Abstract

Indole is a benzopyrrole resulting from the fusion of a benzene ring on (α) and (β) carbons of pyrrole. It is a substance that is related to a great number of natural compounds, which play a considerable biochemical role.

The theoretical study of Fischer reaction, which is a general way of indole synthesis, was carried out by means of ab-initio and semi-empirical calculations. Three mechanisms were proposed for this reaction.

Energies and heats of formation obtained are based on primarily on geometries optimization calculations, resulted initially from a multi-conformational research on different hypothetical intermediates in the three mechanisms. Transition states calculations allows the clarification of Fischer reaction regioselectivity

The comparative theoretical study made on the proposed mechanisms, shows that the Robinson's mechanism is the most favourable.

Key words : Fischer indole synthesis, ab-initio and semi-empirical calculations, geometries optimization calculations, transition states calculations.

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