The Mean Dissociation Enthalpy of the N-O Bond for 2,2´-Bipyridine N,N´-Dioxide

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A large variety of organic compounds contain terminal (N-O) dative-covalent bonds (amine-oxides, pyridine N-oxides, nitrile N-oxides, nitrones, azoxycompounds, furoxans, azo-N,N´-dioxides, quinoxaline 1,4-dioxides, or pyrazine 1,4-dioxide), and they have the potential to act as oxidizing agents, leading to the large variety of their applications. Recently, a lot of attention has been devoted to the study of aromatic heterocyclic di-N-oxides, particularly due to the fact that they are thought to be involved in selective biological activities.

The thermodynamic properties of compounds play a critical role to understand their chemical behavior. During the last decade, energetic studies have being expanded in order to update the data for several types of compounds with terminal N-O bonds [1], as the result of experimental thermochemical measurements performed for those oxygenated compounds, RN-O, and, whenever possible, the measurement of the thermochemical properties for the corresponding compounds without the N-O bonds, RN. The dissociation enthalpy of the (N-O), being very influenced by the immediate environment of the bond, can be derived from the enthalpies of formation of RN-O, RN and O, in the gaseous state.

The present work reports the thermochemical study of a new compound, the 2,2´-bipyridine N,N´-dioxide. The values of the enthalpy of formation, in the condensed state, and the enthalpy of sublimation, measured by static bomb calorimetry and Knudsen effusion technique, respectively, are combined to derive the standard molar enthalpy in the gaseous state of compound. The standard molar mean dissociation enthalpy of the (N-O) bonds is derived as one half of the enthalpy of the reaction described by the following equation, with the reactants and products in their standard states.

$$\text{2,2´-bipyridine N,N´-dioxide (g)} \leftrightarrow \text{2,2´-bipyridine (g)} + 2\ \text{O (g)}$$

Thanks are due to Fundação para a Ciência e Tecnologia, F.C.T., Lisbon, Portugal, for financial support to Centro de Investigação em Química. Thanks are also due to F. C. T. and to FEDER for financial support to the research project (POCTI / 44471 / QUI / 2002).

[1] W. E. Acree, Jr., M. D. M. C. Ribeiro da Silva, G. Pilcher, *J. Phys. Chem. Reference Data*, **34**, 553 (2005).