Hydroxide in kyanite: A quantitative determination
of the absolute amount and calibration of the IR spectrum

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ABSTRACT

The hydrogen contents of four natural kyanites were determined by ¹⁵N nuclear reaction analysis and used to calibrate an IR spectroscopic method for a more convenient quantitative H analysis of kyanite. Hydrogen is present as the OH⁻ ion and (expressed as ppm H₂O by weight) ranges from near zero up to 230 ppm. Its content is best determined from integrated absorbance of the OH bands in the 3200-3450 cm⁻¹ range. Approximate concentrations can be determined from measurements of either summed peak heights or integrated areas of spectra obtained from just the two principal optical directions in the cleavage plane. The present calibration leads to estimates of the OH concentration in kyanite that are about a factor of 18 lower than the earlier calibration of Beran and Götzinger (1987).
INTRODUCTION

Initial infrared studies of kyanite determined that OH commonly occurs in this mineral (Beran 1970, 1971; Wilkins and Sabine 1973; Beran et al. 1983; Beran et al. 1989). OH is likewise identified in the infrared spectra of the other aluminosilicate polymorphs, andalusite and sillimanite. (Beran and Zemann 1969; Wilkins and Sabine 1973; Beran et al. 1983; Beran et al. 1989, Bell and Rossman, 1992a). The aluminosilicates are widespread components of crustal rocks and an improved knowledge of their hydrous components may lead to a further understanding of metamorphic conditions and processes. Of particular interest is the observation that the greatest concentrations of OH are generally found in samples from mantle eclogites (Beran and Götzinger 1987; Rossman and Smyth, 1990; Beran et al. 1993). This observation supports speculation that kyanite may transport some water in subducted crust and, after potential transformation to AlSiO$_3$OH, may transport some water into the deep Earth (Bell and Rossman, 1992a; Schmidt et al. 1998).

Wilkins and Sabine (1973) used electrolytic water analysis and found between 90 and 600 ppm H$_2$O in kyanites from a variety of localities. From the infrared spectra they presented, we now recognize that most of the major features in many of the spectra are from layer silicates or liquid water. However, a common feature in many of their infrared spectra and those of all other studies are a series of relatively sharp OH absorption bands in the infrared spectrum in the 3200 to 3450 cm$^{-1}$ region that are now attributed to bound OH in the kyanite structure.

IR spectroscopy is currently the most sensitive technique for quantifying OH in most minerals but requires an independent calibration for each phase. The first attempt to provide a mineral specific calibration of the kyanite spectrum was presented (Beran and Götzinger
1987) using a moisture analyzer (thermal release) to determine the water content. An alternative approximate approach to calibration is a relationship between absorption frequency and molar absorptivity, based on data for OH groups in stoichiometrically hydrous minerals as most recently revised by Libowitzky and Rossman (1997). While mineral-specific calibrations for different minerals containing OH with weak hydrogen bonds can vary up to a factor of three from the general, approximate trend (Bell et al. 2003), the kyanite calibration of Beran and Götzinger (1987) deviates by a factor of 15 in the direction of high water content.

Such a large deviation is exceptional. Based on our own experience with the tendency of thermal release experiments to overestimate the bound water content of the nominally anhydrous minerals, we elected to analyze the H concentration of four spectroscopically well-characterized kyanite crystals by $^{15}$N NRA, which yields absolute H concentration values and, thus, water concentration values. We use the results to provide a new calibration of the integrated IR absorbance and peak heights of the OH bands in kyanite.

**ANALYTICAL METHODS**

**Samples**

The study forms part of an ongoing effort to refine the quantitative analysis of trace quantities of H in minerals, in which a number of different minerals have been analyzed to date (Rossman et al. 1988, Hammer et al. 1996; Maldener et al. 2001, Bell et al. 2003). The samples were chosen to span a range of IR absorbance and most importantly, to provide a surface that minimized cracks or imperfections that might host contaminant H. Sample origins and compositions are given in Tables 1 and 2.
FSM-15 is a uniformly medium blue 5.0 x 4.1 mm crystal, extracted from a kyanite- and corundum-bearing eclogite from the Frank Smith kimberlite, South Africa. The composition and OH content of garnet in this rock were reported by Bell and Rossman (1992b). LTL-3, also derived from a kyanite eclogite xenolith in kimberlite, from Letlhakane, Botswana, is a uniformly light blue 3.2 x 2.5 mm oval slab with only a small number of inclusions. H-85943 from St. Gotthard, Switzerland, is a near-colorless 6.8 x 3.5 mm rectangular slab with a 0.3 mm blue streak running down the center of the slab. It is nearly free of internal inclusions. H-105650, from Itabira, Minas Gerais, Brazil, is a uniformly medium blue 5.6 x 2.7 mm rectangular slab with a few tubular inclusions running the width of the sample. Samples were initially prepared by exposing a cleavage surface, followed by grinding and polishing down to a final polish with 1 µm alumina. To obtain spectra with the electric vector perpendicular to the cleavage plate, two cuts with a 50 µm wire saw were made on an end of each sample. The cut surface was then polished with diamond Mylar® film down to a 1 µm final polish. Only sample H105650 had a tendency to cleave during this stage of preparation.

