An Analysis of the Isomerization Energies of Pyridazine/Pyrimidine, Pyrazole/Imidazole, and 1,2-/1,3-Diazacyclobutadiene with the Turn-Upside-Down Approach

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Abstract

The isomerization energies of 1,2- and 1,3-diazacyclobutadiene, pyrazole and imidazole, and pyridazine and pyrimidine are 10.6, 9.4, and 20.9 kcal/mol, respectively, at the BP86/TZ2P level of theory. These energies are analyzed using a Morokuma-like energy decomposition analysis in conjunction with what we have called turn-upside-down approach. Our results indicate that, in the three cases, the higher stability of the 1,3-isomers is not due to lower Pauli repulsions but because of the more favorable σ-orbital interactions involved in the formation of two C–N bonds in comparison with the generation of C–C and N–N bonds in the 1,2-isomers.[1]

1. Majid El-Hamdi, William Tiznado, Jordi Poater, Miquel Solà. Journal of Organic Chemistry.Submitted.