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# Identification of gemstones using portable sequentially shifted excitation Raman spectrometer and RRUFF online database: A proof of concept study[⋆] [⋆⋆]

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**Abstract.** Portable Raman spectrometers offer a good option for fast *in situ* analyses and discrimination of gemstones in the cultural heritage and gemmology applications. Their relative affordability and ease of use makes them ideal tools able to complement traditional instruments in a gemmology lab. A test scenario of blind study based on identification of cut gemstones solely using their Raman spectra and online RRUFF database is proposed. A portable Raman spectrometer equipped with a sequentially shifted excitation (PSSERS) that allows recording of Raman spectra with supressed fluorescence background was used for acquisition of Raman spectra of a series of 20 previously unidentified cut minerals in gemstone quality. Obtained spectra were loaded into the freeware CrystalSleuth program that permits to search in the online database of Raman spectra of minerals RRUFF. In this way 19 out of 20 (with the exception of apatite) cut minerals or gemstones were correctly identified based on multiple similar matches of their Raman spectra in the database. These findings and the straightforward process described in this study suggest that a highly practical application such as basic gemstone discrimination using only portable Raman spectrometer and a free online spectral library is feasible even for a user not experienced in Raman spectroscopy and traditional spectroscopic references in the literature.

## 1 Introduction

Raman spectroscopy has long been established in the fields of mineralogy, materials science and gemmology to a lesser degree. The main advantages of this molecular spectroscopy technique are its non-destructive characteristic, which is complemented with generally little to no preparation of the samples for analyses. When coupled with a microscope, this method can achieve fast point analyses on micrometric scale, ideal for phase identification or confirmation as information about both the chemistry and structure of analyzed materials is contained in the Raman spectrum. This process of fast point analyses can be further expedited and automated to the point, where construction of Raman maps in 2D or 3D with the modern micro Raman spectrometers is possible. A selection of lasers used for excitation is available from a wide spectral range: UV, VIS and IR lasers. All carry both advantages and drawbacks, and it is important to select the most appropriate excitation for each application to obtain best results. Needless to stress that this highly advanced analytical equipment is basically only operated in research, teaching or industry environments.

In contrast to these laboratory instruments there also exists a wide group of highly miniaturized and lightweight portable Raman spectrometers. Initially, these instruments were designed as tools for fast *in situ* identification of unknown and possibly dangerous substances by state law-enforcement agencies, such as police, customs or firefighters. Consequently, other applications were developed for example in quality control and later in scientific fields of mineralogy, cultural heritage studies and gemmology [1–4]. Fast and non-destructive analyses of objects *in situ* can be especially appealing for the latter two fields, as some works of art are either too sizeable or priceless for a laboratory

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analysis. This may apply also to gemstones or jewels, that sometimes are not allowed to be transported or borrowed for study in the lab [5]. Portable Raman spectroscopy, as a more affordable alternative for gemstone identification or confirmation, can conveniently complement the more traditional optical tools for the discrimination of minerals, such as refractometer, spectroscope and microscope, for smaller businesses or even private gemmologists. It should be mentioned, however, that portable Raman spectroscopy is not an all-powerful tool in gemmology, because there also exist cases that require an experience of a gemmologist and other methods. For example the distinction between natural and synthetic gems, or possible chemical or heat treatments.

The diverse applications as well as differences in design of portable Raman spectrometers are reviewed in Vandenabeele *et al.* [2]. Studies performed using portable Raman equipment include applications in mineralogy [4,6], in cultural heritage and gemmology [3,5,7,8] fields. Portable Raman spectrometers with commonly used excitation wavelengths (532 and 785 nm) that were used in these studies can be currently complemented by a new instrumentation in the form of a portable sequentially shifted excitation Raman spectrometer, that was designed to use two sequentially shifted laser excitations and mathematically reconstruct Raman spectra in order to minimise unwanted fluorescence. Several studies related to mineralogy and gemmology illustrate the feasibility of this new instrumentation [6,8–11], and show how in several cases the quality of acquired Raman spectra of natural samples such as minerals (gemstones) is improved. Another instrumental approach that allows for a complete elimination of fluorescence is based on time-gated technology, where the Raman signal is collected before the onset of fluorescence using a sub-nanosecond pulsed excitation. An instrument of this type is available recently [12]; its weight of 19 kg is significantly higher than that of the instrument used in this study, and could be described to fall between the categories of mobile and portable instruments according to the overview of mobile Raman instrumentation [13].

