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**Raman spectroscopic study of the uranyl sulphate mineral jáchymovite  
(UO<sub>2</sub>)<sub>8</sub>(SO<sub>4</sub>)(OH)<sub>14</sub>•13H<sub>2</sub>O**

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**Raman spectra of jáchymovite, (UO<sub>2</sub>)<sub>8</sub>(SO<sub>4</sub>)(OH)<sub>14</sub>•13H<sub>2</sub>O, were studied, complemented with infrared spectra, and compared with published Raman and infrared spectra of uranopilite, [(UO<sub>2</sub>)<sub>6</sub>(SO<sub>4</sub>)O<sub>2</sub>(OH)<sub>6</sub>(H<sub>2</sub>O)<sub>6</sub>] •6H<sub>2</sub>O. Bands related to the stretching and bending vibrations of (UO<sub>2</sub>)<sup>2+</sup>, (SO<sub>4</sub>)<sup>2-</sup>, (OH)<sup>-</sup> and water molecules were assigned. U-O bond lengths in uranyl and O-H...O hydrogen bond lengths were calculated from the Raman and infrared spectra.**

**KEYWORDS:** jáchymovite, uranyl, sulphate, Raman spectroscopy, infrared spectroscopy, U-O bond lengths, O-H...O hydrogen bond lengths

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## INTRODUCTION

Uranyl sulphate minerals are widespread around uranium bearing mine sites<sup>1-3</sup>. They may be considered similar to uranyl carbonates classified as intermediates and are formed in regions rich in sulfides, the alteration of which leads to the origin of acid solutions containing sulfate anions. Uranyl sulfate minerals originate by evaporation of such solutions e.g. on the walls of worked out mining tunnels, pits and tailing dumps. Such minerals typically occur close to actively oxidizing uraninite and sulfide minerals in moist surroundings<sup>4</sup>. These minerals usually occur as admixtures of species consisting of fine grained mats and coatings, making their characterization difficult<sup>5-9</sup>. Natural uranyl sulfates, i.e. uranyl sulfate minerals, may be divided in four groups: (a) minerals in the system  $UO_3 - SO_3 - H_2O$ , represented by uranopilite<sup>6,10,11</sup> jáchymovite<sup>12</sup>, insufficiently described metauranopilite<sup>5,7</sup>, and some insufficiently described phases in the system  $UO_3 - SO_3 - H_2O$  by Jensen<sup>13-15</sup> – this indicates that a set of mineral species may be expected in the series uranopilite - schoepite; (b) zippeite group minerals (U:S = 2:1), containing monovalent and/or divalent cations<sup>6</sup>; (c) uranyl sulfates (U:S = 1:1), containing divalent cations, such as johannite and deliensite<sup>5</sup>; (d) uranyl sulfate containing other anions, such as schroekingerite, xiangjiangite and coconinoite<sup>5</sup>. For all known uranyl sulfate minerals are characteristic sheet structures<sup>16</sup>.

Jáchymovite, monoclinic  $(UO_2)_8(SO_4)(OH)_{14} \cdot 13H_2O$ , is formed as one of alteration products of strongly weathered uraninite. It occurs in the dolomite-uraninite veins at Jáchymov, Krušné hory Mts., the Czech Republic, in association with gypsum, uranopilite and uraninite. It was also found at the hydrothermal uranium deposit La Creusaz, the Aiguilles Rouges massif in the Western Swiss Alps (Switzerland)<sup>17,18</sup> and at the Grant Uranium Region, New Mexico, USA<sup>19</sup>. No X-ray single crystal structure data are as yet available. Chemical composition and formula, X-ray powder pattern and unit cell parameters, infrared spectrum and thermal analysis of jáchymovite were described and interpreted by Čejka *et al.*<sup>20</sup> and compared with those for uranopilite and discussed also by Čejka<sup>16</sup>. Infrared spectrum of jáchymovite was also published by Sejkora<sup>21</sup> without any interpretation. Raman spectra of uranopilite were presented by Frost *et al.*<sup>22-25</sup>

As part of a comprehensive study of the molecular structure of secondary minerals containing oxy-anions<sup>22,26-35</sup>, inclusive of uranyl minerals, formed in the oxide zone, using IR and Raman spectroscopy, we report the Raman properties of a holotype specimen of jáchymovite from Jáchymov, Czech Republic, and compare the infrared spectra of jáchymovite and also with published Raman and infrared spectra of uranopilite. The spectra are related to the mineral structure.

