Chemistry Research Journal, 2016, 1(5):26-27

Available online www.chemrj.org

Research Article

ISSN: 2455-8990
CODEN(USA): CRJHA5

Vaporization and Gaseous Phase Formation Enthalpies for 4-Nitrobenzyl alcohol by Quantum Chemistry Composite and Semi-empirical Methods

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Abstract In the present work it is presented, for the first time, the standard gaseous formation enthalpy and the vaporization enthalpy for 4-Nitrobenzyl alcohol. Such thermochemical data wereobtained byquantum chemistry composite and semi-empirical methods, as well as experimental data from literature. The $\Delta_f H_m^0$ $(_g)$ and $\Delta_{vap} H_m^0$ values (kJ mol^{-1}) are 115.07 ± 0.73 and 66.43 ± 0.73, respectively.

Keywords 4-Nitrobenzyl alcohol, Gaseous formation enthalpy, Vaporization enthalpy, Quantum chemical calculations

Introduction

The combustion and solid state formation enthalpies, as well as low-temperature heat capacities for 4-Nitrobenzyl alcohol ($C_7H_7NO_3$; 4-NBA, CAS Nº 619-73-8) have been measured by combustion calorimetry and precision automated adiabatic calorimeter experiments [1], respectively. In the present work, the gaseous formation enthalpy for 4-Nitrobenzyl alcohol is calculated by quantum chemistry composite, as well as semi-empirical methods. Based on this value and on experimental data [1] the standard vaporization enthalpy for 4-NBA is calculated.

Experimental

Gaseous phase formation enthalpy for 4-nitrobenzyl alcohol was calculated by using Spartan´14 (version 1.1.8) [2].The enthalpy of formation in gaseous phase was provided by the T1 recipe, as well as semi-empirical (MP6 and RM1) methods. By using the gaseous formation enthalpy values, as well as the experimental melting enthalpy value [1], the vaporization enthalpy was calculated. The main characteristic of T1 is that it follows the G3(MP2) recipe, substituting an HF/6-31G* for the MP2/6-31G* geometry, eliminating both the HF/6-31G* frequency and QCISD(T)/6-31G* energy and approximating the MP2/G3MP2 large energy using dual basis set RI-MP2 techniques [3].

Results and Discussion

The melting enthalpy at the melting temperature was measure as 20.97 kJ mol^{-1}. $SE^{\#}$ = Semi-Empirical. As can be verified, the T1 and semi-empirical gaseous phase formation values are in good agreement with each other. Taking this value, as well as the experimental value to the melting enthalpy [1], the vaporization enthalpy was calculated.
The obtained results are summarized in Table 1.

Table 1: Calculated and experimental values for combustion and formation enthalpies (kJ mol^{-1}) for 4-nitrobenzyl alcohol.

	$\Delta_c H_m^0$ (s)	$\Delta_f H_m^0$ (s)	$\Delta_f H_m^0$ (l)	$\Delta_f H_m^0$ (g)	$\Delta_{vap} H_m^0$
Exp. [Ref. 1]	-3548.49 ± 1.47	-206.49 ± 2.52	-181,51*	_	_
Calc. (T1)				-114.38	67.13
Calc. SE# (MP6)				-115.00	66.51
Calc. SE# (RM1)				-115.84	65.67
			Average	115.07 ± 0.73	66.43 ± 0.73

*This value it is not directly provided by the authors. It was calculated by using the (H_{375k}-$H_{298.15K}$) - (H_{345K}-$H_{298.15K}$) = 35.62-10.64 = 24.97 kJ mol^{-1} as the standard melting enthalpy (the measured melting temperature was 366.4 K).

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