The aim of this study was to examine the possibility of a fast and unambiguous identification of various minerals presented in cut form, solely based on their Raman spectra acquired by a modern portable Raman instrument and an online database of Raman spectra. The emphasis was placed on the documenting whether even users with minimal knowledge in Raman spectroscopy can perform this process of mineral identification, which uses the data from the latest generation of portable Raman spectrometers and a freely available reference data from the RRUFF database. This brief study should illustrate that the significant quality of data from both sources and the very simple process of identification enable users such as gemmologists to capitalize on the advantages of Raman spectroscopy and at the same time even avoid the usual searching for the references in literature.

## 2 Materials and methods

### 2.1 Samples

A total of 20 cut gemstones and minerals were analyzed in this study. Table 1 lists all samples with some additional information and macro photographs of the samples are shown in fig. 1. The samples represented a selection of cut gemstones (some more common and some less frequently used) that was used as a teaching set for the students of gemmology, to be determined by traditional optical methods for gemstone identification. The stones were obtained from reputable sources. Also, some stones were faceted from a known gem rough and thus the gemstones were properly identified. A skilled gemmologist using standard gemmological methods (refractive index, birefrigence, fluorescence, optical character, etc.) then checked all stones for confirmation. Sanidine is impossible to distiguish from orthoclase, but the studied stone is from Volkesfeld, Eifel Mts., Germany, and triphylite is from the Cigana mine near Galileia, Minas Gerais, Brazil. No information about the identity of the gemstones was provided prior to the Raman analyses.

### 2.2 Portable sequentially shifted excitation Raman spectroscopy

The miniaturized Raman spectrometer used for analyses in this study was a portable sequentially shifted excitation Raman spectrometer Bravo from Bruker (Ettlingen, Germany). It weighs 1.5 kg, is battery powered, and can be operated either using the buttons or through the connection (wired or wireless) to the control computer. Spectral range for this specific instrument is 300–3200 $\text{cm}^{-1}$ at a 10–12 $\text{cm}^{-1}$ resolution. This instrument uses a combination of two excitation wavelengths in near infrared region (785 nm and 853 nm, determined using a UV-Vis spectrometer Specord S600, Analytik Jena), and each of these wavelengths is additionally sequentially shifted in order to suppress the fluorescence in the acquired Raman spectra. Therefore, the portable sequentially shifted excitation Raman spectrometer records a total of six spectra, we call them “raw spectra”, that can also be accessed and reviewed in the OPUS software as all the data is stored in the *.0 files. A Raman spectrum is then computed from these raw spectra, based on the different behaviour of fluorescence background or bands, and the actual Raman bands to the sequentially shifted wavelengths of the lasers. This final Raman spectrum is presented as a main result by the intrument, ideally free of any fluorescence and only including Raman bands. A more detailed description of this method, and how this approach is advantageous for fluorescence removal in geological samples is given here [6,10]. The PSSERS was operated at the automatic settings, where the laser power and the acquisition times are regulated by the instrument itself, and usually this mode provides good quality results.

