

Raman Spectrum of Berlinite [α -AlPO₄]

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ISSN: 2576-8840



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Submission:  September 15, 2026

Published:  September 30, 2026

Volume 23 - Issue 2

How to cite this article: Rainer Thomas*.
Raman Spectrum of Berlinite [α -AlPO₄].
Res Dev Material Sci. 23(2). RDMS. 001059.
2026.
DOI: [10.31031/RDMS.2026.23.001059](https://doi.org/10.31031/RDMS.2026.23.001059)

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Abstract

Raman spectroscopy was used to characterize a synthetic, defect-poor berlinite [α -AlPO₄] single crystal and compare its spectral features with published data and natural reference samples. Measurements were performed with a 532nm laser over 0-4000cm⁻¹ using calibrated silicon and diamond standards, with spectra collected from rhombohedral and prismatic crystal planes. The principal diagnostic Raman bands occurred near 220, 461, and 1110-1112cm⁻¹, while the strongest bands were observed at approximately 462 and 1112cm⁻¹. Their positions were consistent with handbook data obtained using 514nm excitation and with measurements from berlinite samples from Sweden and Germany. Comparison of the examined orientations indicates that the principal band positions are relatively stable, although the available data does not establish complete orientation independence. Further measurements involving additional crystals, controlled polarization, and quantitative intensity analysis are required to define orientation effects more rigorously.

Keywords: Berlinite; α -AlPO₄; Raman spectroscopy; Diagnostic raman bands; Crystal orientation; Synthetic single crystal; Mineral characterization

Introduction

During the study of pegmatites of the Variscan Ehrenfriedersdorf tin deposit, we frequently found berlinite crystals [1]. At that time, we used, at first, reference material from Vestanå and Hålsjöberg from the Naturhistoriska Riksmusset in Stockholm/Sweden arranged by Hans-Jürgen Wilke [2]. Later, we used as a reference a synthetic single crystal of berlinite from the AMNH, which Dr. G. Harlow provided.

Sample Material and Method

As a sample, we used a water-clear, defect-poor, single berlinite crystal of about 17x10x8mm from the American Museum of Natural History, New York, USA (No. 99035). Figure 1 shows that crystal.

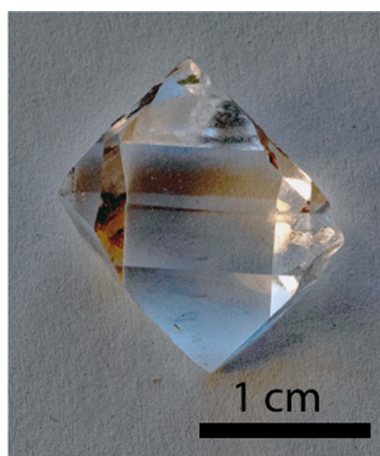


Figure 1: Synthetic berlinite crystal used for Raman spectroscopy.

Microscopic investigations were performed using a Zeiss JENALAB POL microscope in transmitted and reflected light. Raman measurements were performed with an Olympus BX43 microscope and an EnSpectr R532 system using a 532nm laser. Spectra were collected from 0-4000 cm^{-1} with an approximate resolution of 4 cm^{-1} . Calibration used silicon and diamond standards; minerals were identified with Crystal Sleuth [3].

Results

Raman spectra of berlinite are shown in Figures 2 & 3. Three typical Raman bands of berlinite are diagnostically: 221, 462, and 1112 cm^{-1} . Table 1 shows the results on the synthetic berlinite crystal and the reference material from Lyon [4]. The composition is 58.20% P_2O_5 and 41.8% Al_2O_3 .

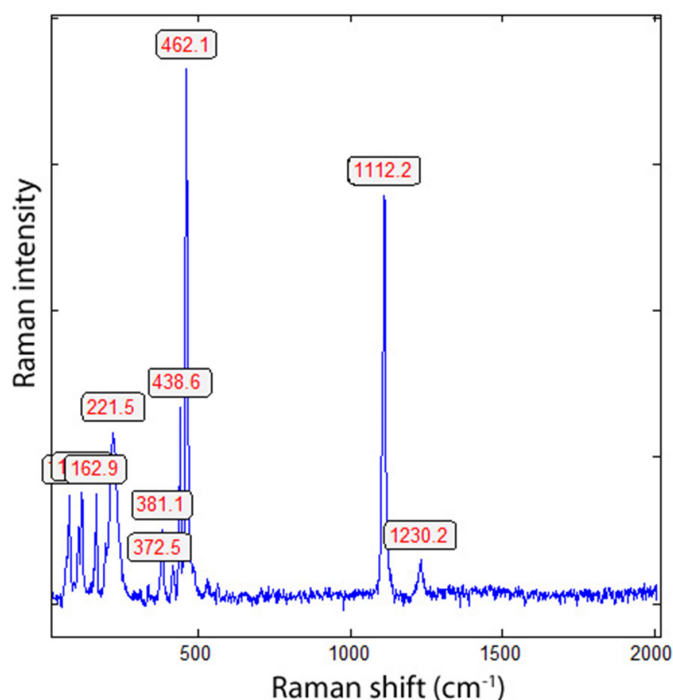


Figure 2: Raman spectrum of a rhombohedral plane.

