

Ag, Cu, Hg, Pt, and Te substitutions in the synthetic analogue of palladseite, Pd₁₇Se₁₅: an experimental mineralogical study

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Palladseite, Pd₁₇Se₁₅ was described as a new mineral by Davis et al. [1] from residual concentrates from gold washing at Itabira, Minas Gerais, Brazil. Palladseite has an ideal chemical composition of Pd₁₇Se₁₅. Ag, Cu, Hg and Pt are common elements to occur in the palladseite structure and are regarded as non-essential elements for palladseite; e.g. Cabral and Lehmann [2] indicated 3.89 wt.% of Hg and 4.43 wt.% of Ag for palladseite-like mineral from Gongo Soco, Brazil. Crystal structure of synthetic Pd₁₇Se₁₅ was solved by Geller [3].

In order to explain the incorporation of reported significant amounts of Ag, Cu, Hg, Pt and Te and define the range of their solubility in the palladseite structure, an experimental study of solubility of above-mentioned elements in the synthetic analogue of palladseite at 400 °C was performed. Silica glass tube technique was used. To document the impact of these elements on the palladseite crystal structure, Rietveld refinement analysis of powder X-ray diffraction data of experimental products was carried out.

Palladseite (Pd₁₇Se₁₅) crystallizes in the *Pm-3m* space group (*a* = 10.607 Å) and contains four Pd and three Se sites. It has a framework crystal structure formed by three types of polyhedra: [PdSe₆] octahedra, [PdSe₄] squares and [PdSe₄] flattened tetrahedra. Three way of substitution mechanism were revealed to occur in the palladseite structure. Cu, Ag and Hg enter the palladseite structure in a significant amount (e.g. up to 8.8 wt% of Hg) and occupy a new position 3*d* of the *Pm-3m* space group, which was empty in pure Pd₁₇Se₁₅. As a consequence, Pd occupancy of adjacent [Pd(4)Se₆] octahedron is reduced to 0.5 for Cu and Ag - bearing palladseite. Incorporation of Hg cases vacancy of this [Pd(4)Se₆] position. Contrary to that, Pt substitutes Pd at the Pd(2) position in the palladseite structure and shows square-planar coordination by Se atoms. This is in agreement with expected coordination preference of Pt. Te enters palladseite structure in an significant amount (6.50 wt. %) and substitutes Se atoms without further modification of the palladseite structure.

Incorporation of Cu, Ag and Hg to the palladseite causes significant changes of its powder X-ray diffraction pattern and hence can be easily detected.

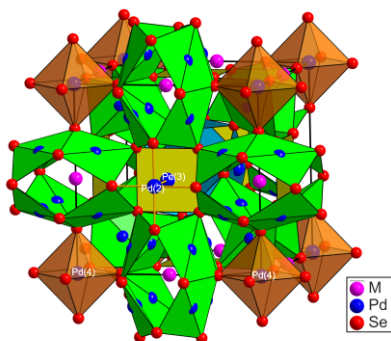


Figure 1. Crystal structure of substituted palladseite (M = Ag, Cu or Hg). For Hg-bearing palladseite, the Pd(4) site is empty. Note three types of coordination polyhedra including [PdSe₄] squares (yellow), [PdSe₄] flattened tetrahedra (green) and [PdSe₆] octahedra (orange).

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[2] Cabral, A.R., Lehmann, B. (2007). *Ore Geology Reviews*, **32**, 681.

[3] Geller, S. (1962) *Acta Cryst.* **15**, 713.

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