**Table 1.** Detailed information about the samples of cut gemstones.

| Stone # | Colour | Mineral name, variety determined by CrystalSleuth | Gemmologist | Weight [ct][(a)] | Largest dimension [mm] | Formula |
|---|---|---|---|---|---|---|
| 1 | Blue | Cordierite, iolite | Iolite | 1.85 | 12.80 | $(\mathrm{Mg}, \mathrm{Fe})_2\mathrm{Al}_3(\mathrm{Si}_5\mathrm{AlO}_{18})$ |
| 2 | Green | Beryl, emerald | Emerald | 1.37 | 8.26 | $\mathrm{Be}_3\mathrm{Al}_2(\mathrm{SiO}_3)_6$ |
| 3 | Green | Diopside | Diopside | 0.91 | 7.21 | $\mathrm{MgCaSi}_2\mathrm{O}_6$ |
| 4 | Yellow | Chrysoberyl | Chrysoberyl | 0.56 | 5.62 | $\mathrm{BeAl}_2\mathrm{O}_4$ |
| 5 | Green | Kornerupine | Kornerupine | 0.87 | 8.02 | $(\mathrm{Mg}, \mathrm{Fe}^{2+})_4(\mathrm{Al}, \mathrm{Fe}^{3+})_6(\mathrm{SiO}_4, \mathrm{BO}_4)_5(\mathrm{O}, \mathrm{OH})_2$ |
| 6 | Brown | Andalusite | Andalusite | 1.57 | 7.90 | $\mathrm{Al}_2\mathrm{SiO}_5$ |
| 7 | Brown | Triphylite | Triphylite | 1.52 | 7.68 | $\mathrm{LiFe}^{2+}\mathrm{PO}_4$ |
| 8 | Orange | Grossular | Grossular, hessonite | 2.43 | 9.33 | $\mathrm{Ca}_3\mathrm{Al}_2(\mathrm{SiO}_4)_3$ |
| 9 | Yellow | Quartz, citrine | Citrine | 1.30 | 8.14 | $\mathrm{SiO}_2$ |
| 10 | Red | Andradite | Andradite | 0.39 | 5.52 | $\mathrm{Ca}_3\mathrm{Fe}_2(\mathrm{SiO}_4)_3$ |
| 11 | Orange | Topaz | Topaz | 0.56 | 5.98 | $\mathrm{Al}_2\mathrm{SiO}_4(\mathrm{F}, \mathrm{OH})_2$ |
| 12 | Brownish | x | Apatite | 0.50 | 4.80 | $\mathrm{Ca}_5(\mathrm{PO}_4)_3(\mathrm{F}, \mathrm{Cl}, \mathrm{OH})$ |
| 13 | Colourless | Phenakite | Phenakite | 0.94 | 7.02 | $\mathrm{Be}_2\mathrm{SiO}_4$ |
| 14 | Brownish | Baryte | Baryte | 1.89 | 7.90 | $\mathrm{BaSO}_4$ |
| 15 | Yellowish | Labradorite | Labradorite | 0.97 | 7.80 | $(\mathrm{Ca}, \mathrm{Na})(\mathrm{Al}, \mathrm{Si})_4\mathrm{O}_8$ |
| 16 | Colourless | Hydroxylherderite | Hydroxylherderite | 0.58 | 5.99 | $\mathrm{CaBe}(\mathrm{PO}_4)(\mathrm{F}, \mathrm{OH})$ |
| 17 | Brownish | Orthoclase | Sanidine | 0.41 | 5.87 | $\mathrm{KAlSi}_3\mathrm{O}_8$ |
| 18 | Colourless | Datolite | Datolite | 0.28 | 4.13 | $\mathrm{CaBSiO}_4(\mathrm{OH})$ |
| 19 | Colourless | Danburite | Danburite | 0.40 | 4.72 | $\mathrm{CaB}_2(\mathrm{SiO}_4)_2$ |
| 20 | Colourless | Pollucite | Pollucite | 0.34 | 4.70 | $(\mathrm{Cs}, \mathrm{Na})_2\mathrm{Al}_2\mathrm{Si}_4\mathrm{O}_{12} \cdot 2\mathrm{H}_2\mathrm{O}$ |

[(a)] 1 carat (ct) is equal to 0.2 g.