Compositions were determined by wavelength-dispersive X-ray analysis using the JEOL-733 electron microprobe at Caltech. Accelerating voltage was 15 kV, but beam currents and counting times were varied, depending on the concentration of the elements of interest. Natural and synthetic mineral standards were employed, and the K-ratios were converted to concentrations with the φ(ρ,z) correction scheme of Armstrong (1988).

15N Nuclear Reaction Analyses

The NRA measurements were performed using the 15N technique (Lanford, 1978), that is based on the nuclear reaction \(^1\text{H}(^{15}\text{N},\alpha\gamma)^{12}\text{C}\). They were conducted at the accelerator laboratory of the Institut für Kernphysik, Frankfurt am Main, with a 2 mm \(^{15}\text{N}^{2+}\) beam
delivered by the 7 MV Van de Graaff accelerator. The apparatus used has been specially
designed for the analysis of low H concentrations in mineral samples. A detailed description
of the experimental design can be found in Endisch et al. (1994) and a discussion of the
analytical method and a typical NRA profile has been presented for olivine (Bell et al.,
2003). Salient aspects of the kyanite analyses include a Pb-shielded bismuth germanate
(BGO) scintillation detector with anti-coincidence counting system for reduction of cosmic-
ray background, with the samples placed in a high-vacuum chamber at 2 x 10^{-9} torr.

Despite the extensive measures employed to minimize background H, a finite background
or blank level may contribute to the amount of H measured. Due to the evolving methods of
background reduction, the absolute background contribution to each analysis may vary
somewhat. In the most recent set of procedures, analysis of anhydrous silica glass and a
silicon wafer place this estimate at 2 ± 2 ppm H_2O.

**IR Spectroscopy**

Infrared spectra were determined at Caltech on either a Nicolet 60SX or a Nicolet Magna
860 spectrometer fitted with an air-spaced Glan-Foucault type LiIO_3 prism polarizer
producing linearly polarized IR radiation of high polarization purity and operating at 2 cm^{-1}
resolution. We used the sample preparation and spectrometric techniques for biaxial
minerals described by Miller et al. (1987) and Bell et al. (2003). All samples were
independently run at least twice in the β and γ polarizations to confirm that reproducible
results could be obtained.

The background correction is often not well constrained and is a potential source of
inaccuracy in the IR analysis of all minerals, particularly those with low H contents. In the
case of kyanite, the subtraction of a dehydrated mineral spectrum was not necessary because
of the simple, flat background to the OH absorptions of this mineral. Band intensities were
determined through a variety of methods as discussed in the respective sections.

RESULTS

NRA analysis

High H contents occur at the sample surface, with counts decreasing as the
comparatively H-poor interior is penetrated with higher energy ions. Figure 1 shows a
representative total profile for the FSM-15 sample and the interior profiles for the other
samples converted to their depth equivalent. The concentration profile levels off at depths of
a few hundred nm to a value that represents the intrinsic H content of the kyanite. H
concentrations determined from the NRA measurements, expressed as ppm H$_2$O by weight,
are reported in Table 1. The uncertainties reported are based on counting statistics and also
include uncertainties in stopping cross section of the $^{15}$N ions and in gamma ray detection
efficiency. The cause of the deviation from a constant H content that is obvious in the
expanded plot is the main source of uncertainty in the water content of the kyanite. Whether
this arises from inhomogeneity in the samples themselves, or from factors associated with the
analysis, is unknown. This ‘noise’ in the kyanite determinations is much greater than the
variation observed in the olivine analyses of Bell et al. (2003).

IR spectroscopy

Kyanite IR spectra are shown in Figures 2a-c and are similar to previously published
spectra. The dominant absorption in all three polarizations is between 3650 and 3450 cm$^{-1}$.
Intensity data derived from the spectra are reported in Table 1. Both integrated areas and
summed peak heights were measured in an attempt to determine the optimal way to
determine the water content of kyanite. Additional details on the exact methods are provided in the sections below on the different calibration methods.

