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A Raman spectroscopic study of the natural carbonophosphates $Na_3MCO_3PO_4$ (M = Mn, Fe, and Mg)

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Along with some other Na-minerals, carbonophosphates indicate a high initial Na activity in carbonatite and kimberlite melts, which is beneficial for petrological reconstructions. Because carbonophosphates are capable of incorporating large-ion lithophile and rare earth elements (REEs) in their structure, they can participate in the transport of these elements. Moreover, due to the presence of both $[PO_4]^{3-}$ and $[CO_3]^{2-}$ groups in carbonophosphates, these mineral phases play an important role in the Earth's global carbon and phosphate cycles. With all these properties, carbonophosphates have long attracted the attention of geologists. Raman spectroscopy appears to be one of the most suitable tools for their diagnosis, since they commonly present in rocks as small inclusions in other mineral grains. Despite this profit, only a few publications contain Raman characteristics of either natural or synthetic carbonophosphates.

We studied and compared Raman spectra of three natural carbonophosphate phases (sidorenkite, bonshtedtite, and bradleyite) with the general formula $Na_3MCO_3PO_4$ (M = Mn, Fe, and Mg, correspondingly). These spectra showed from 21 to 24 vibrational bands, of which the two most intense (963±5 cm^{-1} и 1074±3 cm^{-1}) correspond to the ν1(P–O) and ν1(C–O) modes. These two bands split due to the occurrence of isomorphic impurities. It was found that the crystallographic orientation of the sample influences the intensity of most bands. A natural increase in the Raman shift was observed for most bands assigned to the same vibrations (the smallest shift in the spectrum is characteristic of sidorenkite, an intermediate - of bonshtedtite, and the largest - of bradleyite).

We propose the following algorithm for the diagnosis of carbonophosphates:

- Checking minerals for belonging to the group of carbonophosphates by the main bands and the characteristic profile of the spectrum;
- Testing the hypothesis that the mineral of question is bradleyite based on the analysis of the estimated shift of the main bands;
- Diagnosis of a mineral species by peaks located between the main bands;
- Validation of the diagnostics by considering the position of the bands at 185±9 cm^{-1}, 208±7 cm^{-1}, 255±5 cm^{-1}, and 725±6 cm^{-1}.

The proposed algorithm allows one to perform Raman diagnostics of carbonophosphates in inclusions even in the absence of EPMA data. In the study of carbonatites, kimberlites, and other rocks, the diagnostics of the mineral species of the carbonophosphate group can be important in the petrological aspect.

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