Data in Brief 42 (2022) 108282

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

# Data on FTIR spectra of the clays KGa-1b and STx-1b and their mixtures at different moistures

T. Nazdracheva, A. Morozov, V. Yavna*, A. Kochur

*Rostov State Transport University, Narodnogo Opolcheniya Sq., Rostov-on-Don, 344038 Russia*

ARTICLE INFO

*Article history:*
Received 17 February 2022
Revised 3 May 2022
Accepted 9 May 2022
Available online 16 May 2022

*Keywords:*
Minerals
Clays
Hydration
Infrared spectroscopy

ABSTRACT

Kaolinite and smectite are among the main soil-forming minerals, and therefore their properties are constantly being refined. This article provides data on the IR spectra of the clays KGa-1b and STx-1b containing 96% and 67% of those minerals [1], and their mixtures in equal mass proportions at different moisture contents. These data were used in the article "Study of hydration of kaolinite and montmorillonite mixture by IR spectroscopy" [2], to study the dynamics of the formation of water layers on the surface of clay particles. The data presented can be used to test experimental methods for studying the adsorption properties of mixtures, and to create new laboratory methods for determining the plastic properties of soils [3]. In addition, the data presented can be used to verify theoretical approximations and computer models for calculating the structure and electronic properties of minerals and their mixtures [4].



DOI of original article: 10.1016/j.molstruc.2021.131871
* Corresponding author.
*E-mail address:* vay@rgups.ru (V. Yavna).

https://doi.org/10.1016/j.dib.2022.108282

## Specifications Table

.

| | |
|---|---|
| **Subject** | Chemistry |
| **Specific subject area** | FTIR spectra reflecting the peculiarities of the formation of water layers on the surface of particles of clays KGa-1b, STx-1b, and their mixture at different sample moisture contents. |
| **Type of data** | Figures, Excel data tables |
| **How data were acquired** | The data were obtained by an infrared spectrometer (Bruker Optik GmbH, Ettlingen, Germany) with Alpha-E module and OPUS software, climatic chamber HD KWGDS62IF (Hyde Science and Technology Limited), AB 1200-1 analytical balance (OKB VESTA, Russia) |
| **Data format** | Raw |
| **Description of data collection** | The effect of moisture of samples on the characteristics of the IR spectra was studied. The samples were prepared by crushing in a porcelain mortar for 10 min and then dried to constant weight at a temperature of 105° C. Mixture samples were prepared from dried clay samples taken in equal mass ratios with an accuracy of 0.1%. After drying the clays to constant weight, the samples still contained some bound water and some unknown small moisture content. We take this residual moisture as the reference zero, and thus the moistures obtained during sample preparation are increments to the residual moisture. When preparing a sample with a given moisture $w$, 200 mg of dry clay or a mixture of clays, and $2w$ mg of double distillation water were used, the mass of water was also determined with an accuracy of 0.1%. After adding water, each prepared sample was subjected to thorough mixing and stored in a sealed vessel.IR spectra were recorded in the mid-infrared range from 500 to 4000 $cm^{-1}$. The IR spectra were recorded with the resolution of 2 $cm^{-1}$ and averaged over 25 scans. |
| **Data source location** | Rostov State Transport University, 2 Narodnogo Opolcheniya Sq., Rostov-on-Don, 344038, Russia |
| **Data accessibility** | Repository name: Mendeley Data<br>Data identification number: 10.17632/h3rg5htwxx.1<br>Direct link to the dataset: https://data.mendeley.com/datasets/h3rg5htwxx/draft?a=5f48926b-2a9e-4798-a1f1-3f90d37cd277 |
| **Related research article** | T. Nazdracheva, A. Morozov, V. Yavna, A. Kochur, Study of hydration of kaolinite and montmorillonite mixture by IR spectroscopy, J. Mol. Struct. 1250, Part 3 (2022) 131871. https://doi.org/10.1016/j.molstruc.2021.131871 |

## Value of the data

- The data are useful for studying the dynamics of the liquid phase in mixtures of clay minerals.
- The data will be of interest to scientists working in the field of surface properties modification.
- Data analysis methods can be used to test experimental and theoretical methods for studying the adsorption properties of mixtures.
- Further development of data analysis methods may lead to the creation of new technologies for determining the properties of clay soils for use in engineering applications.

