

## Experimental and Theoretical Study of Thermodynamic Properties of Levoglucosan

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Levoglucosan (1,6-anhydro- $\beta$ -D-glucopyranose) is a carbohydrate formed during thermal decomposition of cellulose and cellulosic materials. It can be used for production of biodegradable polymers, antibiotics and other materials. In this work, we present the results of the comprehensive study of thermodynamic properties for this substance. Heat capacity of levoglucosan was measured over the temperature range (5 to 370) K by adiabatic calorimetry. The temperatures and enthalpies of a transition into the plastic crystal phase and fusion determined by DSC were in good agreement with literature. The obtained results allowed us to calculate thermodynamic properties of crystalline levoglucosan in the temperature range (0 to 384) K. Enthalpy of sublimation for the low-temperature crystal phase was derived from the temperature dependence of saturated vapor pressure from the Knudsen effusion method. Thermodynamic properties of levoglucosan in the ideal-gas state were found by methods of statistical thermodynamics using molecular parameters from quantum chemical calculations. A theoretical value of the standard entropy at  $T = 370$  K for gaseous levoglucosan agreed well with that derived from the experimental data. Enthalpy of formation of the crystalline compound was found from experiments in a combustion calorimeter. The gas-phase enthalpy of formation obtained at the G4 level of theory was too negative compared to that found from the experimental data even if isodesmic reactions were used. Thermodynamic analysis of equilibria of levoglucosan formation from cellulose, starch and glucose demonstrated that this process is possible only if the product is formed in the gas phase and then quickly removed from the reaction zone.

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