HEAT CAPACITIES AND FORMATION FUNCTIONS OF SOME 1,5-DIAZABICYCLO[3.1.0]HEXANES

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The compounds studied in this work belong to the class of diaziridine derivatives. Compounds of this class play an important role in various fields of science and technology.

The heat capacity of three diaziridine derivatives 6-phenyl-, 6-(4-methoxyphenyl)- and 6-(4-ethoxyphenyl)-1,5-diazabicyclo[3.1.0]hexanes (PDABH, MeOPDABH and EtOPDABH, respectively) was determined by low-temperature adiabatic calorimetry.

The studied compounds were synthesized and purified. The structure of the obtained compounds was monitored by spectroscopic methods. The purity of the sample of each compound was assessed by elemental analysis and by gravimetric analysis of combustion products.

The heat capacity of PDABH and MeOPDABH was determined in the temperature range of 6–350 K, where the calorimetric cell was cooled with liquid helium and nitrogen. The heat capacity of EtOPDABH was determined in the range of 80–350 K; its heat capacity in the temperature range of 5–80 K was estimated empirically by the Kelly method. Extrapolation to 0 K was performed using the Debye cube law. The data obtained in the temperature range of 5–350 K were smoothed by power polynomials of the $C_{p,m}(T) = \sum A_i\,(T)^i$, where A_i are the polynomial coefficients and i is the polynomial degree. By integrating these polynomials, the main thermodynamic functions, S^0_{m}, $\Delta^{\mathrm{T}}_0 H^0_{\mathrm{m}}$, $\Delta^{\mathrm{T}}_0 G^0_{\mathrm{m}}$, and the entropy of formation at 298.15 K, $\Delta_{\mathrm{f}} S^0_{\mathrm{m}}$, were found.

Using the obtained experimental data and literature data on the enthalpies of formation, $\Delta_{\mathrm{f}} H^{\circ}_{\mathrm{m}}$, the Gibbs free energy of formation was calculated, $\Delta_{\mathrm{f}} G^0_{\mathrm{m}}$ (Table).

Thermodynamic functions at 298.15 K of the studied compounds

	PDABH	MeOPDABH	EtOPDABH
$C_{\mathrm{p,m}}$(cr)/ J K^{-1} mol^{-1}	201.18 ± 0.40	241.97 ± 0.48	270.37± 0.81
$\Delta_{\mathrm{f}} S^0_{\mathrm{m}}(cr)$/ J K^{-1} mol^{-1}	-1017.8 ± 1.4	-819.1±1.3	-1118.4 ± 3.1
$\Delta_{\mathrm{f}} G^0_{\mathrm{m}}(cr)$/ kJ mol^{-1}	373.1 ± 4.1	490.6±1.8	376.4 ± 2.8
$\Delta_{\mathrm{f}} H^{\circ}_{\mathrm{m}}$(cr)/ kJ mol^{-1}	246.4 ± 1.8 [1]	69.6 ± 4.1 [2]	43.0 ± 2.6

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