

CRYSTAL STRUCTURE STUDY OF JACUTINGAITE (Pt_2HgSe_3) AND TISCHENDORFITE ($\text{Pd}_8\text{Hg}_3\text{Se}_9$)

LAUFEK, F.^{1*}, VYMAZALOVÁ, A.¹, DRÁBEK, M.¹ & DRAHOKOUPIL, J.²

¹ Czech Geological Survey, Geologická 6, 152 00 Praha 5, Czech Republic

² Institute of Physics AS CR v.v.i., Na Slovance 2, 182 21, Praha 8, Czech Republic

* E-mail: frantisek.laufek@geology.cz

Two naturally occurring phases Pt_2HgSe_3 and $\text{Pd}_8\text{Hg}_3\text{Se}_9$ 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. $\text{Pd}_8\text{Hg}_3\text{Se}_9$ 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 Pt_2HgSe_3 and $\text{Pd}_8\text{Hg}_3\text{Se}_9$ were determined from powder X-ray diffraction data. The programs EXPO2004 and SuperFlip were used for structure determinations; subsequent Rietveld refinements were performed with FullProf program.

Pt_2HgSe_3 phase, which was recently described as a new mineral jacutingaite (VYMAZALOVÁ *et al.*, 2012), crystallizes in space group $P\bar{3}m1$, ($a = 7.34 \text{ \AA}$,

$c = 5.29 \text{ \AA}$, $V = 247 \text{ \AA}^3$) and $Z = 2$. Its crystal structure is composed of layers of $[\text{PtSe}_6]$ octahedra and $[\text{PtSe}_4]$ 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, PtSe_2 .

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

References

- CABRAL, A.R., GALBIATTI F.H., KWITKO-RIBERIO, R. & LEHMANN, B. (2008): Terra Nova, 20: 32–37.
 STANLEY, C.J., CRIDDLE, A.J., FÖRSTER, H.J. & ROBERTS, A.C. (2002): Canadian Mineralogist, 40: 739–745.
 VYMAZALOVÁ, A., LAUFEK, F., DRÁBEK, M., CABRAL, A.R., HALODA, J., SIDORINOVÁ, T. & LEHMANN, B. (2012): Canadian Mineralogist, 50: in press.

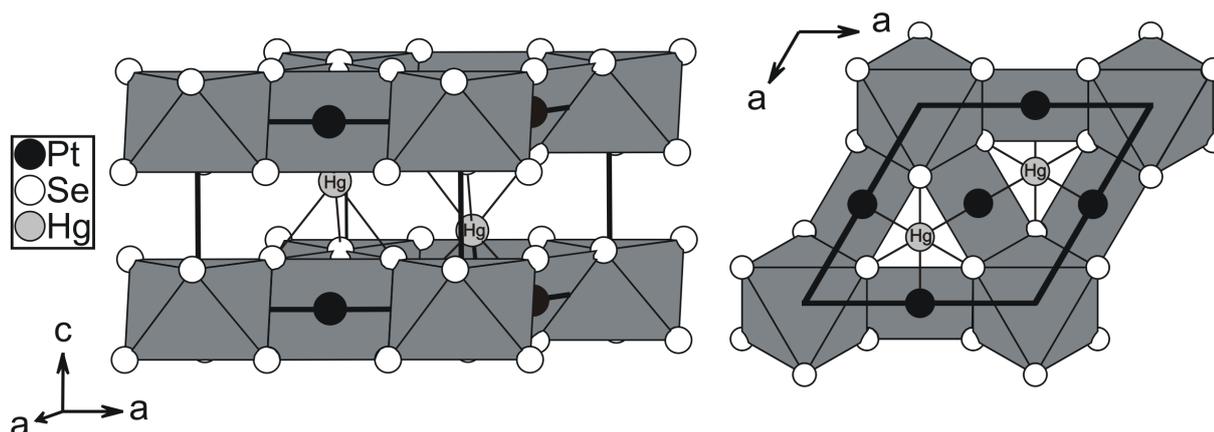


Fig.1. Polyhedral depiction of the jacutingaite (Pt_2HgSe_3) crystal structure. $[\text{PtSe}_6]$ octahedra and $[\text{PtSe}_4]$ squares are emphasised (adapted from VYMAZALOVÁ *et al.*, 2012).