**CALIBRATION OF THE IR SPECTRUM**

Our first approach for determining the OH concentration from the IR spectrum in the OH region in kyanite is to determine the integrated area under the OH absorption bands and to calibrate this area with the NRA results. This method previously worked well with garnets and olivines. Ideally, we would obtain spectra along the three principal axes of the indicatrix (the three principal extinction directions corresponding to the X, Y and Z axes). In the case of kyanite, the triclinic crystal system renders such measurements inconvenient. Instead, we measured the two extinction directions occurring in the plane of the (100) cleavage. These are oriented within about 30° to the Y and Z directions. The third direction measured was a vibration direction perpendicular to the cleavage plane that is within about 15° of the X direction. As Libowitzky and Rossman (1996) have shown, the total water content can be determined by spectral measurement in any three orthogonal extinction directions.

After the appropriate baselines are subtracted, the integrated areas of the three individual absorption spectra are normalized to a unit thickness and added together to obtain a ‘total’ integral absorbance, $\text{Abs}_{\text{tot}}$,

$$\text{Abs}_{\text{tot}} = \frac{1}{t_1} \int_{v_1}^{v_2} \text{Abs}_1 dv + \frac{1}{t_2} \int_{v_1}^{v_2} \text{Abs}_2 dv + \frac{1}{t_3} \int_{v_1}^{v_2} \text{Abs}_3 dv$$

(1)

where the thicknesses of the slices in the three directions are given by $t_1$, $t_2$ and $t_3$, and $\text{Abs}_1$ is the integrated absorbance in the $E \parallel 1^{\text{st}}$ direction, etc. For the purposes of our work, the unit of thickness to which data are normalized is 1.00 cm and the region of integration is usually
from 3700 to 3050 cm\(^{-1}\). This includes the three sharp bands in the 3340 to 3480 cm\(^{-1}\) region and the two overlapping bands near 3270 cm\(^{-1}\) and variable bands in the 3600 cm\(^{-1}\) region. The baseline correction is taken as a straight line between the two ends of the integration region. The results are shown in Figure 3.

Our second method is similar to the first, but uses only the two extinction directions in the cleavage plane. This method is more convenient as a practical matter due to the ease of preparation of kyanite cleavage slabs. The results are also shown on Figure 3.

Our third approach for determining the OH concentration from the IR spectrum is to determine the summed peak heights of the five bands in the 3200 – 3450 cm\(^{-1}\) in the beta spectrum. The peak height of each band is determined from the same straight baseline used for the integrations. Because the bands near 3270 cm\(^{-1}\) are overlapped and differ from spectrum to spectrum in the amount of overlap, we compared both visual estimates of the two band heights and heights determined through the PeakFit v4.05 (SPSS Inc.) program. The results of these two approaches barely differed. This approach also has the advantage that it can also be used with easily prepared cleavage fragments. Furthermore, because the spectrum consists of comparatively sharp bands on a nearly flat background, errors due uncertainty in the baseline are much less important than is the case for methods based on integration of band areas. Figure 4 shows the results.

Our fourth method was to determine just the peak height of the band at 3387 cm\(^{-1}\) in the beta spectrum. The result is shown in Figure 5 along with a point that represents Beran and Götzinger’s (1987) calibration determined as discussed in a following section. The third and fourth approaches work in the case of kyanite because the spectrum does not show large variations from sample to sample, unlike the cases of garnet and olivine.
EVALUATION OF THE RESULTS AND THE IR CALIBRATION

Our results are reported in Table 1. Using our first method of integrating three extinction directions (Fig. 3), we find significant deviation from a straight-line calibration between the infrared intensities and the water content determined with the NRA method if we include all four samples. However, if the LTL-3 data are eliminated from consideration, an excellent linear correlation exists between the integrated infrared area and the NRA water contents.

Likewise, the methods based on integration of two directions and on the sum of peak heights also deviate greatly from straight lines if the LTL-3 data are included, but exhibit a trend much closer to linear if this datum is excluded. The decision to exclude this datum is motivated by two facts. First, the kyanite spectra are similar in band positions, halfwidths, and relative heights. Thus we conclude that the spectra are coming from essentially the same chemical species. Second, in view of the spectral similarity, we expect that the IR intensities would be correlated with the absolute OH concentrations as exhibited by the other three samples. The reason for the anomalous result is not apparent, but could represent analytical error or an unrecognized heterogeneity in OH content near the surface of the sample. Thus, we elect to disregard the LTL-3 datum in order to proceed with usable results.