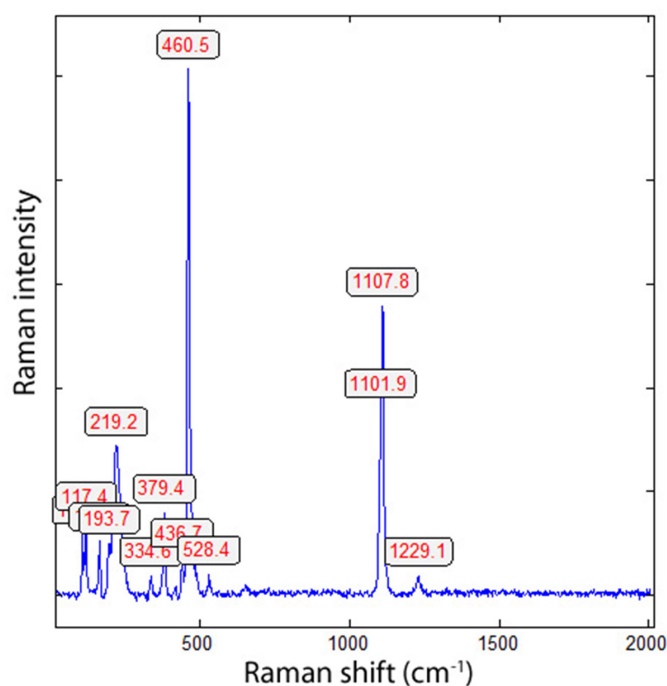


Figure 3: Raman spectrum of a prismatic plane (30° rotated).

Table 1: Important Raman lines of berlinite (in cm^{-1}).

Own Measurements (532nm)	Handbook of Raman Spectra (514nm)
75.7 $\pm$ 0.9	-
117.2 $\pm$ 0.9	120
161.7 $\pm$ 1.0	164
219.6$\pm$0.8	222
379.0 $\pm$ 1.4	375
416.6 $\pm$ 1.2	418
437.7$\pm$1.0	439
461.1$\pm$1.1	462
529.6	567
-	703
1110.0$\pm$1.2	1113
1230.5 $\pm$ 2.8	-

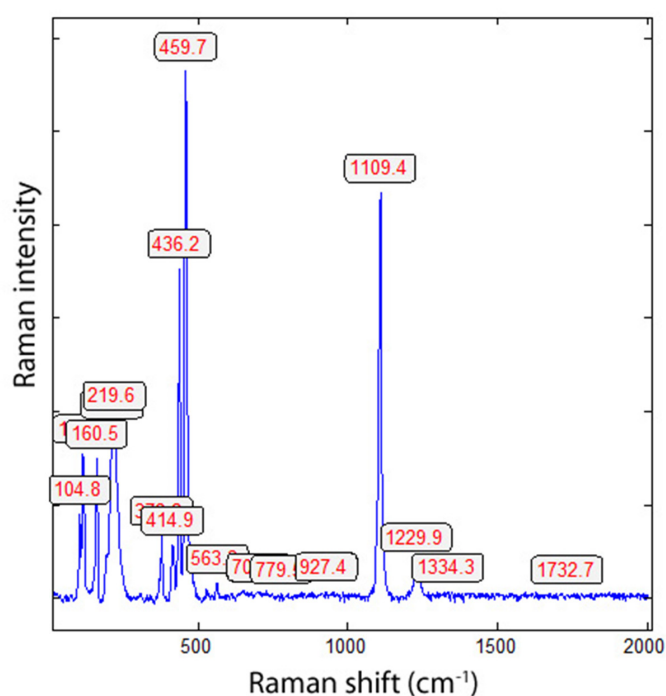
Number of measurements: n = 20.

Table 2: Diagnostic Raman bands of different berlinite samples.

Sample	$\sim 220\text{cm}^{-1}$	$\sim 461\text{cm}^{-1}$	$\sim 1110\text{cm}^{-1}$
Synthetic berlinite (AMNH)	219.6$\pm$0.8	461.1$\pm$1.1	1110.0$\pm$1.2
Vestanå/Sweden (No. 24607)	219.9	461.0	1111.0
Hålsjöberg/Sweden (No. 870025)	220.9	461.4	1111.4
Ehrenfriedersdorf/Germany, Pegmatite Qu8	214.4	460.8	1112.8

The Raman spectra are characterized by two strong bands at 462 and 1112 cm^{-1} , which are the strongest and are $\pm$ independent of orientation. Table 1 gives a comparison between our measurements and the data from the Handbook of Raman spectra [4]. Table 2 summarizes the diagnostic Raman bands of different berlinite samples.

The data from Vestanå, Halsjöberg (Sweden), and Ehrenfriedersdorf, Saxon Erzgebirge/Germany are from Thomas and Webster [1] using the Dilor XY Laser Raman Triple 800mm spectrometer with the 514nm laser. According to Figure 4 and comparison with Figure 3, we see that the Raman line at 436 cm^{-1} depends strongly on the orientation of the berlinite crystal.

**Figure 4:** Raman spectrum of berlinite of prismatic plane (120° rotated).

Discussion

Berlinite [α -AlPO₄] is isomorphous to α -quartz, showing a doubling of the unit cell along the c-axis as a result of the alternance of AlO₄ and PO₄ tetrahedral [5].

The principal claim is that berlinite exhibits a Raman spectrum that is largely insensitive to crystal orientation, with particularly strong bands near 462 and 1112cm⁻¹. This interpretation is plausible because the measurements were obtained from a well-characterized single crystal using calibrated instrumentation and multiple crystal planes. The comparison of rhombohedral and prismatic orientations provides a relevant, although limited, basis for assessing orientation dependence.

Accordingly, the data supports the more cautious conclusion that the principal Raman bands appear stable across the orientations examined, rather than demonstrating complete orientation independence. The reported variation of the 436cm⁻¹ line further indicates that orientation effects should not be dismissed, even if they are less pronounced for the strongest bands. Additional

measurements on several natural and synthetic crystals, with controlled polarization and quantitative intensity comparisons, would be required to establish the scope and reproducibility of the observed behavior.

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