## EXPERIMENTAL

### Mineral

The studied specimen of the mineral jáchymovite was obtained from National Museum Prague (holotype sample No. P1N 68.905) and originated from the Jáchymov ore district, northern Bohemia, Czech Republic. It was analysed for phase purity by X-ray powder diffraction. No minor significant impurities were found. Its refined unit-cell parameters for monoclinic space group  $P2_1/m-C^2_{2h}$  or  $P2_1-C^2_2$  are:  $a=18.553(8)$ ,  $b=9.276(2)$ ,  $c=13.532(7)$  Å,  $\beta=125.56(2)^\circ$ ,  $V=1894(2)$  Å<sup>3</sup> and  $Z=2$  (Čejka *et al.* 1996). This holotype sample of jáchymovite was analysed by wet chemical analyses<sup>20</sup> with the following mean results: UO<sub>3</sub> 84.20, SO<sub>3</sub> 2.79, H<sub>2</sub>O 13.32, sum 100.31 wt. %. The resulting empirical formula on the basis of 47 (O,OH) is  $(UO_2)_{8.01}(SO_4)_{0.95}(OH)_{14.12}\cdot 13.06H_2O$ .

### Raman spectroscopy

The crystals of jáchymovite were placed and oriented on the stage of an Olympus BHSM microscope, equipped with 10x and 50x objectives and part of a Renishaw 1000 Raman microscope system, which also includes a monochromator, a filter system and a Charge Coupled Device (CCD). Further details have been published<sup>36-44</sup>. Raman spectra of jáchymovite are shown in Figs. 1-5.

## Infrared spectroscopy

The FTIR spectrum of jáchymovite was obtained with the FTIR Nicolet 740 spectrometer using the conventional KBr-disk technique. Infrared spectrum in the range 4000 - 400  $\text{cm}^{-1}$  were obtained by the co-addition of 32 scans with a resolution of 2  $\text{cm}^{-1}$  and a mirror velocity of 1496  $\text{cm/s}$ . Spectral manipulation such as baseline adjustment, smoothing and normalization were performed using the OMNIC software package (Thermo Electron Corporation). Band component analysis was undertaken using the same software package which enabled the type of fitting function to be selected and allows specific parameters to be fixed or varied accordingly. Band fitting was done using a Lorentz-Gauss cross-product function with the minimum number of component bands used for the fitting process. The fitting process was undertaken until reproducible results were obtained with minimum value of standard errors (usually lower than 2, the range for jáchymovite spectra is 1.36-0.22).

Infrared spectra of jáchymovite are given in the supplementary information Figs. 1S-6S.

## RESULTS AND DISCUSSION

Four normal vibrations of linear  $(\text{UO}_2)^{2+}$  ion (point group symmetry  $D_{\infty h}$ ) exhibit three fundamentals: the symmetric stretching vibration  $\nu_1$ , ( $\sim 900\text{-}700 \text{ cm}^{-1}$ , Raman active), the doubly degenerate bending vibration  $\nu_2$  ( $\delta$ ) ( $\sim 350\text{-}180 \text{ cm}^{-1}$ , infrared active), and the antisymmetric stretching vibration  $\nu_3$  ( $\sim 1000\text{-}850 \text{ cm}^{-1}$ , infrared active). The uranyl group symmetry lowering can result in splitting of the doubly degenerate bending vibration  $\nu_2$  and up to the Raman and infrared activation of all vibrations.

In the case of a free  $(\text{SO}_4)^{2-}$  ion (point group symmetry  $T_d$ ), there are 9 normal vibrations characterized by four fundamentals: the symmetric stretching vibration  $\nu_1$  ( $\sim 1010\text{-}975 \text{ cm}^{-1}$ , Raman active), the doubly degenerate bending vibration  $\nu_2$  ( $\sim 470\text{-}362 \text{ cm}^{-1}$ , Raman active), the triply degenerate antisymmetric stretching vibration  $\nu_3$  ( $\sim 1160\text{-}1015$ , Raman and infrared active), and the triply degenerate bending vibration

$\nu_4$  ( $\sim 680\text{-}570\text{ cm}^{-1}$ , Raman and infrared active). The symmetry lowering causes infrared activation of the  $\nu_1$  and  $\nu_2$  vibrations and splitting of the doubly degenerate  $\nu_2$  vibration. Simultaneously, the  $\nu_3$  and  $\nu_4$  triply degenerate vibrations can be split into two or three components<sup>16,20</sup>.

Molecular water (point group symmetry  $C_{2v}$ ) is characterized by three fundamentals: the symmetric stretching vibration  $\nu_1$  and the antisymmetric stretching vibration  $\nu_3$  ( $\sim 3600\text{-}2900\text{ cm}^{-1}$  - usually these two vibrations are not distinguished and separated), and the bending vibration  $\nu_2$  ( $\delta$ ) ( $\sim 1700\text{-}1590\text{ cm}^{-1}$ ). Libration modes of water molecules can occur in the range approximately  $1100\text{-}300\text{ cm}^{-1}$ . Hydroxyls,  $(\text{OH})^-$  ions, (point group symmetry  $C_{\infty v}$ , will be usually indicated by sharp bands between  $3700\text{-}3450\text{ cm}^{-1}$  sometimes lower if any appreciable amount of hydrogen bonding is involved. The restricted rotational or librational motion occurs with a wavenumber usually in the  $600\text{-}300\text{ cm}^{-1}$  range. A M-OH bending vibration may be observed over a wide range usually below  $1450\text{ cm}^{-1}$ . All these vibrations are infrared and Raman active<sup>16</sup>.

