

Thermodynamic Properties of 1,1'-biadamantane

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Thermodynamic properties of 1,1'-biadamantane have been determined. 1,1'-Biadamantane was prepared by Wurtz reaction from 1-bromadamantane and sodium in toluene. The sample was purified by double crystallization from toluene and subsequent sublimation in vacuum. The final mass fraction purity of the sample was determined by g.l.c. to be 0.999.

The low-temperature heat capacity in the solid state in the temperature range (5 to 370) K were measured in a vacuum adiabatic calorimeter. The heat capacities in the range (290 to 610) K were measured with a scanning calorimeter of the heat-bridge type. Two solid-to-solid transitions were discovered at 336 and 531 K. The melting temperature of 1,1'-biadamantane was 591 K. Standard molar thermodynamics functions of the crystal at $T = 298.15$ K were obtained from the experimental heat capacities: heat capacity was (335.3 ± 1.3) J/K/mol; standard entropy was (298.9 ± 1.3) J/K/mol; standard enthalpy was (45.88 ± 0.20) kJ/mol. The vapor pressures measured by the integral effusion Knudsen method in the range (392.8 to 442.7) K were fitted by the equation $\ln(p/\text{Pa}) = (32.82 \pm 0.37) - (13126 \pm 153)(K/T)$. According to this equation, the molar enthalpy of sublimation was (109.1 ± 1.3) kJ/mol at $\langle T \rangle = 417.8$ K. The enthalpy of combustion of 1,1'-biadamantane was determined in a bomb calorimeter with an isothermal water shell. Thermodynamic properties of 1,1'-biadamantane in the ideal gas state were calculated by the statistical thermodynamic methods.