**Effect of Lone Pairs on the Conformational Energies of Piperazine and Morpholine Derivatives**

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Conformational analysis of non-aromatic six-membered heterocyclic rings is an active field of research and includes the study of the axial/equatorial equilibrium of substituted cyclohexanes and heterocycles and the influence of steric and stereoelectronic effects on the conformational properties.[1,2] In the present study, we succeeded in identifying the following conformations on the Potential Energy Surface (P.E.S.) of the cyclohexane and its 1,4-diheteroanalogues (1-4).



|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Compound** | **X1** | **X2** |  |
|  | 1 | CH2 | CH2 |  |
|  | 2 | N-H | N-H |  |
|  | 3 | N-H | N-CH3 |  |
|  | 4 | N-H | O |  |

We investigated these conformations using Density Functional Theory (B3LYP/6-31+G\*) and determined their energies. These relative energies could be rationalised on the basis of 1,3-diaxial and lone-pair-lone-pair interactions.

(1) Juaristi,E.; Cuevas,G.; *Chem.Phys.Chem.,***1992**,*48*(24), 5019–5087.

1. Booth,H.; Lemieux,R.U.; *Canad. J . Chem****.,* 1971,** *49*,776.

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