## **Raman spectroscopy**

### ***U-O vibrations in $\text{UO}_2\text{O}_5$ pentagonal dipyramidal coordination polyhedra***

No band which could be attributed to the  $\nu_3$   $(\text{UO}_2)^{2+}$  antisymmetric stretching vibration was observed in the Raman spectrum of jáchymovite and also in uranopilite (Fig. 1)<sup>22,23,25</sup>. In the infrared spectrum of jáchymovite, two bands at  $902$  and  $923\text{ cm}^{-1}$  were observed. All these wavenumbers are close to those in uranopilite<sup>16</sup>. The wavenumbers  $902$  and  $923\text{ cm}^{-1}$  (IR) were used for the calculation of U-O bond length in uranyl with the empirical relation  $R_{\text{U-O}} = 91.41\nu_3^{-2/3} + 0.804\text{ \AA}$  (Fig 1S)<sup>45</sup>. Obtained values are  $1.783$  and  $1.768\text{ \AA}$ , respectively. This is in agreement with average U-O bond length in uranyl in the single crystal structure of uranopilite  $1.794\text{ \AA}$ <sup>10</sup> and U-O bond lengths in uranyles inferred from crystal structures of uranyl compounds and minerals with uranyl pentagonal dipyramidal coordination polyhedra<sup>6,11</sup>.

Raman bands at 839, 828, 807 and 800  $\text{cm}^{-1}$  (Fig 1) and infrared bands at 857 and 807  $\text{cm}^{-1}$  (Fig 1S) were attributed to the  $\nu_1 (\text{UO}_2)^{2+}$  symmetric stretching vibrations. Infrared bands close to 845  $\text{cm}^{-1}$  were observed in the uranopilite infrared spectra<sup>12</sup> and a set of bands in the Raman of infrared spectra of some uranopilite samples studied by Frost *et al.*<sup>22,25</sup>. Some of these bands, however, may be connected with  $\delta$  U-OH. The empirical relation  $R_{\text{U-O}} = 106.5\nu_1^{-2/3} + 0.565 \text{ \AA}$ <sup>45</sup> was used for the calculation of U-O bond length in uranyl. Obtained values are ( $\text{\AA}/\text{cm}^{-1}$ ): 1.772/839, 1.783/828, 1.804/807 and 1.811/800 (Raman), and 1.755/857 and 1.804/807 (infrared). These values are also close to those for uranopilite and compounds and minerals possessing uranyl pentagonal dipyramidal coordination polyhedra. Some of these bands, however, may be related to the  $\delta$  U-OH bending vibrations.

A set of bands was observed in the range 322-474  $\text{cm}^{-1}$  (322, 337, 357, 405, 434, 454, 474  $\text{cm}^{-1}$  (Raman) (Fig. 2), 439 and 459  $\text{cm}^{-1}$  (infrared)) (Fig. 1S). These bands may be understood as coinciding bands connected with  $\nu_2 (\text{SO}_4)^{2-}$  bending vibration,  $\nu$  U-O<sub>ligand</sub> vibrations and librations of water molecules as were attributed in the infrared spectra of phases in the  $\text{UO}_3\text{-H}_2\text{O}$  system<sup>46</sup> and uranopilite<sup>20,22,25</sup>. Bands at 276 and 261  $\text{cm}^{-1}$  (Raman) were assigned to the split doubly degenerate  $\nu_2 (\delta)$  ( $\text{UO}_2$ )<sup>2+</sup> bending vibration (Fig. 3). In the same region were found bands related to this vibration in Raman spectra of some uranopilite samples<sup>22,25</sup>.

Bands at 1348  $\text{cm}^{-1}$  (Raman) (Fig. 4) and 1259, 1300, 1400, 1418, 1455, 1467, 1520 and 1538  $\text{cm}^{-1}$  (infrared) (Fig. 4S) were assigned to the  $\delta$  U-OH bending vibrations. A set of bands in this region was also observed in some uranopilite samples<sup>22,25</sup>. An infrared band at 1740  $\text{cm}^{-1}$  may be connected with the  $((\nu_1 + \nu_3) (\text{UO}_2)^{2+})$  combination band.

