FEATURES OF VAPORIZATION AND THERMODYNAMIC PROPERTIES OF SOME LOW-VOLATILE AMINO ACIDS

Korobov M.A., Kaplin A.S., Motalov V.B., Dunaev A.M.
Ivanovo State University of Chemistry and Technology
153000, Ivanovo, Sheremetevskiy ave., 7

The work presents the results of a study of low-volatile proteinogenic amino acids L-histidine, L-aspartic acid, L-asparagine, L-glutamine, L-glutamic acid, L-lysine, and L-arginine using Knudsen effusion mass spectrometry. There are no sublimation thermodynamics data for these compounds. Commercial samples (Aladdin, Macklin; mole fraction 0.99) were loaded into a Knudsen cell (Mo; an evaporation-to-effusion area ratio of ~400) coupled with a MI1201 single-focusing magnetic mass spectrometer.

The main task of the study was to select experimental conditions (temperature range, heating duration) for congruent sublimation. The thermal stability of the substances was monitored using IR spectroscopy and visual observation. Most of the studied amino acids were found to decompose at any conditions. Only L-histidine (L-His) and L-aspartic acid (L-Asp) could be sublimed congruently in the limited temperature and time ranges. Due to these limitations, the saturated vapor pressure could not be determined by classical Knudsen effusion method. Therefore, the pressure was obtained by a mass spectrometric method of ion current comparison; L-methionine [1] was used as a standard. The vapor pressures for L-histidine and L-aspartic acid were fitted by equations presented in Table.

Saturated vapor pressure equations ln(p, Pa), temperature range ΔT, K, enthalpy of sublimation $\Delta_{sub}H°$, kJ·mol^{-1} at 298.15 K

Subst.	$\ln p = -a/T+b$		ΔT	$\Delta_{sub}H°$(298.15 K)	
	a	b		2nd law	3rd law
L-His	21983 ± 485	42.411 ± 1.029	448-480	184.7 ± 4.4	183.5 ± 4.2
L-Asp	22350 ± 600	43.757 ± 1.351	420-450	186.8 ± 5.2	183.2 ± 3.6

Sublimation enthalpy was obtained by the methods of the second and third laws of thermodynamics; see Table. The data obtained by the independent approaches agree within the uncertainties. The third law values were used in further derivation of the formation enthalpies for the gaseous amino acids: −283.2 ± 5.0 kJ·mol^{-1} (L-His), and −791.1±4.6 kJ·mol^{-1} (L-Asp); they agree reasonably with the corresponding values from [2]: −289.4 ± 4.0 kJ·mol^{-1} (L-His) and −796.8 ± 4.0 kJ·mol^{-1} (L-Asp), obtained by isodesmic reaction approach.

1. Motalov, V. B.; Korobov, M. A.; Dunaev, A. M.; Dunaeva, V. V.; Tyunina, E. Y.; Kudin, L. S. J. Chem. Eng. Data 2022, 67, 1326–1334.
2. Dorofeeva, O. V.; Ryzhova, O. N. J. Phys. Chem. A 2014, 118, 3490–3502.
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