

## Quadrupole splitting distributions in triclinic astrophyllite

ZHE LI<sup>1</sup>, ZHESHENG MA<sup>2</sup>, MING XIONG<sup>2</sup>, NICHENG SHI<sup>2</sup>, DANIAN YE<sup>1</sup> and ALEXANDR KHOMYAKOV<sup>3</sup>

<sup>1</sup> Institute of Geology and Geophysics, Chinese Academy of Sciences, P.O. Box 9825, Beijing 100029, China

<sup>2</sup> China Geoscience University, Beijing 100083, China

<sup>3</sup> Department of Geology, Moscow State University, Moscow, Russia

**Abstract:** The mineral, triclinic astrophyllite, was investigated using the Mössbauer effect. The Mössbauer spectra of triclinic astrophyllite at 298 K, 180 K and 90 K were measured, and the quadrupole splitting distributions (QSDs) from the Mössbauer spectra were obtained by using a Voigt-based method for line shape analysis. The distortion parameters, the variances of the octahedral bond angles for triclinic astrophyllite, were calculated, and a site assignment was tentatively given based on the distortion parameters. According to the ratios of ferric to total iron obtained by the Mössbauer effect and the mean value of  $f(\text{Fe}^{3+}(\text{O}))/f(\text{Fe}^{2+}(\text{O}))$ , the chemical formula of triclinic astrophyllite was rewritten.

**Key-words:** Mössbauer effect, quadrupole splitting distributions, astrophyllite.

### Introduction

Astrophyllite, mica-like titanium silicate, is known to have several polymorphic modifications with different symmetries and compositions. Triclinic astrophyllite,  $\text{K}_2\text{Na}(\text{Fe}, \text{Mn}, \text{Mg})_7[\text{Ti}_2(\text{Si}_4\text{O}_{12})_2\text{O}_3](\text{OH}, \text{F})_4$ , is a mineral belonging to the astrophyllite group. It is characterized chemically by the presence of large amounts of sodium, titanium or zirconium, and the almost complete absence of aluminium. Astrophyllite occurs as accessory or pegmatite mineral in alkaline igneous rocks and has been reported from several localities including Kraemers Island, East Greenland (Layne *et al.*, 1982), Egypt (Abdel-Rahman, 1992) and Eastern Tibet (Liu *et al.*, 1997). The crystal structure of triclinic astrophyllite has been investigated by several authors (Peng & Ma, 1963, 1964; Woodrow, 1967; Yamnova *et al.*, 2000; Ma *et al.*, 2001). Although the crystal structure of triclinic astrophyllite has been studied in detail, the Mössbauer effect has not been applied to study triclinic astrophyllite. The Mössbauer spectra of triclinic astrophyllite at 298 K, 180 K and 90 K were measured in this work, and the quadrupole splitting distributions from the Mössbauer spectra were obtained by using a Voigt-based method.

### Samples and experimental

The sample of triclinic astrophyllite investigated here are from Khibina alkaline massifs, Kola Peninsula, Russia (sample no. 3098), and it is rice-straw-yellow in color. X-ray diffraction method was used to check purity of the sample, and no other phases were found. The electron micro-

probe analysis for the sample yields the formula  $(\text{K}_{1.579}\text{Na}_{0.990}\text{Ca}_{0.524})_{3.093}(\text{Fe}^{2+}_{5.182}\text{Mn}_{0.988}\text{Mg}_{0.372})_{6.542}[(\text{Ti}_{1.775}\text{Nb}_{0.056}\text{Zr}_{0.052}\text{TR}_{0.005}\text{Ba}_{0.012})_{1.900}(\text{Si}_{7.388}\text{Al}_{0.475})_{7.863}\text{O}_{24}](\text{O}_{1.430}(\text{OH})_{4.428}\text{F}_{1.142})_7$  or  $(\text{K}_{0.790}\text{Ca}_{0.262})_2\text{Na}_{0.990}(\text{Fe}_{0.740}\text{Mn}_{0.141}\text{Mg}_{0.053})_7[(\text{Ti}_{0.888}\text{Nb}_{0.028}\text{Zr}_{0.026}\text{Ba}_{0.006}\text{TR}_{0.003})_2((\text{Si}_{1.847}\text{Al}_{0.119})_4\text{O}_{24})/(\text{O}_{0.477}(\text{OH})_{0.523})_3]((\text{OH})_{0.715}\text{F}_{0.286})_4$  for triclinic astrophyllite, where TR represents total amount of rare earth elements.

Transmission  $^{57}\text{Fe}$  Mössbauer spectra of triclinic astrophyllite were collected with an M-500 spectrometer in conjunction with a CANBERRA 35 1024 multichannel analyzer. A  $\sim 10$  mCi  $^{57}\text{Co}/\text{Pd}$  matrix single-line source was used to measure the Mössbauer spectra. The detector used was a xenon (methane) proportional counter. The velocity range was  $\pm 4.89$  mm/s and the spectrometer velocity was regularly calibrated by using a thin high-purity  $\alpha$ -Fe foil. The isomer shifts are given relative to  $\alpha$ -Fe. The spectra at 180 K and 90 K were obtained by means of an OXFORD MD 306 cryostat. This model is capable of changing the temperature in the range of 77–300 K using nitrogen with a variation of 0.5 K. Approximately 8 mg  $\text{Fe}/\text{cm}^2$  for the sample was used in this study.

The two symmetric spectra (512 channels each) were calibrated, folded, and analyzed using the Voigt-based quadrupole splitting distribution (QSD) method. The methodology was described in detail by Rancourt & Ping (1991), Ping *et al.* (1991) and Rancourt (1994). In an absorption experiment using a thin absorber, the width of Lorentzian line  $\Gamma$  has a precise physical meaning, and is not an adjustable parameter. Since  $\Gamma = 0.24$  mm/s is a typical value for silicates in our laboratory without using the QSD method, the Lorentzian width  $\Gamma$  was constrained to be this value