

Prospecting for spodumene pegmatites by statistical evaluation of trace elements in magmatic muscovite

SCHUBERTH-HLAVAC GERALD ¹⁾, MALI HEINRICH ²⁾, SCHUSTER RALF ¹⁾, STEINER RALF ²⁾, ROHRHOFER SANDRO ²⁾, ZAHRL MARCEL AARON ²⁾, SWEDA MARTIN ²⁾, HORVAT CHRISTIAN ²⁾, KNOLL TANJA ¹⁾

Introduction

During the past years, pegmatite occurrences belonging to the Austroalpine Unit Pegmatite Province were investigated in the frame of the projects MRI_Pegmatite I/II. These projects are part of "Initiative GBA-Forschungspartnerschaften Mineralrohstoffe – MRI" and aim to investigate the economic potential of the rocks with respect to lithium and other rare elements.

Based on the appearance in the field and the mineralogical composition pegmatite bodies of about 1400 sites are categorized as pegmatite, leucogranite or spodumene-pegmatite. Field and analytical data (whole-rock and mineral geochemistry, geochronological age data, isotopic composition, ...) concerning these pegmatite occurrences are available in a database, which allows visualizing certain parameters in maps.

Of special interest are major and trace elements of magmatic muscovite, which allow to determine regional fractionation trends and prospective areas. In this contribution, we present results of a data mining method applied on muscovite geochemistry, which was applied to infer the pegmatite categories recognized in the field. Thus, data analysis helps in prospecting for additional spodumene pegmatite bodies and to identify further target areas.

Regional geology

The investigated Austroalpine Unit Pegmatite Province formed during Permian lithospheric extension by anatectic melting of aluminum rich metapelites. Simple pegmatite, evolved pegmatite, leucogranite and spodumene pegmatite appear in different levels of the Permian middle and lower crust embedded in certain host rocks [1].