A linear regression of the data in Fig. 3 gives a slope of $0.149 \pm 0.012$ and intercept of $-2.74 [\pm 0.12]$ ppm H$_2$O. When constrained to pass through the origin, the regression leads to the following calibration equation:

$$
\text{H}_2\text{O (in ppm by weight)} = 0.147 [\pm 0.002] \times \text{Integrated-Abs}_{\text{tot}},
$$

(2)

where the integral absorbance is calculated for a sample of 1 cm thickness. An alternative way to express this calibration is through equation (3):

\[ \text{H}_2\text{O (in ppm by weight)} = 0.149 [\pm 0.012] \times \text{Integrated-Abs}_{\text{tot}}, \]
Integrated-Abs$_{tot}$ = $I \times$ thickness (cm) $\times$ c$_{H2O}$ \hspace{1cm} (3)

where $I$ is the integral molar absorption coefficient and c$_{H2O}$ is in units of moles$_{H2O}$/liter. In the case of kyanite, our calibration with three polarizations leads to $I = 32900$ L$\times$mol$^{-1}\times$cm$^{-2}$. This is between the corresponding $I$ values for olivine (28450) and clinopyroxene (38300) (Bell et al. 2003; Bell et al. 1995). Because kyanite varies so little in composition from the ideal endmember, c$_{H2O}$ can be determined from this calibration, within the uncertainty of our measurements, without concern for a density correction. While it has been recognized for other systems that the intensity of OH bands (as expressed through the Beer’s Law calibration constant, $\varepsilon$) tends to decrease with increasing wavenumber (Libowitzky and Rossman, 1997), we do not have enough data to determine if this is an important factor for kyanite, particularly with respect to comparison of mantle and crustal samples that have differences in the proportions of the different OH bands.

DISCUSSION

Comparison to a previous calibration

The current calibration, even with its uncertainty, differs significantly from the calibration of Beran and Götzinger (1987) (B&G). The methods used for the calibrations are different; the previous calibration used unpolarized infrared light on a cleavage slab of kyanite from Pizzo Forno, Switzerland, and an elemental analyzer for the water determination (thermal release). We can compare our results to the previous calibration in the following way. The spectrum presented for B&G’s Pizzo Forno sample (in %T) was digitized and converted to absorbance. A sample of kyanite (CIT 3750) from the same locality was run in our laboratory, both unpolarized and polarized. The ratio of the
intensities of the bands in the unpolarized spectra of the two samples at 3380 cm$^{-1}$ was used as a factor to estimate what would be the intensity of the polarized spectrum of the B&G sample with the knowledge of the intensity of the polarized spectrum of our sample. The estimate is that the 3380 cm$^{-1}$ band of the B&G sample would have an absorbance of 0.24. This value is plotted in the lower right of Figure 5 and deviates far from the calibration trend of this study. Whereas B&G found 230 ppm H$_2$O (± 12% relative uncertainty from the B&G water determination), our calibration would bring the H$_2$O content of their sample to about 13 ppm and the range of H$_2$O contents in the kyanites they studied from <0.005-0.180 wt.% to <0.0003 – 0.010 wt%.

There are two possible reasons for the difference between the two calibrations. It is now recognized that the sample of B&G contained hydrous contaminants such as kaolinite mica and chlorite (Beran, pers comm.) that would decompose during the hydrogen determination and become part of the analysis. Furthermore, the propensity of kyanite to develop incipient cleavages at the edges of the grains contributes to the analytical difficulties. These cleavages can entrap water that will also be released in the course of the analysis.

Previously, Beran et al. (1989) noted that the majority of the OH content of sillimanite was held in a form that was easily driven off at less than 700°C, and that did not contribute to the sharp OH bands in this phase. This water was believed to reside in incipient cleavages, and surface damage at the edge of the easily cleaved mineral. Kyanite is likewise subject to cleavage, and often displays internal cleavages manifested by interference colors, and incipient cleavages at the edge of the crystals. These damage sites may well be coated with water that would be released in a thermal release experiment. In contrast, because the NRA method places the sample under ultrahigh vacuum and does not analyze the edge region
of the sample where the cleavages occur, it should be nearly immune to these effects and should produce lower, but more accurate, H-contents.

**Other forms of H in kyanite**

The spectral features of layer-silicates have been identified in the 3700 – 3450 cm\(^{-1}\) region by Beran and Götzinger (1987). They become more significant in turbid regions of samples and are most prominent in crustal metamorphic samples. Because it was our goal to measure the intrinsic OH content of kyanite, rather than the OH contained in alteration products, samples for our analysis were chosen to be free as possible of any visible clay or other alteration products. However, the infrared spectra used in this calibration did include bands indicative of the presence of small amounts of clays. Consequently we included all OH bands in the integration. Because the nuclear reaction analysis interacts with only a small fraction of the entire volume of the sample, there is the possibility of a significant error in the calibration if the hydrous components are not homogeneously distributed. The amount of contribution of clays and related phases to the \(\text{Abs}_{\text{tot}}\) is typically on the order of 10% or less. The contribution to the total integrated absorbance from the bands assigned to layer silicates is small in the case of high OH-content samples (e.g. 2.3% for FSM-15) but becomes more significant for the lower OH-content samples.