### ***S-O vibrations in $(\text{SO}_4)^{2-}$ tetrahedra***

Raman bands at 1015, 1010 and 1003  $\text{cm}^{-1}$ , and an infrared band at 1011  $\text{cm}^{-1}$  were attributed to the  $\nu_1 (\text{SO}_4)^{2-}$  symmetric stretching vibrations (Fig. 4). In the same region were also observed infrared bands in uranopilite (Fig. 3S)<sup>16,22,25</sup>. Raman bands at 1125, 1094 and 1068  $\text{cm}^{-1}$  and infrared bands at 1158, 1100 and 1076  $\text{cm}^{-1}$  were

assigned to the split  $\nu_3$  ( $\text{SO}_4$ )<sup>2-</sup> antisymmetric stretching vibrations. In the region 1032-1186  $\text{cm}^{-1}$  were observed these bands in the Raman and infrared spectra of uranopilite samples<sup>22,25</sup>.

Raman bands at 667, 562 and 542  $\text{cm}^{-1}$  and infrared bands at 672, 627, 583, 551 and 513  $\text{cm}^{-1}$  may be connected with the split triply degenerate  $\nu_4$  ( $\text{SO}_4$ )<sup>2-</sup> bending vibrations. However, there may be some coincidence with libration modes of water molecules. As mentioned above, Raman bands at 474, 454, 434, 405, 357, 337 and 322  $\text{cm}^{-1}$  and infrared bands at 481, 459 and 438  $\text{cm}^{-1}$  may be, respecting any coincidence, assigned to the  $\nu_2$  ( $\text{SO}_4$ )<sup>2-</sup> bending vibration,  $\nu$  U-O<sub>ligand</sub> and libration modes of water molecules. Similar bands were observed in the Raman and infrared spectra of uranopilite<sup>22,25</sup>

### ***Vibrations of water molecules and hydroxyl ions***

$\nu$  OH stretching vibrations of water molecules and hydroxyl ions were observed at 3504 and 3180  $\text{cm}^{-1}$  (Raman) (Fig. 5) and 3738, 3604, 3515, 3303, 3202, 3121 and 3010  $\text{cm}^{-1}$  (infrared) (Fig. 6S). A set of bands in this region was found also in the Raman and infrared spectra of uranopilite<sup>16,22,25</sup>. Wavenumbers of the bands prove that hydrogen bonds are present in the crystal structure of jáchymovite which may be important for the origin and stability of this mineral species. Approximate O-H...O hydrogen bond lengths were inferred from these wavenumbers ( $\text{\AA}/\text{cm}^{-1}$ ): 2.9/3504 and 2.7/3180 (Raman),  $>3.2/3738$ ,  $>3.2/3604$ , 2.92/3515, 2.75/303, 2.7/3202, 2.69/3121 and 2.61/3010 (infrared)<sup>47</sup>. A Raman band at 2257  $\text{cm}^{-1}$  may be assigned to an overtone and/or a combination band and bands at 252, 242, 208, 195, 172, 147 and 114  $\text{cm}^{-1}$  to lattice vibrations. Infrared bands at 2932, 2961 and 2852  $\text{cm}^{-1}$  are probably connected with CH- impurities.

## **CONCLUSIONS**

(a) Raman spectra of jáchymovite were measured, interpreted, complemented with infrared spectra and compared with published Raman and infrared spectra of uranopilite.

- (b) The stretching and bending vibrations of  $(\text{UO}_2)^{2+}$ ,  $(\text{SO}_4)^{2-}$ ,  $(\text{OH})^-$  units and water molecules were assigned.
- (c) Bands related to the  $\delta$  U-OH bending vibrations and water libration modes were attributed.
- (d) Possible coincidences of bands were mentioned.
- (e) The presence of hydrogen bonds in the crystal structure of jáchymovite was inferred from the spectra.
- (f) U-O bond lengths in uranyl and O-H...O hydrogen bond lengths were calculated from the Raman and infrared spectra. U-O bond lengths observed are close to those inferred for uranopilite on the basis of its X-ray single crystal structure<sup>10</sup> and uranyl synthetic and natural compounds possessing uranyl pentagonal dipyramidal coordination polyhedra in their crystal structures.