Raman spectra obtained with the Bravo instrument were converted to Data point table (.dpt) format (basically x, y plaintext data) to be loaded in the CrystalSleuth program first with no additional manipulation of any type, such as baseline correction.

### 2.3 RRUFF free online database of Raman spectra of minerals

The RRUFF project [14], accessible at web address `rruff.info` provides a searchable integrated database of Raman, X-ray diffraction and chemistry data for minerals. It is one of few freely accessible databases of Raman spectra of minerals. Currently, more than 20 000 Raman spectra are included in the database. Each mineral species can be represented by several different specimens from various localities, and therefore several entries of Raman spectra are available for each mineral. The overall quality of the Raman spectra is good for majority of entries, although occasionally, some entries contain only fluorescence signals, etc. Raman spectra of minerals in the database were recorded using 514.5, 532, 780 and 785 nm excitations, and crystal orientations may differ from sample to sample.

The authors of the RRUFF database additionally provide a simple frontend software called CrystalSleuth that enables users to load their own spectra in x, y ASCII format to be compared against the database. This program currently searches from the 5129 of the Raman spectra.

## 3 Results and discussion

The results of the identification process that is described in more details in the Supplementary Material (SM) are presented in table 2 and fig. 2. For simplicity, results obtained on the same samples with two other portable Raman spectrometers equipped with lasers of common excitation wavelengths (532 and 785 nm) are also included in the SM. Raman spectra recorded with the PSSERS (black colour) given in fig. 2 correspond very well with the best match from the database (grey colour) for correctly identified gemstones (minerals). Typically, the pairs of Raman spectra for each mineral contain similar number of Raman bands at very similar positions. This is reflected in generally high certainty matches for a majority of the analyzed gemstones (see table 2). Intensity of some Raman bands differed probably mostly due to the slightly different orientation of the crystals. Closely located Raman bands or doublets

**Fig. 1.** Macro photographs of samples of cut gemstones.

in some spectra (see, *i.e.*, in andradite, labradorite, and danburite spectra) were not so well resolved in the spectra taken with the PSSERS due to the lower spectral resolution compared to the entries in the database that were taken most certainly with full-fledged laboratory Raman spectrometers. This instrument however provides Raman spectra consistently with very precise values for Raman bands (with almost non-existent shift in the bands positions between consecutive analyses), and this compensates for the average spectral resolution in the field of portable instruments. Thus, some minerals with closely located pairs of bands such as calcite/aragonite can still be distinguished. Raman spectra of many minerals contain medium to strong intensity bands at wavenumber positions lower than $300\,\mathrm{cm}^{-1}$, sometimes these bands are the most intense and very characteristic (see spectra of andalusite and most clearly of topaz). Additionally, the upper spectral limit of $3200\,\mathrm{cm}^{-1}$ poses a limitation, since useful information, for example presence and type of OH groups (Raman bands due to stretching OH vibrations occur at around $3600\,\mathrm{cm}^{-1}$) in gemstones can be utilised in for instance in provenience/genesis studies of emeralds [15] or to distonguish polymorphs for instance variscite/metavariscite [16]. This is the most obvious limitation of the PSSERS in this kind of application. Nevertheless, in our set of samples, the remaining detected Raman bands were enough for a good identification of 19 gemstones out of 20.

The fluorescence removal process that this instrument is using sometimes introduces changes in the shapes of Raman bands of analyzed materials. For example, the Raman spectrum of diopside (see fig. 2) clearly contains at least two strong bands with skewed and asymmetrical band shapes at around 400 and $700\,\mathrm{cm}^{-1}$ wavenumbers. Another such unwanted change to the Raman spectra can be spotted in the spectrum of mineral kornerupine, where the general shape of a group of naturally wider Raman bands (at around $1000\,\mathrm{cm}^{-1}$) is modified which is accompanied in the shift in position of the $1020\,\mathrm{cm}^{-1}$ band to $1046\,\mathrm{cm}^{-1}$.