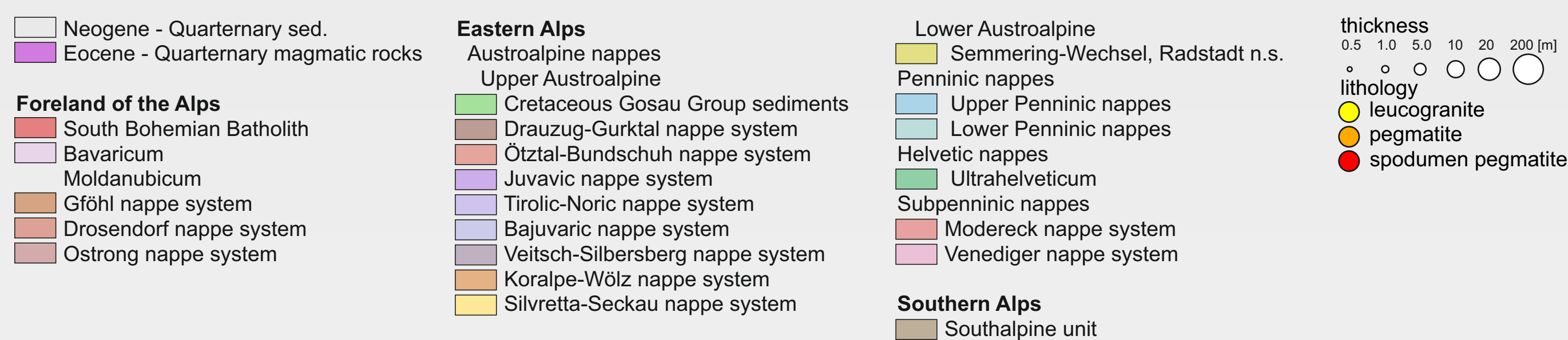
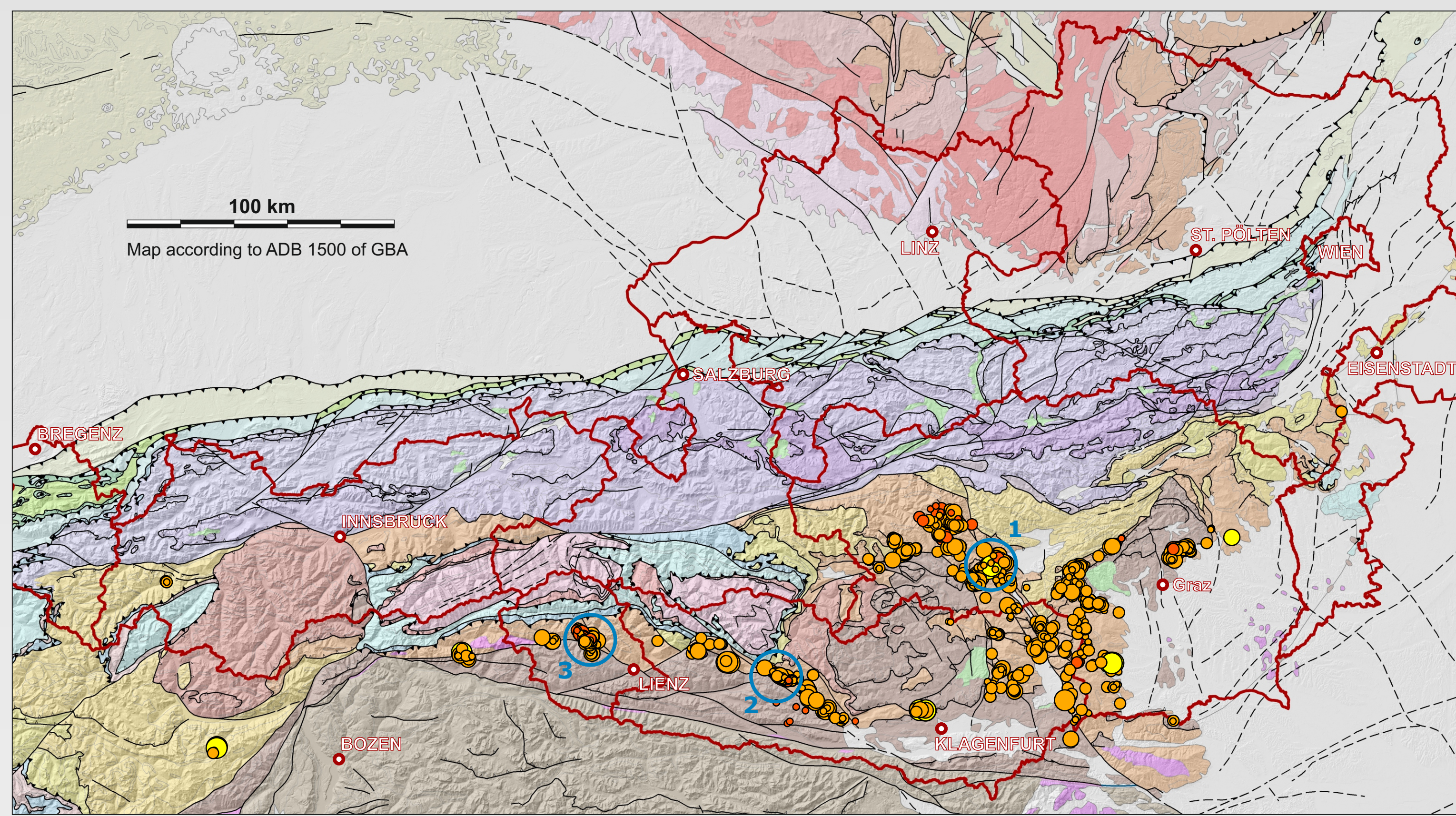


Fig. 1: Map showing investigated sites of pegmatite, leucogranite and spodumene pegmatite. Tectonic map of Austria after ADB 1500 of GBA. Most prospective areas are indicated by blue numbers: (1) Falkenberg, (2) Millstätter See-Rücken, (3) Ratzell

Data set

For statistical evaluation, 1943 analyses of 43 major and trace elements of magmatic muscovite grains of at least 5 mm in diameter from leucogranite (40, 2%), pegmatite (1821, 94%), and spodumene pegmatite (82, 4%) bodies were used. These analyses are from 921 sample points.

