Heat Capacity and Derived Thermodynamic Properties of Rimantadine in the Condensed State Between T = (5 and 370) K

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Rimantadine (1-(1'-adamantyl)ethylamine hydrochloride) is widely used for treating and preventing infections caused by the flu (influenza A). The study of its thermodynamic properties is necessary for optimization of the conditions of its manufacturing. In this work the investigation of the low-temperature heat capacity of crystalline rimantadine has been carried out.

A commercial sample of rimantadine with its mass fraction purity >0.99 was additionally exposed to vacuum at ambient temperature in order to remove volatile impurities and moisture.

The heat capacity of crystalline rimantadine in the range from (5 to 370) K was measured with an automatic vacuum adiabatic calorimeter with a titanium calorimetric cell of 1 cm^3 volume. The device uncertainty of the measurements was found to be 0.4 % from (20 to 370) K. When temperature decreases below 20 K the error rises but does not exceed 2 % from (5 to 10) K.

A reproducible hump-shaped anomaly between (170 and 250) K was revealed in the curve of the temperature dependence of the heat capacity. The heat capacity increased all over the region and exceeded the 'normal' heat capacities of the compound by <10%. The excess enthalpy and entropy of the phase anomaly obtained by integration amounted to ΔH = (248 +/- 5) J/mol and ΔS = (1.16 +/- 0.02) J/(K mol). Possible explanations of such behavior could be gradual development of the hindered rotation of NH_3-top or slight changes of the crystal structure.

The standard thermodynamic functions of crystalline rimantadine between (5 and 370) K were calculated on the base of the smoothed values of the heat capacity. The derived thermodynamic properties at T = 298.15 K were;

$$C_{p,m} = (268.1 \pm 1.1)\ \mathrm{J/(K\ mol)}$$
$$S_T - S_0 = (281.3 \pm 1.2)\ \mathrm{J/(K\ mol)}$$
$$H_T - H_0 = (41.99 \pm 0.17)\ \mathrm{kJ/mol}$$