CRYSTAL STRUCTURE STUDY OF JACUTINGAITE (Pt₂HgSe₃) AND TISCHENDORFITE (Pd₈Hg₃Se₉)

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Two naturally occurring phases Pt_2HgSe_3 and $Pd_8Hg_3Se_9$ were synthesised and structurally characterized. Recently, Pt_2HgSe_3 phase was discovered in hematite-rich auriferous veins, known as jacutinga, from Cauê iron-ore deposit (Itabira district, Minas Gerais, Brazil) (CABRAL *et al.*, 2008). This Pt-Hg selenide was observed in one polished section as a grain with size of 50 µm and occurs on an aggregate of atheneite, potarite and hematite. $Pd_8Hg_3Se_9$ phase is known from Tilkerode (Harz, Germany) as a mineral tischendorfite (STANLEY *et al.*, 2002). Crystal structures of these phases have not been hitherto known.

Because of extremely low amount of natural samples and difficulties connected with their isolation, the two above-mentioned phases were synthesized from elements by conventional solid-state reactions using silica glass tube technique. All attempts to prepare single crystals suitable for single-crystal examinations failed; hence the crystal structures of Pt₂HgSe₃ and Pd₈Hg₃Se₉ were determined from powder X-ray diffraction data. The programs EXPO2004 and SuperFlip were used for structure determinations; subsequent Rietveld refinements were performed width FullProf program.

Pt₂HgSe₃ phase, which was recently described as a new mineral jacutingaite (VYMAZALOVÁ *et al.*, 2012), crystallizes in space group $P\overline{3}m1$, (a = 7.34 Å,

c = 5.29 Å, V = 247 Å³) and Z = 2. Its crystal structure is composed of layers of [PtSe₆] octahedra and [PtSe₄] squares running parallel to (001) planes. The Se atoms are arranged in layers perpendicular to the **c**-axis forming the *Kagomé*-nets. The Hg atoms are located in voids, defined by Se atoms, between these layers. Jacutingaite is structurally related to the sudovikovite, PtSe₂.

The tischendorfite crystal structure shows *Pmmn* symmetry (a = 7.18 Å, b = 16.80 Å, c = 6.48 Å, Z = 2). Its crystal structure has two Hg sites, three Pd sites, and four Se sites and can be described as a three-dimensional framework.

References

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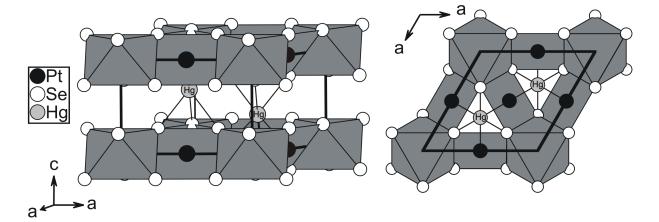


Fig.1. Polyhedral depiction of the jacutingaite (Pt₂HgSe₃) crystal structure. [PtSe₆] octahedra and [PtSe₄] squares are emphasised (adapted from VYMAZALOVÁ et al., 2012).