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Thermochemistry of guest-free melanophlogite

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ABSTRACT

Melanophlogite is a naturally occurring clathrasil possessing a framework of linked silicate tetrahedra surrounding small, isolated cages, which can host small molecules. The energetics of a guest-free natural sample was determined by oxide-melt solution calorimetry. Melanophlogite is energetically metastable with respect to α-quartz by 9.5 ± 0.5 kJ/mol, a value similar to that for amorphous silica and for synthetic small-pore zeolitic silicas (Petrovic et al. 1993, Piccione et al. 2001). Thus, its occurrence in nature, for example in environments where it can occlude volcanic gases, is reasonable on energetic grounds.

Molecular modeling of the internal pore volume of melanophlogite confirms that this enthalpy follows the trend previously established for a variety of silica zeolites, which defines an internal surface energy of 0.093 ± 0.010 J/m^2, similar to that of the external surface energy of amorphous silica. Thus melanophlogite, despite its unique topology and isolated cages, behaves energetically as predicted from the enthalpies of more-open zeolitic frameworks.