Muscovite grains were analyzed by SEM-EDX (major elements) and LA-ICP-MS (trace element). Trace element contents from LA-ICP-MS were corrected to an ideal muscovite (Si 21.15 wt%) using silicon content from SEM-EDX. The data set is partially incomplete because some elements were measured in some muscovite grains only (Fig. 2).

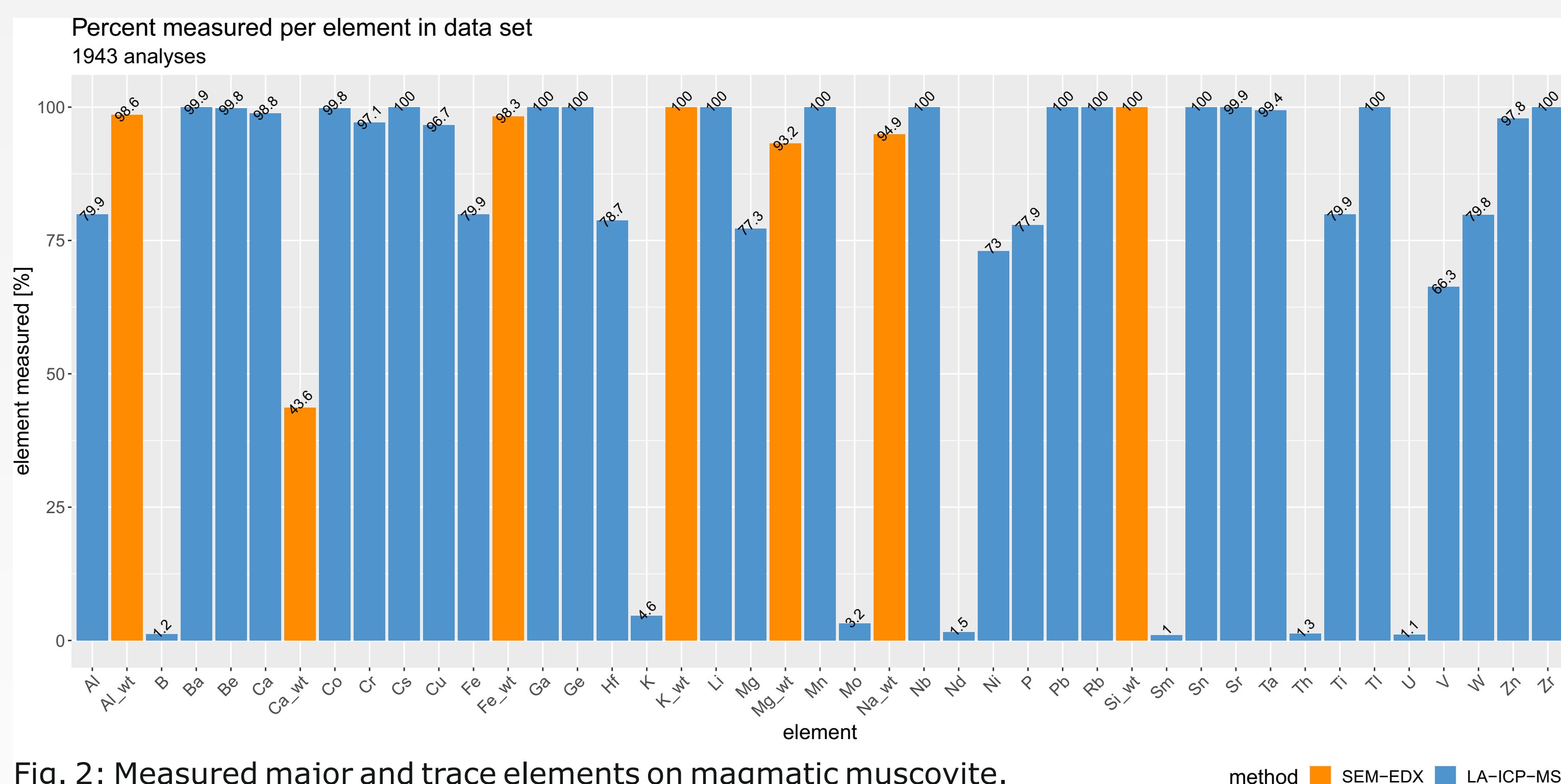


Fig. 2: Measured major and trace elements on magmatic muscovite.

References

- [1] KNOLL, TANJA ; SCHUSTER, RALF ; HUET, BENJAMIN ; MALI, HEINRICH ; ONUK, PETER ; HORSCHINEGG, MONIKA ; ERTL, ANDREAS ; GIESTER, GERALD: Spodumene Pegmatites and Related Leucogranites from the Austroalpine Unit (Eastern Alps, Central Europe): Field Relations, Petrography, Geochemistry, and Geochronology. In: The Canadian Mineralogist vol. 56, Mineralogical Association of Canada (2018), Nr. 4, pp. 489–528
- [2] BREIMAN, L. ; FRIEDMAN, J. H. ; OLSHEN, R. A. ; STONE, C. J.: Classification and regression trees: Wadsworth, Inc., 1984
- [3] OKRUSCH, MARTIN ; MATTHES, SIEGFRIED: Mineralogie: Eine Einführung in die spezielle Mineralogie, Petrologie und Lagerstättenkunde. Neunte. : Springer Spektrum, 2014
- [4] R CORE TEAM: R: A Language and Environment for Statistical Computing. Vienna, Austria : R Foundation for Statistical Computing, 2021
- [5] THERNEAU, TERRY ; ATKINSON, BETH: rpart: Recursive Partitioning and Regression Trees, 2019. — R package version 4.1-15

Statistical method

In order to classify pegmatites by analyzing their magmatic muscovite grains, methods of multivariate statistics and data mining are useful. Two requirements should be met here:

- 1) Little data preparation should be necessary, so that one can easily work with the whole data set and little specific knowledge about data analysis is needed.
- 2) The result should be understandable and interpretable also by non-experts.

Here, classification and regression trees (CART) [2] were used, this well-known method is well suited for the problem at hand: On the one hand, it is possible to work with an incomplete data set and on the other hand, the generated decision trees are easy to visualize and understand - in contrast to black-box models like artificial neural networks.

Data quality check: The data set was subjected to a plausibility check to see whether the many data to be evaluated represent muscovite (Fig. 3). Further, correlation matrices were generated to check whether the corresponding correlations are present for certain elements.

