

# Thermodynamics of the Antiviral and Antiparkinsonian Drug Amantadine Hydrochloride: Condensed State Properties and Decomposition

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## Abstract

© 2017 American Chemical Society. Heat capacities of the antiviral and antiparkinsonian drug amantadine hydrochloride in the crystalline state were measured by adiabatic and differential scanning calorimetry in the temperature range from 5 K to 470 K. Two unresolved low-enthalpy solid-to-solid phase transitions with peak maxima at 120.0 K and 123.1 K were detected. Thermodynamic functions for crystalline amantadine hydrochloride were derived from the data obtained. Decomposition of amantadine hydrochloride was studied by the Knudsen effusion method. Quantum chemical calculations supported completeness of the amantadine hydrochloride ionic pair disintegration under the effusion conditions. A data treatment model considering the difference in effusion rates of the decomposition products, anisotropy failure in the vicinity of the orifice, and vapor undersaturation in the effusion cell was developed. Thermodynamic parameters for the decomposition were thus derived and shown to be consistent with available literature data on decomposition of similar organic hydrochlorides and with the entropy of reaction calculated directly from the entropies of the decomposition reaction participants. The obtained set of thermodynamic properties of the medication is expected to provide new key information necessary for optimization of production and storage conditions. (Graph Presented).

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