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### *List of Figures*

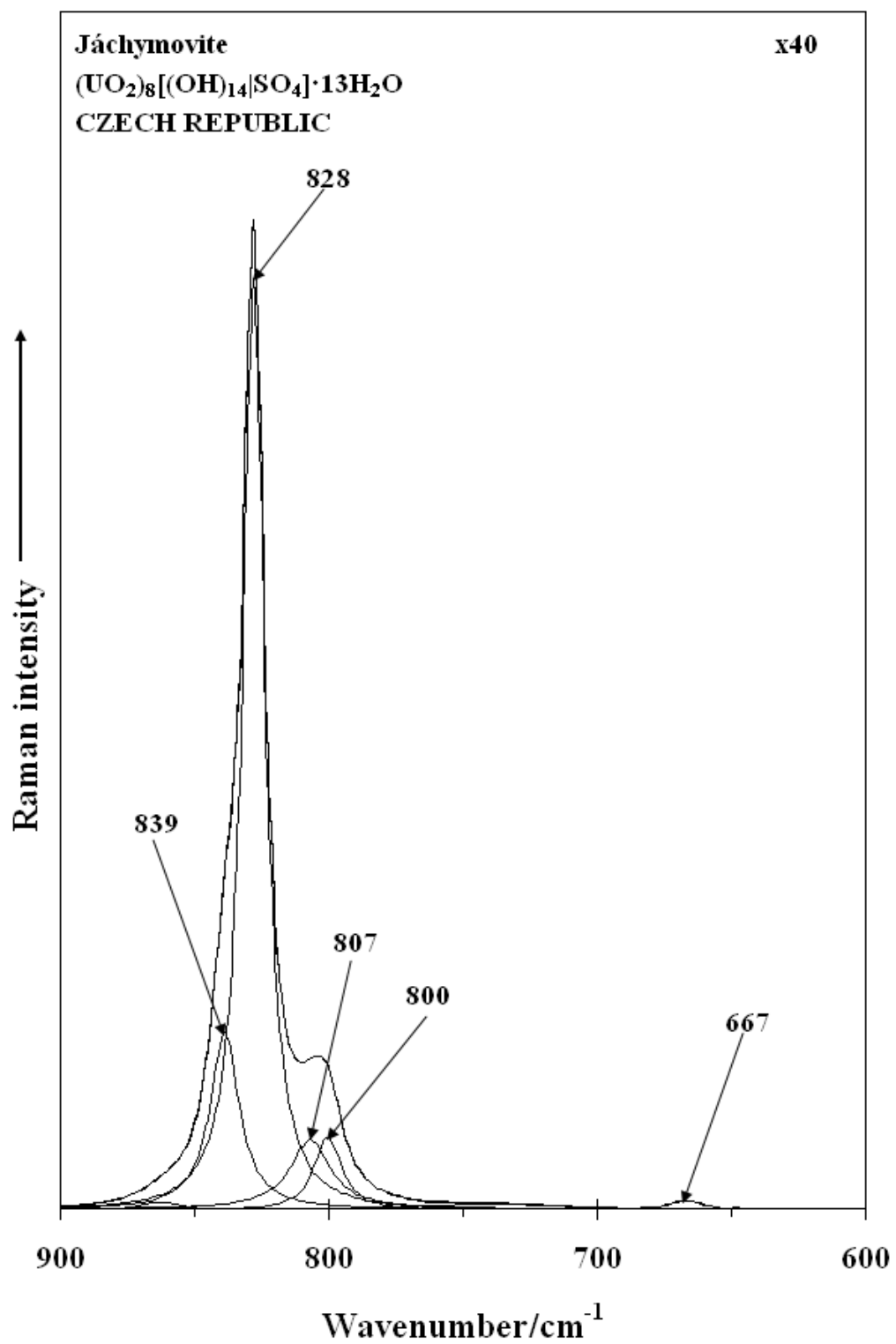
Fig. 1 Raman spectrum of jachymovite in the 600 to 900  $\text{cm}^{-1}$  region

Fig. 2 Raman spectrum of jachymovite in the 300 to 600  $\text{cm}^{-1}$  region

Fig. 3 Raman spectrum of jachymovite in the 100 to 300  $\text{cm}^{-1}$  region

Fig. 4 Raman spectrum of jachymovite in the 900 to 1200  $\text{cm}^{-1}$  region

Fig. 5 Raman spectrum of jachymovite in the 3100 to 3700  $\text{cm}^{-1}$  region