**Implications for crustal and mantle water contents**

Kyanite is a minor phase overall in the crust and the mantle and the calibration presented here shows that it does not contribute significantly to the global hydrogen reservoir on the Earth. Based on the natural minerals analyzed to date, it is unlikely that kyanite transports significant quantities of water to the mantle during subduction. However, as Schmidt et al. (1998) speculate, after potential transformation to AlSiO\(_3\)OH, it may transport
some water into the deep Earth. Perhaps more significantly, this calibration lays a quantitative foundation for developing a better understanding of the role of water in metamorphic processes in the lithosphere, where kyanite and other aluminosilicates are widespread in metamorphic rocks.

ACKNOWLEDGEMENTS

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REFERENCES CITED


**FIGURE CAPTIONS**

Figure 1. a) NRA profile for kyanite FSM-15. Representative error bars based on counting statistics and nuclear corrections are illustrated for some points. The profile shows the high water content at the surface (left) and represents about 2000 nm depth into the sample on the right. b) Expanded graph of the NRA profile of the interior portion of the sample. c) NRA profiles of LTL-3 (squares), H85943 (triangles), and H105650 (circles). A horizontal line indicates the average interior water content of each sample.

Figure 2. Infrared spectra of kyanite standards scaled to 1.0 mm thickness. The spectra are displaced vertically for clarity. a) Spectra polarized in the X direction (alpha spectrum). b) Spectra polarized in the Y direction (beta spectrum). c) Spectra polarized in the Z direction (gamma direction).

Figure 3. Correlation of the infrared integrated intensities vs. water content determined by NRA for kyanite. The graph compares integrations of all three extinction directions with the two extinction directions (β’ and γ’) in the cleavage plate. The line through the 3-polarization data is a linear regression that does not include the datum for LTL-3. The
dotted line through the 2-polarization data is not based on a regression; it is only intended
to suggest an approximate working curve for 2-polarization data.

Figure 4. Relationship between the summed infrared band heights in the beta spectrum on the
cleavage plane vs. the water content determined by NRA.

Figure 5. Comparison of our calibration to the calibration of Beran and Götzinger (1987) as
expressed through the height of the 3380 cm$^{-1}$ band.
Table 1. Sample details and the results of NRA and IR H$_2$O analyses.

<table>
<thead>
<tr>
<th>Sample number</th>
<th>H105650*</th>
<th>H85943*</th>
<th>LTL-3</th>
<th>FSM-15</th>
</tr>
</thead>
<tbody>
<tr>
<td>Locality</td>
<td>Itabira, Minas Gerais</td>
<td>Letlhakane Mine</td>
<td>Frank Smith Mine</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Brazil</td>
<td>Brazil</td>
<td>Botswana</td>
<td>South Africa</td>
</tr>
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<td>H$_2$O (ppm by weight by NRA)</td>
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<td>22</td>
<td>27</td>
<td>230</td>
</tr>
<tr>
<td>IR integ/cm ($\alpha+\beta+\gamma$)</td>
<td>46</td>
<td>165</td>
<td>803</td>
<td>1560</td>
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<tr>
<td>IR integ/cm ($\beta+\gamma$)</td>
<td>1</td>
<td>142</td>
<td>393</td>
<td>780</td>
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<tr>
<td>Peak height per mm at 3380 cm$^{-1}$</td>
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<td>0.371</td>
<td>0.567</td>
<td>1.679</td>
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<tr>
<td>Sum of 5 peak heights in beta</td>
<td>0</td>
<td>0.67</td>
<td>1.66</td>
<td>3.73</td>
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* Harvard University Mineral Museum Sample Number
Table 2. Composition of kyanite samples in wt. % determined by electron microprobe analysis.

<table>
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<tr>
<th>Sample</th>
<th>Na&lt;sub&gt;2&lt;/sub&gt;O</th>
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<th>MnO</th>
<th>Fe&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;3&lt;/sub&gt;</th>
<th>NiO</th>
<th>P&lt;sub&gt;2&lt;/sub&gt;O&lt;sub&gt;5&lt;/sub&gt;</th>
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* not determined