Ba₈{Cu,Zn,Pd}_xGe_{46-x} CLATHRATES

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Formation, crystal chemistry and physical properties were investigated for the solid solutions $Ba_8Cu_xGe_{46-x-v}\Box_v$, $Ba_8Pd_xZn_yGe_{46-x-y-v}\Box_v$, and $Ba_8Cu_xZn_yGe_{46-x-y-v}\Box_v$ (\Box is a vacancy). The phase boundary of the clathrate phases was determined from metallography, EMPA and X-ray powder and X-ray single crystal data. Structural investigations for all specimens confirm isotypism with the cubic primitive clathrate type I structure (lattice parameters a = ~1.1 nm and space group type Pm-3n). Temperature dependent X-ray spectra and the heat capacity define a low lying, almost localized, phonon branch. Studies of transport properties evidence electrons as the majority charge carriers in the system. Thermal conductivity exhibits a pronounced low temperature maximum, dominated by the lattice contribution, while at higher temperatures the electronic part gains weight.

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