**Figure 1**

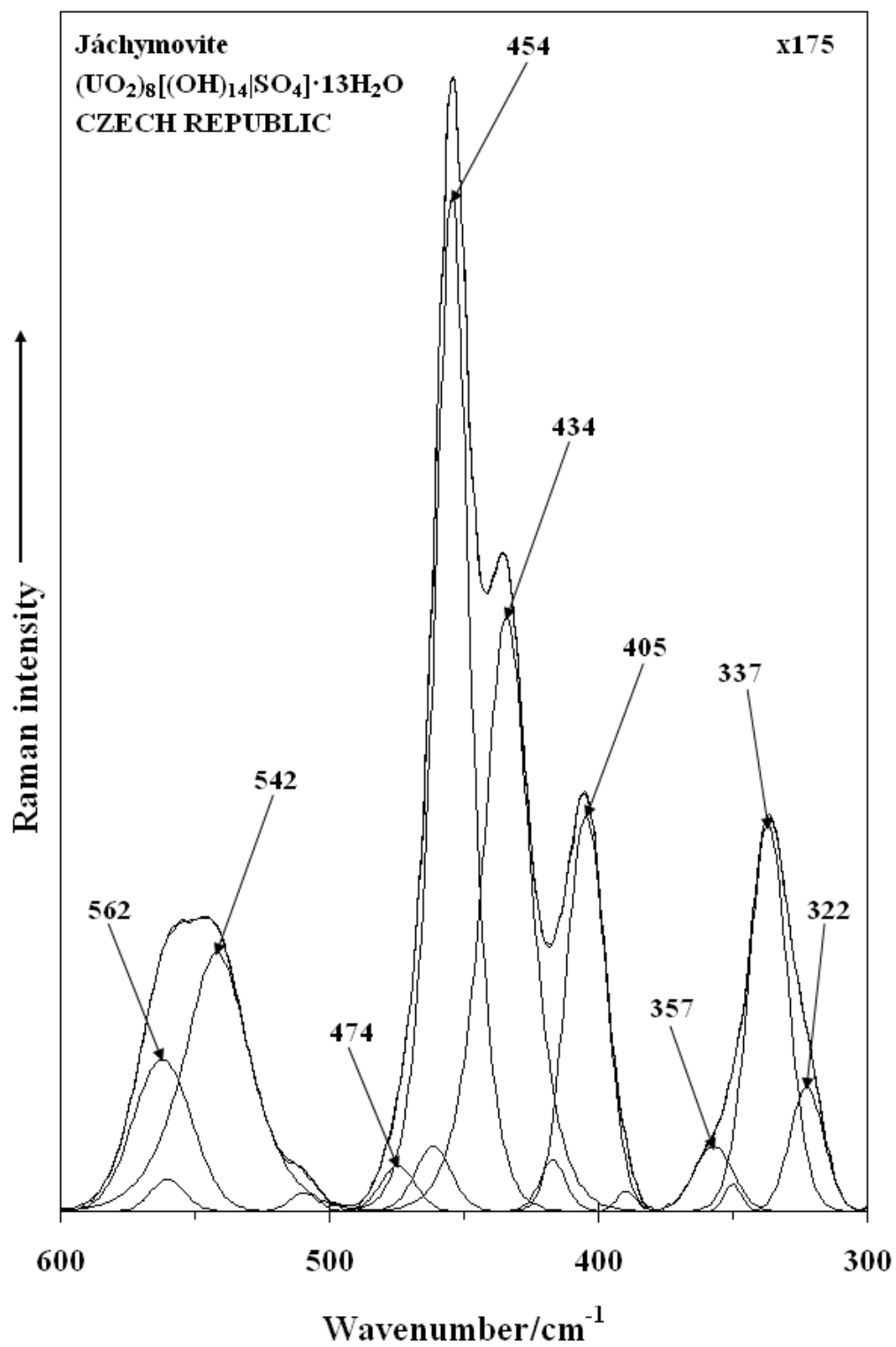
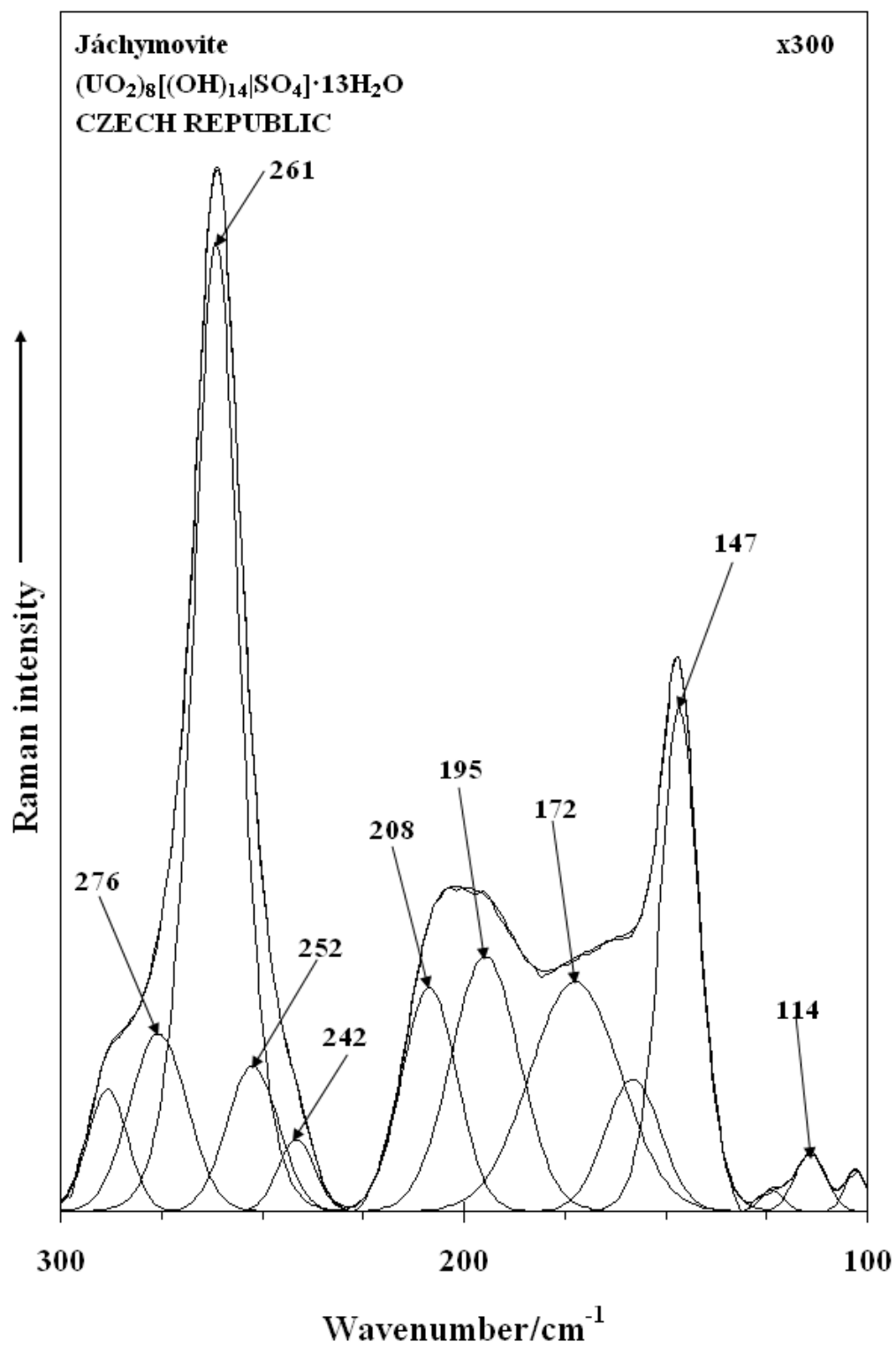


