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论文

烟酸钠$Na(C_6H_4NO_2)(s)$的低温热容和热化学

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摘要:

选择分析纯烟酸和无水醋酸钠作为反应物, 用室温固相合成方法合成了无水烟酸钠. 利用FTIR和X射线粉末衍射等方法进行了表征, 利用化学分析和元素分析确定其组成为$Na(C_6H_4NO_2)$. 用精密自动绝热热量计测量其在78~400 K温度区间的低温热容. 研究结果表明, 该化合物在此温度区间无热异常现象发生. 用最小二乘法将实验摩尔热容对温度进行拟合, 得到热容随温度变化的多项式方程. 用此方程进行数值积分, 得到在此温度区间每隔5 K的舒平热容值和相对于298.15 K时的热力学函数值. 在此基础上, 通过设计合理的热化学循环, 选用1 mol/L NaOH溶液作为量热溶剂, 利用等温环境溶解-反应热量计分别测得固相反应的反应物和产物在所选溶剂中的溶解焓, 得到固相反应的反应焓. 最后, 计算出无水烟酸钠的标准摩尔生成焓为: $\Delta_f H_m^0[Na(C_6H_4NO_2), s]=-(548.96\pm1.11)$ kJ/mol.

关键词: 烟酸钠 绝热量热法 低温热容 溶解-反应量热法 标准摩尔生成焓

Low-temperature Heat Capacities and Thermochemistry of Sodium Nicotinate $Na(C_6H_4NO_2)(s)$

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Abstract:

Nicotinic acid and sodium acetate were chosen as the reactants, a compoundsodium nicotinate was synthesized by the method of room temperature solid phase synthesis. FTIR and X-ray powder diffraction technique were applied to characterize its structure, and its composition was determined to be $Na(C_6H_4NO_2)$ by chemical and elemental analyses. Low-temperature heat capacities of the compound were measured by a precision automated adiabatic calorimeter over the temperature range from 78 K to 400 K. A polynomial equation of the heat capacities as a function of the temperature was fitted by the least square method. On the basis of the fitted polynomial, the smoothed heat capacities and thermodynamic functions of the compound relative to the standard reference temperature 298.15 K were calculated at the interval of 5 K. A reasonable thermochemical cycle was designed on the basis of the solid phase preparation reaction of the substance, 1 mol/L NaOH solution was chosen as the calorimetric solvent, and the standard molar enthalpies of dissolution for the reactants and products of the solid phase reaction in the selected solvents were measured by an isoperibol solution-reaction calorimeter, respectively. In addition, the enthalpy change of the solid phase reaction was determined to be (23.232±0.509) kJ/mol from the data of the above standard molar enthalpies of dissolution. Eventually, the standard molar enthalpy of formation of sodium nicotinate was derived to be: $\Delta_f H_m^0[Na(C_6H_4NO_2), s]=(-548.96\pm1.11)$ kJ/mol, by the combination of the enthalpy change of the solid phase reaction with other auxiliary thermodynamic quantities.

Keywords: Sodium nicotinate Adiabatic calorimetry Low-temperature heat capacity Solution-reaction calorimetry Standard molar enthalpy of formation

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