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Perkin Transactions 2

Physical Organic Chemistry

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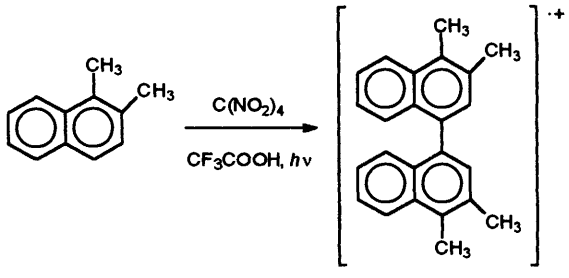

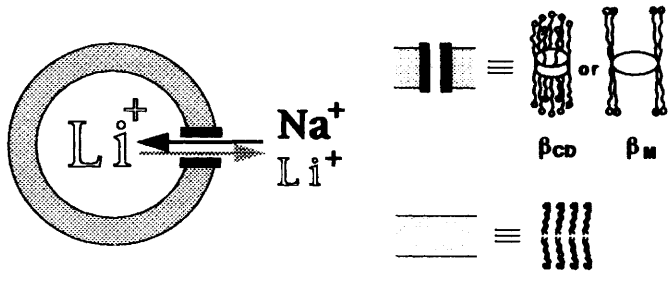

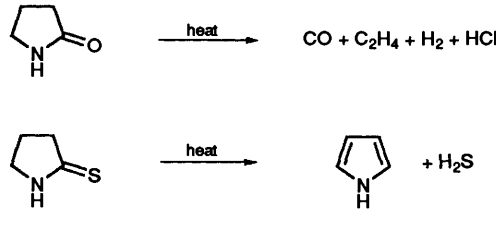

The molecular electrostatic potentials of a series of imidazoles and pyrazoles have been mapped to their respective pK_a values and proton affinities using a backpropagation neural network. Predictions made by the trained network remain sensitive to the quality of the semiempirical and *ab initio* methods used.

6-31G* > 3-21G ≫ MNDO > STO-3G > AM1 ≫ PM3

AUTHOR INDEX

NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.

International Society of Heterocyclic Chemistry

HONG KONG INTERNATIONAL SYMPOSIUM ON HETEROCYCLIC CHEMISTRY

August 13-16 1995

Department of Chemistry, The University of Hong Kong, Hong Kong

Topics

*Biologically Active Heterocycles
*Heterocyclic Ligands in Asymmetric Synthesis
*New Methods of Heterocyclic Synthesis

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H. Takaya	Kyoto University
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