Figure 2



**Figure 3**

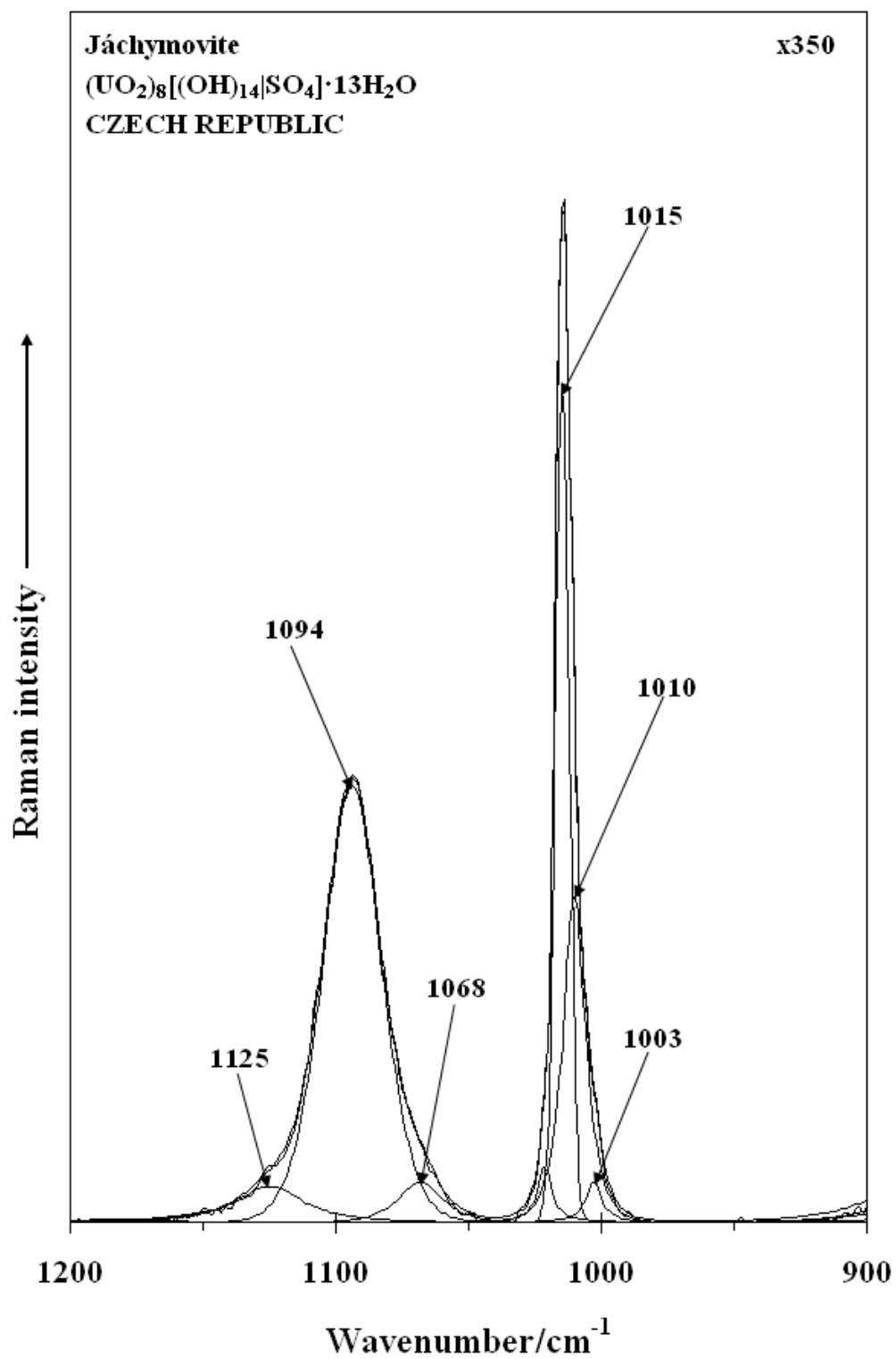


