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Diffraction and spectroscopic characterization of jeffbenite: a high-pressure marker in diamonds

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Jeffbenite is a new mineral, recently approved by IMA (IMA 2014-097), which could cover a key role in determining the depth of formation of the so-called super-deep diamonds. This category of diamonds is thought to crystallize in sub-lithospheric conditions, i.e. below about 250 km (corresponding to ~7-8 GPa; see the *Nature* paper published by Pearson et al. in 2014 on a Brazilian diamond bearing an inclusion of ringwoodite) and represents only 6% of diamonds investigated so far. On the contrary, the so-called lithospheric diamonds represent the remaining 94% and are those typically formed inside the cratons at depths between 120-130 and 250 km. Jeffbenite is a tetragonal high-pressure phase, emerald green in colour (Figure 1), which can be found only in super-deep diamonds and shows a chemical composition very similar to that of Mg-Fe garnets. More in detail, the recently approved jeffbenite has composition $(Mg_{2.62}Fe^{2+}_{0.27})(Al_{1.86}Cr_{0.16})(Si_{2.91}Al_{0.09})O_{12}$ with very minor amounts of Mn, Na and Ca, as it is highlighted by the EDS spectrum (Figure 2). Jeffbenite has unit-cell parameters a = 6.5231(1) Å and c = 18.1756(3) Å; its space group is $I\text{-}42d$ and its X-ray calculated density is 3.576 g/cm^3 (Nestola et al., 2015).

The first crystal structure of jeffbenite was published in 1997 (*Nature*, Harris et al.). Nevertheless, at that time the mineral was simply reported with the acronym "TAPP", due to its similar composition to garnet (Tetragonal Almandine-Pyrope Phase), and never submitted to IMA to get an official approval. Thanks to our new re-investigation of TAPP, we were able not only to give a name to such important marker, but also to provide new mineralogical features besides crystal structure and chemistry. Indeed, in addition to the microprobe WDS and the single-crystal X-ray diffraction analyses, we measured the jeffbenite Raman spectrum, its trace elements composition by Laser ablation ICP-MS, its optical properties and its micro-hardness. Finally, we verified the chemical homogeneity by mapping all its main elements. In terms of vibrational spectroscopy, although jeffbenite has a Raman spectrum close to that of peridotitic garnets, this technique should be able to distinguish the two phases. In detail, the main peaks of

Figure 1. Single crystal of jeffbenite.

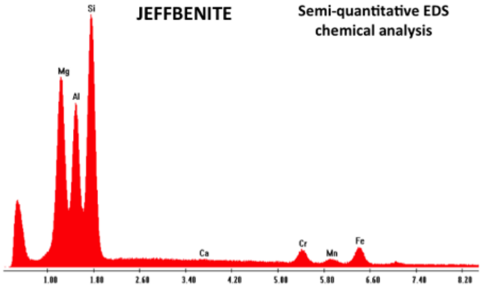

Figure 2. EDS spectrum of jeffbenite.

jeffbenite (in order of decreasing intensity and in cm^{-1}) are: 865, 935, 318, 995, 499, 204, 635. An analysis on a kimberlitic peridotitic garnet performed both by the same instrument and at the same working conditions adopted to measure jeffbenite (ThermoScientific DXR Raman microscope) shows the following main peaks: 919, 362, 860, 560, 600, 643, 1052. This is essential to identify jeffbenite even without breaking the host diamond, basic condition if you want to determine its depth of formation. In this light, we must remark that at present there are not definitive data on the depth of formation of jeffbenite; the unique available experimental work was published by Armstrong and Walter (2012), but their data were obtained on a jeffbenite rich in Ti (totally absent in the IMA-approved jeffbenite) and poor in Fe. However, these authors report for their Ti-rich jeffbenite conditions of formation of ~13 GPa and ~1700 K, which would locate the mineral at about 390 km depth, close to the upper mantle-transition zone boundary.

We are performing new synthesis experiments in order to determine which is the effect of Ti on the jeffbenite stability field and, as a consequence, to figure out if it can be really formed in the transition zone as some authors stated (e.g. Brenker et al., 2002).

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