## 1. Data description

Fig. 1 shows the IR spectra of water and the KGa-1b clay at different moisture contents. The table of raw data used for plotting the graphs in Fig. 1 are in the file Figure_1.xlsx. Fig. 2 shows the IR spectra of water and the STx-1b clay at different moisture contents. The table of raw data used for plotting the graphs in Fig. 2 are in the file Figure_2.xlsx. Fig. 3 shows the IR spectra of a mass 1:1 mixture of the KGa-1b and STx-1b clays prepared at different moistures. The table of

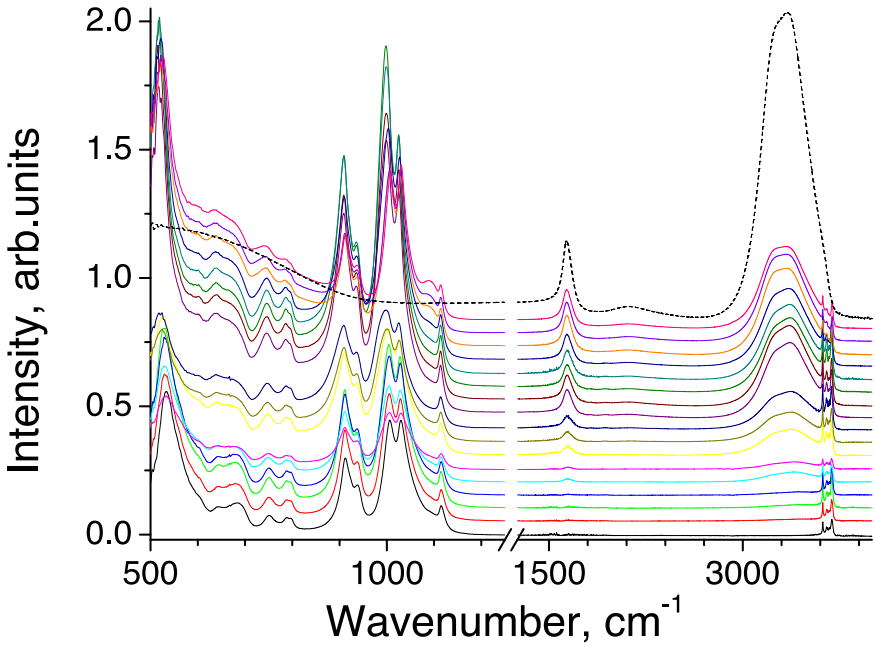


**Fig. 1.** IR spectra of the KGa-1b clay at moisture (*w*%): 0, 3, 6, 9, 15, 18, 20, 25, 30, 32, 35, 40, 50, 60, 65, 70, 80 (bottom to top) and $H_2O$ (dashed line)