During the identification process, it was found that the search algorithm in the CrystalSleuth program is very sensitive to the baseline of loaded Raman spectra. This was not so important for the spectra that were recorded with PSSERS since these spectra are already “baseline corrected” a result of the mathematically reconstructed and cleaned spectra from fluorescence and other factors that appear as a raised baseline in the original Raman spectra. See the generally higher match scores in the third column in table 2. However, the number of identified minerals was identical in both cases.

**Table 2.** A summary of all matches including the match scores (in %) at the first five positions for each gemstone spectrum. The empty lines mean the same mineral identified as in the last line above. * For more details, see SM.

| Spectrum loaded | PSSERS as recorded | PSSERS baselined $< 1500\,\mathrm{cm}^{-1}$ | Spectrum loaded | PSSERS as recorded | PSSERS baselined $< 1500\,\mathrm{cm}^{-1}$ |
|---|---|---|---|---|---|
| 1 Iolite | 85 Cordierite | 96 Cordierite | 11 Topaz | 67 Topaz | 94 Topaz |
| | 84 | 95 | | 65 | 90 |
| | 83 | 93 | | 62 Niahite | 87 Niahite |
| | 82 | 93 | | 62 | 87 |
| | 81 | 92 | | 62 Topaz | 87 Topaz |
| 2 Emerald | 79 Beryl | 97 Beryl | 12 Apatite | *53 Phosphuranylite* | *84 Phosphuranylite* |
| | 79 | 96 | | *52 Kyanite* | *83 Kyanite* |
| | 78 | 96 | [identification failed]* | *52 Wilkinsonite* | *82 Wilkinsonite* |
| | 78 | 96 | | *52 Greenockite* | *82 Greenockite* |
| | 78 | 96 | | *51 Zircon* | *81 Zircon* |
| 3 Diopside | 75 Erdite* | 79 Erdite* | 13 Phenakite | 92 Phenakite | 94 Phenakite |
| | 74 Diopside | 79 Diopside | | 92 | 94 |
| | 74 | 78 | | 92 | 94 |
| | 73 | 78 | | 92 | 93 |
| | 73 Howieite | 78 Howieite | | 92 | 93 |
| 4 Chrysoberyl | 85 Chrysoberyl | 92 Chrysoberyl | 14 Baryte | 94 Baryte | 94 Baryte |
| | 82 | 88 | | 94 | 94 |
| | 80 | 87 | | 94 | 94 |
| | 75 | 81 | | 93 | 94 |
| | 73 | 79 | | 92 Magnesioaubertite | 92 Magnesioaubertite |
| 5 Kornerupine | 77 Kornerupine | 87 Kornerupine | 15 Labradorite | 83 Labradorite | 97 Labradorite |
| | 74 | 84 | | 83 | 97 |
| | 66 | 74 | | 83 | 97 |
| | 64 Pyrophyllite | 73 Pyrophyllite | | 83 | 97 |
| | 64 Muscovite | 72 Muscovite | | 82 | 96 |
| 6 Andalusite | 72 Andalusite | 97 Andalusite | 16 Hydroxyl-herderite | 92 Hydroxyl-herderite | 95 Hydroxyl-herderite |
| | 71 | 96 | | 91 | 95 |
| | 69 | 93 | | 91 | 95 |
| | 69 | 93 | | 91 | 94 |
| | 68 | 92 | | 90 | 93 |
| 7 Triphylite | 91 Triphylite | 97 Triphylite | 17 Orthoclase | 93 Orthoclase | 98 Orthoclase |
| | 91 | 97 | | 93 | 98 |
| | 90 | 97 | | 93 | 98 |
| | 90 Ludlamite | 97 Ludlamite | | 93 | 98 |
| | 90 Triphylite | 96 Triphylite | | 92 | 98 |
| 8 Grossular | 95 Grossular | 99 Grossular | 18 Datolite | 96 Datolite | 97 Datolite |
| | 94 | 98 | | 94 | 95 |
| | 93 | 97 | | 94 | 95 |
| | 93 | 97 | | 93 | 94 |
| | 92 | 96 | | 92 | 93 |
| 9 Citrine | 98 Quartz | 99 Quartz | 19 Danburite | 75 Danburite | 92 Danburite |
| | 98 | 99 | | 74 | 91 |
| | 98 | 99 | | 74 | 91 |
| | 98 | 98 | | 73 Magnesioferrite | 90 Magnesioferrite |
| | 97 | 98 | | 71 Inyoite | 87 Inyoite |
| 10 Andradite | 95 Andradite | 96 Andradite | 20 Pollucite | 96 Pollucite | 99 Pollucite |
| | 95 | 96 | | 95 | 98 |
| | 93 | 94 | | 95 | 98 |
| | 93 | 94 | | 94 | 98 |
| | 92 | 93 | | 94 | 97 |