Figure 4

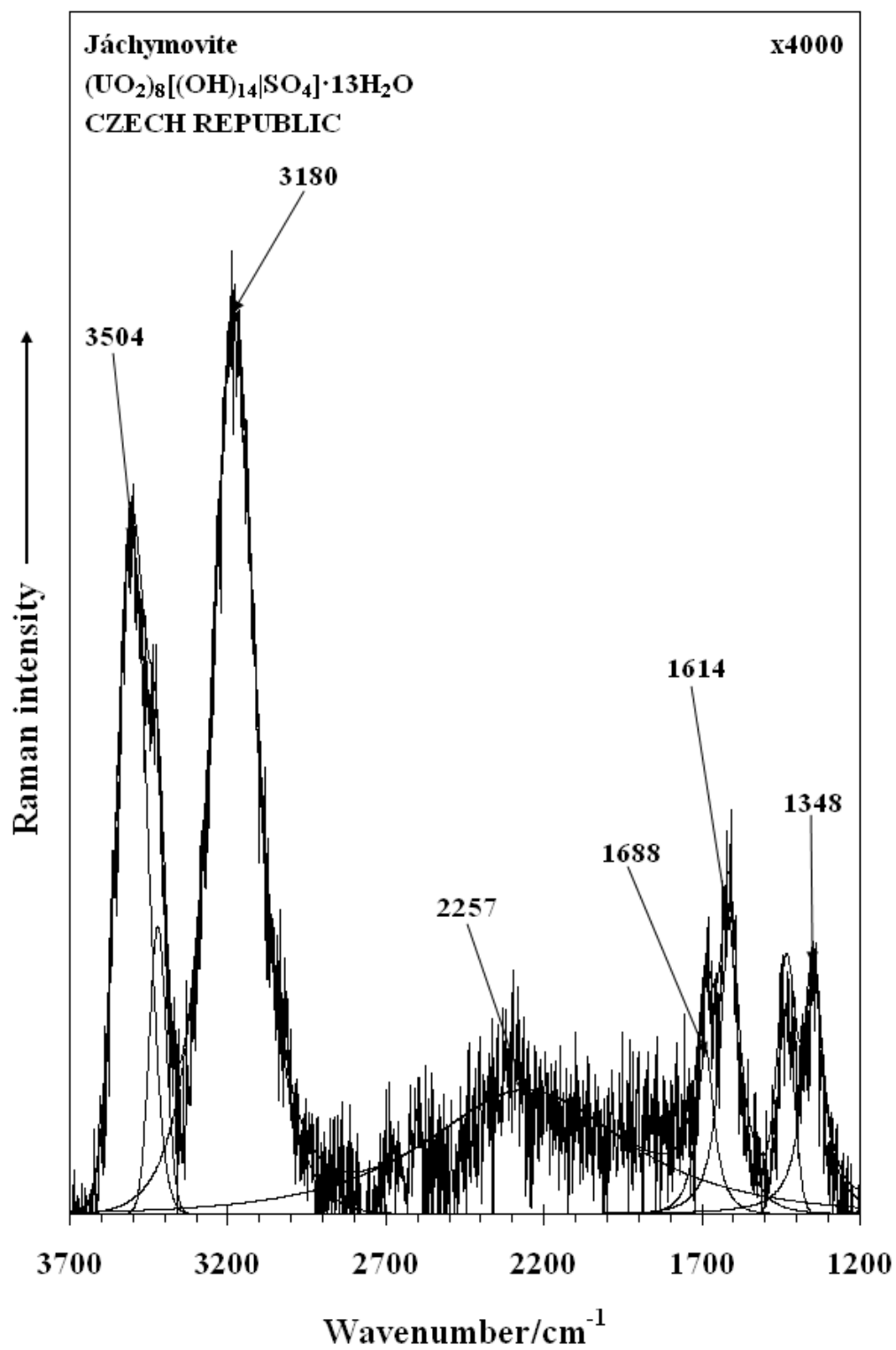


Figure 5