Full Paper

八水氢氧化钡**Ba(OH)$_2$×8H$_2$O(s)**的低温热容和热力学性质

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摘要　　八水氢氧化钡Ba(OH)$_2$×8H$_2$O(s)
因相变潜热大使其作为胶囊化相变储能材料的应用已受到人们的广泛关注, 但是其热力学性质数据依然缺乏.
本文利用精密自动绝热量热计准确测定了八水氢氧化钡Ba(OH)$_2$×8H$_2$O(s)在78－370 K温区的低温热容.
在热容曲线上发现在345－356 K温区有一个明显的吸热峰. 通过分析发现,
这个峰对应着样品的熔化和第一次脱水的焓变之和. 用最小二乘法将78－345 K和356－369
K两个温区的摩尔热容实验值分别拟合成了热容对温度的多项式方程. 通过在温区298－370
K内的三次重复热容测量，得到了相转变所对应的峰温、焓变和熵变分别为：(355.007 ± 0.076) K, (73.506 ±
0.011) kJ×mol^{-1} and (207.140 ± 0.074) J×K^{-1}×mol^{-1}.
通过两个热容多项式方程的数值积分计算出了这个化合物的舒平热容值和相对于298.15 K的热力学函数,(H_T -
$H_{298.15K}$) 和 (S_T - $S_{298.15K}$). 另外, 利用DSC和TG-DTG技术对这个化合物的热分解行为进行了进一步的研究.
从实验结果的分析知, 这个化合物的相转变的潜热之所以变得比正常化合物的大,
主要原因是它融化过程中伴随着7 H$_2$O 和脱出.

关键词　　绝热量热法, 热容, 相变, 热力学函数, 热分解

分类号

Low-Temperature Heat Capacities and Thermodynamic Properties of Octahydrated Barium Dihydroxide, Ba(OH)$_2$•8H$_2$O(s)

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Abstract Low-temperature heat capacities of octahydrated barium dihydroxide, Ba(OH)$_2$•8H$_2$O(s), were measured by a precision automated adiabatic calorimeter in the temperature range from T＝78 to 370 K. An obvious endothermic process took place in the temperature range of 345—356 K. The peak in the heat capacity curve was correspondent to the sum of both the fusion and the first thermal decomposition or dehydration. The experimental molar heat capacities in the temperature ranges of 78—345 K and 356—369 K were fitted to two polynomials. The peak temperature, molar enthalpy and entropy of the phase change have been determined to be (355.007±0.076) K, (73.506±0.011) kJ•mol^{-1} and (207.140±0.074) J•K^{-1}•mol^{-1}, respectively, by three series of repeated heat capacity measurements in the temperature region of 298—370 K. The thermodynamic functions, (H_T－$H_{298.15 K}$) and (S_T－$S_{298.15 K}$), of the compound have been calculated by the numerical integral of the two heat-capacity polynomials. In addition, DSC and TG-DTG techniques were used for the further study of thermal behavior of the compound. The latent heat of the phase change became into a value larger than that of the normal compound because the melting process of the compound must be accompanied by the thermal decomposition or dehydration of 7H$_2$O.

Key words   adiabatic calorimetry   heat capacity   phase transition   thermodynamic function   thermal decomposition

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