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Research Article

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Formation and phase transition enthalpies for captopril

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Abstract Combining solution calorimetry data with quantum chemical thermochemistry, a series of thermochemical parameters for captopril were obtained, as follows: $\Delta_{sol}H^{\theta}$ (in water) = 12.26 ± 0.4kJmol^{-1}; $\Delta_{solv}H^{\theta}$= -53.43kJmol^{-1};$\Delta_{cr}{}^{g}H^{\theta}$ = 65.70 kJmol^{-1}, $\Delta_{cr}{}^{l}H^{\theta}$= 19.53kJmol^{-1};$\Delta_{l}{}^{g}H^{\theta}$= 46.17 kJmol^{-1};$\Delta_{f}{}^{g}H^{\theta}$= -623.10 kJmol^{-1}, $\Delta_{f}{}^{l}H^{\theta}$ = -576.93 kJmol^{-1}; $\Delta_{f}{}^{cr}H^{\theta}$= -557.40 kJmol^{-1}; C_v= 231.72 JK^{-1}mol^{-1}andC_p= 240.03 JK^{-1}mol^{-1}.

Keywords Captopril; Solution Calorimetry; Thermochemistry; Formation enthalpies

Introduction

Captopril, $C_9H_{15}NO_3S$ (CAS nº 62571-86-2), (2S)-1-[(2S)-2-methyl-3-sulfanylpropanoyl]pyrrolidine-2-carboxylic acid,(Fig. 1) , is anorally active antihypertensive agent [1]widely utilized in the treatment of hypertension, congestive heart failure and heart attack in both, mono and combination therapy.

However, thermochemical data for captopril are very scarce. In the present work, solution calorimetry data and quantum chemical thermochemistry, are combined in order to obtain a set of thermochemical parameters for captopril.

Experimental Work

All quantum thermochemical calculation were performed by using Spartan´16[2] at DFT/EDF2/6-31G* level of theory. This computation were employed to calculate the total energy (in vacuum and water), the $\Delta_{f}{}^{g}H^{\theta}$ and C_v values.

Calorimetric measurements (solution calorimetry; ampoule break procedure; water as solvent)were performed in a LKB2277 calorimeter.

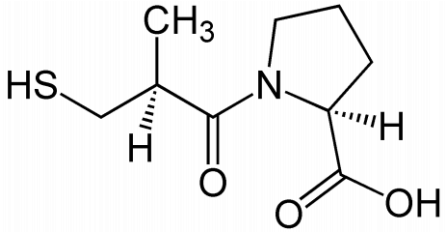

Figure 1: Structural formula of Captopril

Results and Discussion

The obtained thermochemical parameters are summarized in Table 1. The experimental $\Delta_{soln}H^{\theta}$ shown in Table 1 is a mean value obtained over five measurements. The $\Delta_{solv}H^{\theta}$ value was obtained by the total energy values in water and vacuum.

Table 1: Thermochemical parameters for captopril

Total energy/au (in vacuum)	-1030.22390
Total energy/au (in water)	-1030.24425
$\Delta_{solv}H^{\theta}$/kJmol^{-1}	-53.43
$\Delta_{soln}H^{\theta}$/kJmol^{-1} (in water)	12.26 ± 0.4
$\Delta_f{}^{g}H^{\theta}$/kJmol^{-1}	-623.10
$\Delta_f{}^{l}H^{\theta}$/kJmol^{-1}	-576.93
$\Delta_f{}^{cr}H^{\theta}$/kJmol^{-1}	-557.40
$\Delta_{cr}{}^{g}H^{\theta}$/kJmol^{-1}	65.70
$\Delta_l{}^{g}H^{\theta}$/kJmol^{-1}	46.17
$\Delta_{cr}{}^{l}H^{\theta}$/kJmol^{-1}	19.53
C_v/ JK^{-1}mol^{-1}	231.72
C_p/ JK^{-1}mol^{-1}	240.03

Using the C_p value shown in Table 2, and taking into account that the melting temperature for captopril is 379.5 K [3], a melting enthalpy ($\Delta_{cr}{}^{l}H^{\theta}$) of 19.53 kJmol^{-1} can be obtained, in very good agreement with the 20.28 kJmol^{-1} experimental value obtained by DSC [3].

It is known [4,5] that $\Delta_{cr}{}^{g}H^{\theta} = \Delta_{soln}H^{\theta} - \Delta_{solv}H^{\theta}$. Hence, for captopril, a $\Delta_{cr}{}^{g}H^{\theta}$ value of 65.70 kJmol^{-1} is obtained. From this and the $\Delta_{cr}{}^{l}H^{\theta}$ value, $\Delta_l{}^{g}H^{\theta}$ can be calculated as 46.17 kJmol^{-1}.

By using the $\Delta_{cr}{}^{g}H^{\theta}$, $\Delta_{cr}{}^{l}H^{\theta}$, $\Delta_l{}^{g}H^{\theta}$ and the $\Delta_f{}^{g}H^{\theta}$values, the $\Delta_f{}^{l}H^{\theta}$ and $\Delta_f{}^{cr}H^{\theta}$ for captopril can be calculated as -576.93 and-557.40kJmol^{-1}, respectively.

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