaticity and the lower stability of the 1*H*-isomer was explained by the nitrogen lone-pair repulsion that destabilizes cyclic azo-derivatives. Tetrazole has a melting point of 157–158 °C and a Bird index of 72, which is similar to pyrazole (73).



Relative Aromaticity of Five-Membered Ring Heterocycles<sup>1</sup>