Semi Empirical Study of a System Containing a Six-membered Ring

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Semi-empirical AM1 SCF-MO calculations have been used to find the structure optimization and conformational interconversion pathways of a system containing a six-membered ring. The system has the two symmetrical energy-minimum conformations, chair and twist. The chair conformation has the most stable geometry. Some quantum parameters such as HOMO and LUMO energy, the chemical hardness and chemical potential are discussed.

Key words: Six-membered Rings; Conformational Analysis; AM1 Calculations;
                    Quantum Chemical Study.