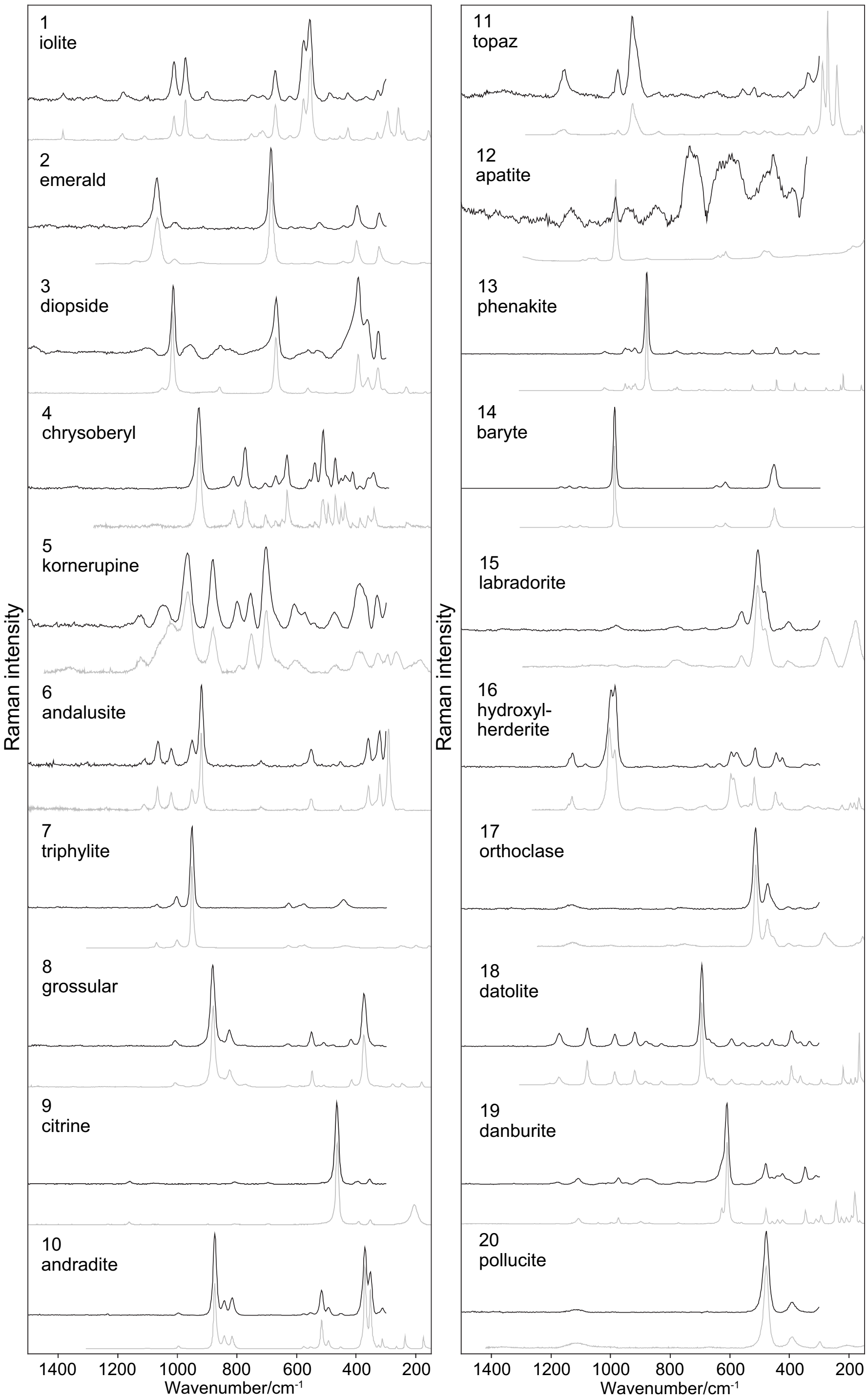

**Fig. 2.** Comparison of Raman spectra of cut gemstones as recorded with a PSSERS (black spectra) and a best match record in the RRUFF database for each sample (grey spectra).

On the other hand, when the same identification process was performed using the raw data obtained by portable instruments with common excitations (532 and 785 nm) only 5 out of 20 samples were identified. After the Remove Background feature in CrystalSleuth was applied, this number vastly improved to 13/20 and 15/20 for the 532 and 785 nm instruments, respectively (see table in SM). This finding shows that it is always recommended to use Raman spectra with as flat baselines as possible as the input for the search, as the chance of a successful identification will improve substantially. This is true mainly for the spectra that still contain raised background due to the fluorescence (data from portable instruments with regular excitations).

### 3.1 Failed identification due to the excessive laser-induced fluorescence

In one case only, for the apatite sample, the identification completely failed. As can be seen very clearly in fig. 2, apatite Raman spectrum taken with the PSSERS contains several high intensity "false bands" that are in fact instrumental artefacts. These artefacts almost completely mask the Raman signal of apatite (a weak intensity band due to the $\upsilon_1(\mathrm{PO}_4)$ symmetrical stretching vibration). Therefore, the search algorithm in the CrystalSleuth program gives completely wrong matches (see table 2). This type of artefacts appears in the Raman spectra of gemstones (or minerals in general) which exhibit a strong special type of laser-induced fluorescence that appears as relatively narrow bands. These unwanted non-Raman bands are often caused by the presence of rare earth elements (REE) such as $\mathrm{Eu}^{3+}$, $\mathrm{Ce}^{3+}$, $\mathrm{Sm}^{3+}$, and $\mathrm{Nd}^{3+}$ which activate fluorescence centres in the samples [17–19].