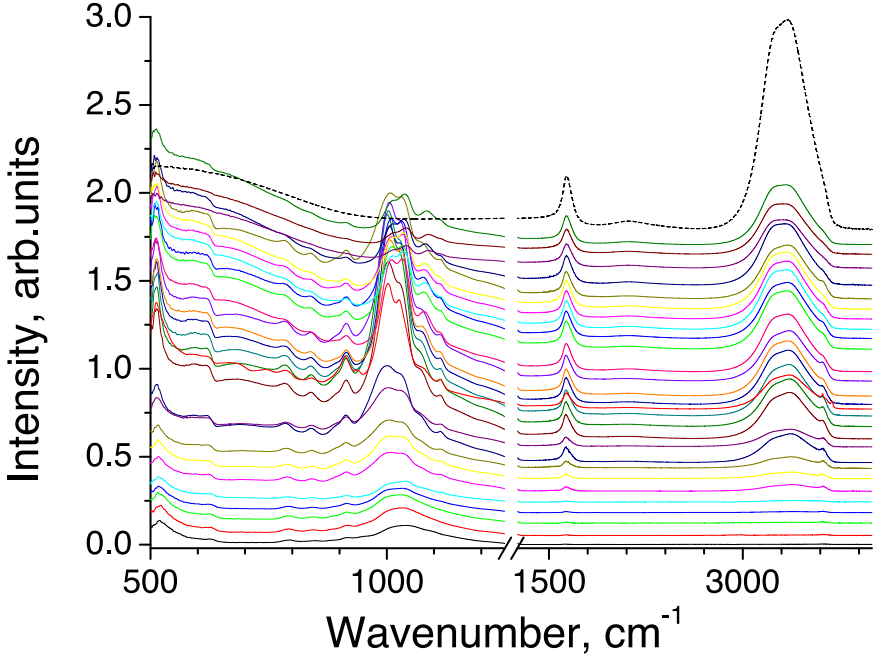


**Fig. 2.** IR spectra of the STx-1b clay at moisture (*w*%): 0, 3, 6, 9, 15, 20, 25, 30, 35, 40, 45, 50, 60, 70, 80, 90, 95, 100, 110, 120, 130, 140, 150, 160, 170, 180, 190, 200 (bottom to top) and $H_2O$ (dashed line)

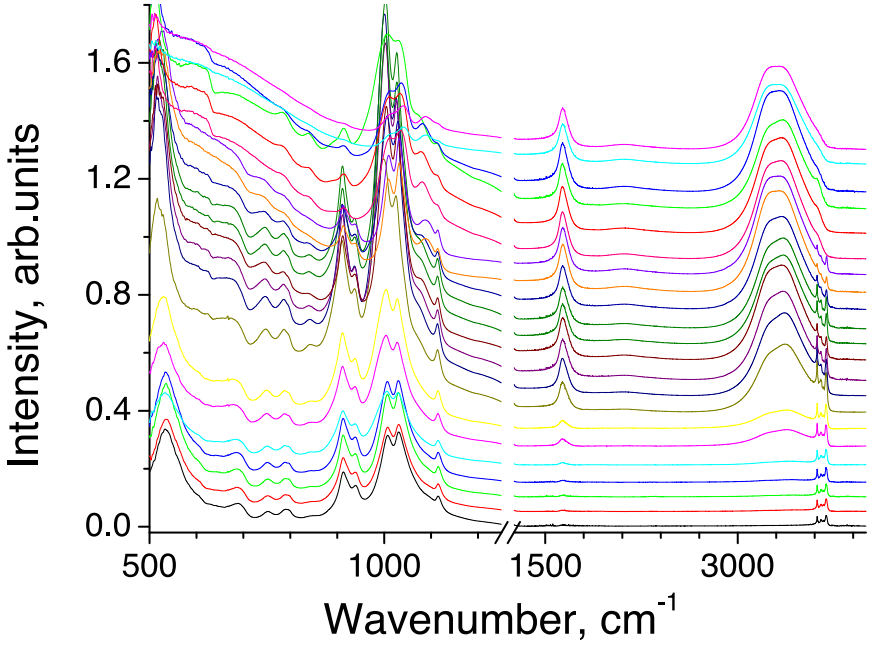


**Fig. 3.** IR spectra of a mixture of KGa-1b and STx-1b clays at moisture (*w*%): 0, 3, 6, 9, 20, 25, 30, 40, 50, 60, 70, 80, 90, 100, 110, 120, 130, 140, 160, 170, 180, 190 (bottom to top).

raw data used for plotting the graphs in Fig. 3 are in the file Figure_3.xlsx. The moistures used are given in the figures captions. Figs. 1 and 2 show the spectra of the liquid phase of distilled water ($H_2O$) for comparison with the spectra of the samples.

In the above figures, the abscissa shows the wavenumbers in the range 500 - 4000 $cm^{-1}$. The ordinate shows the intensities of the IR-ATR spectra in arbitrary units. The spectra of samples of different moisture and water are shifted relative to each other along the ordinate axis. The positions of the spectra were chosen arbitrarily from the condition of the least overlap of the spectra in the figures.