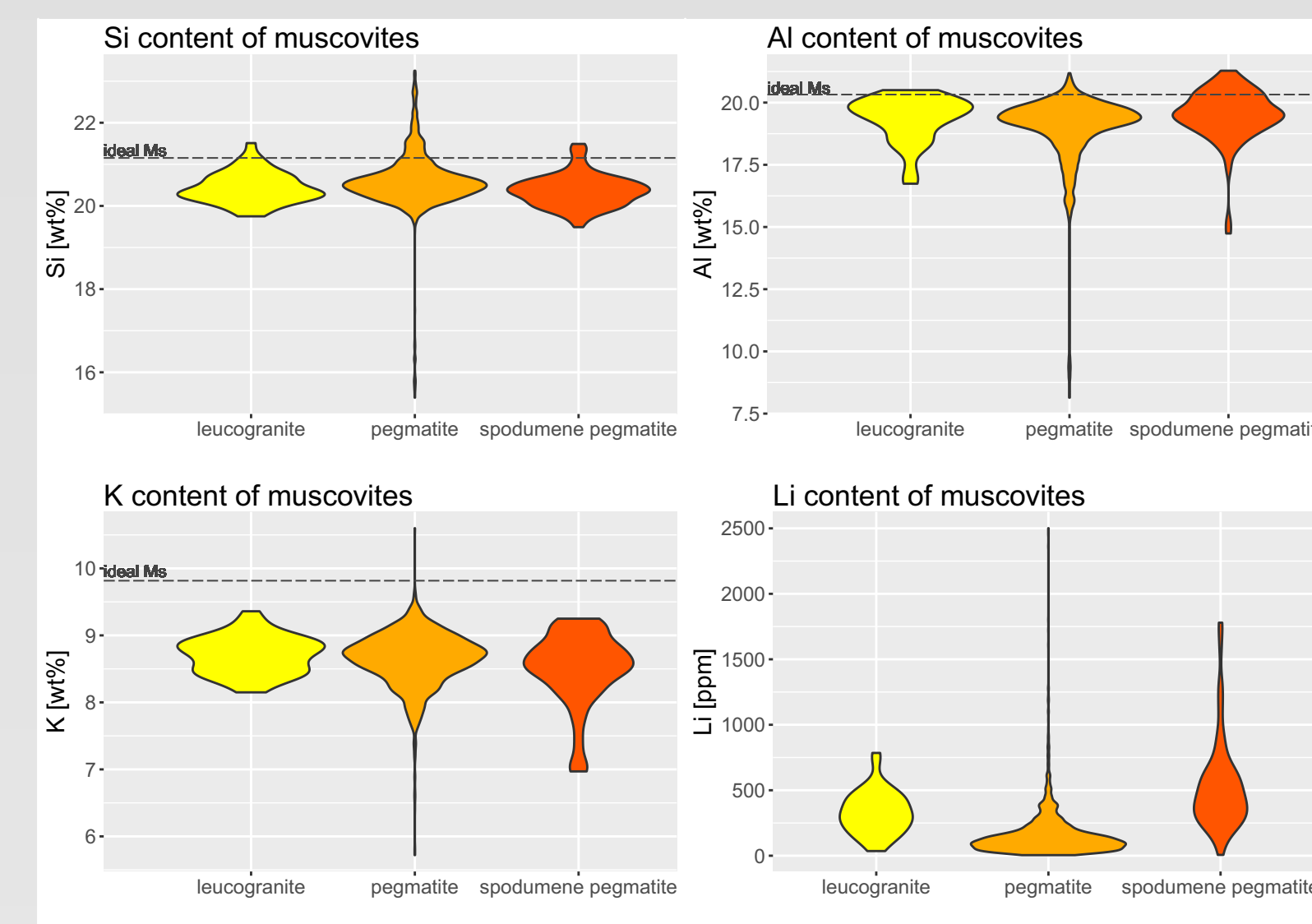


Fig. 3: Violin plots of Si, Al, K, and Li content of the analyzed muscovite grains in different pegmatite categories. The concentration of the respective element in an ideal muscovite is shown as a gray line.

The data check indicates that:

- The available data correlate with an ideal muscovite $KAl_2(Si_3Al)O_{10}(OH)_2$ regarding the major elements Si, Al, K.
- Muscovite crystals from the spodumene pegmatite tend to have a higher Li and Al but lower K contents than muscovite from the other pegmatite categories. This is due to the Li uptake of these muscovites [3].
- The major elements Si, Al and K are not suitable for classification of the pegmatites because their statistical discriminatory power is not high enough
- The data quality seems to be adequate for further calculations.

Classification by decision tree: A binary decision tree (Fig. 4) was generated from all available data using the software R [4] and the library rpart [5] according to the procedure for CART.