The narrow band manifestation of this type of fluorescence that often coincides with the true Raman bands of minerals at close wavenumber positions results in the introduction of the artefact bands as remnants of the fluorescence removal process. These results are similar to previous findings of artefact bands in the PSSER spectra of minerals, such as anhydrite, apatite, and zircon [10], and illustrate some the limits of this method for analyses of natural samples of minerals.

## 4 Conclusions

It was established that the portable sequentially shifted excitation Raman spectrometer was able to provide Raman spectra of sufficient quality for an easy identification using the RRUFF database search program CrystalSleuth with no prior manipulation with the spectra. Nineteen out of twenty samples of cut gemstones were determined this way. One of the main issues that negatively affect the identification process is the background, or baseline, of the user-inputted spectra. The PSSERS provides Raman spectra with flat baselines as a result of fluorescence removal process, which contributes to the higher number of successful identifications, compared to the portable instruments equipped with common excitations. This simple process described in our report suggests that a practical task of basic gemstone discrimination using only portable Raman spectrometer and a free online spectral library is feasible even for a user not experienced in Raman spectroscopy and the traditional approach of searching proper spectroscopic references in literature. Future studies could explore the possibilities of this system for analyses of more spectroscopically challenging geomaterials, such as turquoise, lapis lazuli as well as treated gems and doublets, or important materials of biological origin often used as adornments, such as corals, pearls, amber, etc.

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