In the raw data tables Figure_1.xlsx, Figure_2.xlsx and Figure_3.xlsx, the first line contains information about the units of measurement of wave numbers and moisture, and the second line shows the moistures of the samples. The first column contains 19768 values of the wavenumber, and the following columns show respective intensities of the spectra. In tables Figure_1.xlsx and Figure_2.xlsx, the last column shows the intensities of the spectra of liquid distilled water.

## 2. Experimental design, materials and methods

The clays KGa-1b, STx-1b and their mechanical mixture in equal mass ratios were used as samples for spectroscopic studies. Mineral samples were obtained from Clay Minerals Society [5]. When preparing the samples, the clays were preliminarily ground in a porcelain mortar for 10 min. The applied pressure was low, which made it possible to avoid mechanochemical activation of the samples.

The crushed clays were dried to constant weights at a temperature of 105°C. Mixture samples were prepared from dried clay samples taken in equal mass ratios with an accuracy of 0.1%. After drying the clays to constant weight, the samples still contained some bound water and some

unknown small moisture content. We take this residual moisture as the reference zero, and thus the moistures obtained during sample preparation are increments to the residual moisture.

To prepare a sample with moisture $w$ (in %), the following formula was used: $w=(m_{H2O}/m) \times 100\%$, in which $m$ is the mass of the dry sample, $m_{H2O}$ is the mass of water determined by drying. When preparing a sample with a given moisture w, 200 mg of dry clay or a mixture of clays, and 2w mg of double distillation water were used, the mass of which was also determined with an accuracy of 0.1%. After adding water, each prepared sample was subjected to thorough mixing and stored in a sealed vessel.

For each individual measurement of the IR spectrum, 50 mg of dry clay or 50+w/2 mg of clay with moisture content w was used. The maximum moisture reached 200% for STx-1b clay. This moisture corresponds to the sample mass of 150 mg.

IR spectra in the mid-infrared range (500 - 4000 $cm^{-1}$) are measured by the total reflection method (IR-ATR). The IR spectra were averaged over 25 scans with a resolution of 2 $cm^{-1}$. The spectra were collected from natural surfaces of samples placed on a ZnSe crystal with an area of 19.6 $mm^2$.

The spectra were obtained at different moisture contents for a detailed study of the effect of moisture on spectral characteristics. The moisture contents of the samples were monitored before and after spectroscopic studies. The average value of the half-sum of the results of these measurements rounded to the nearest whole number was used as the moisture content of the sample. In the cases when the moisture content of the samples was above the liquid limit, in order to minimize the effect of gravitational squeezing of water, spectroscopic studies were carried out immediately after sample preparation.

## Ethics statements

None.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## CRediT Author Statement

**T. Nazdracheva:** Data curation, Writing – original draft; **A. Morozov:** Visualization, Investigation; **V. Yavna:** Conceptualization, Methodology, Writing – review & editing.

## Acknowledgments

This work was supported by the Russian Science Foundation (Grant No.21-79-20005).

## References

[1] S.J. Chipera, D.L. Bish, Baseline studies of the clay minerals society source clays: powder x-ray diffraction analyses, Clays Clay Minerals 49 (5) (2001) 398–409.
[2] T. Nazdracheva, A. Morozov, V. Yavna, A. Kochur, Study of hydration of kaolinite and montmorillonite mixture by IR spectroscopy, J. Mol. Struct. v. (2022) 131871 1250, Part 3.
[3] V. Yavna, T. Nazdracheva, A. Morozov, Y. Ermolov, A. Kochur, Ab initio simulation of the IR spectrum of hydrated kaolinite, Crystals 11 (2021) 1146, doi:10.3390/cryst11091146.
[4] T.F. Nazdrachevaa, A.V. Kukharskii, A.S. Kasprzhitskii, G.I. Lazorenko, V.A. Yavna, A.G. Kochur, Opt. Spectroscopy 129 (2) (2021) 270–275.
[5] https://www.clays.org/sourceclays_data.html