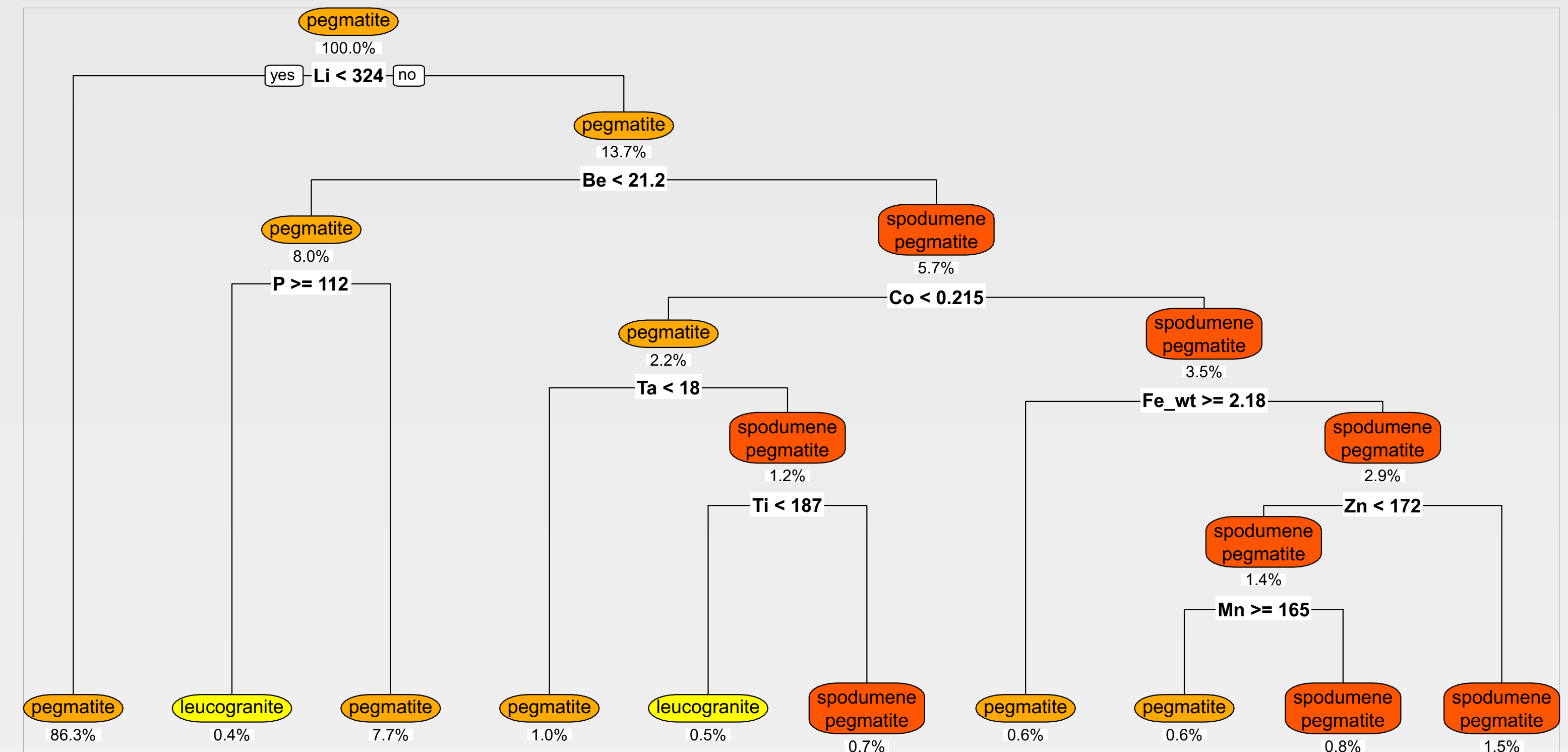


Fig. 4: Decision tree applied on 43 elements of magmatic muscovite.

The following **insights** can be gained from the visualization:

- Li and Be are the **most indicative elements** to infer spodumene pegmatite of the Austroalpine Unit Pegmatite Province by the geochemistry of magmatic muscovite.
- Using this tree, 1878 samples or 97% are correctly classified, whereas 65 samples or 3% are misclassified. This in-sample test overestimates the prediction accuracy, of course. However, even when dividing the available data set into random training and evaluation sets - which then yield other trees - accuracy below 94% has never been determined with the available data set.
- **Simple rules** are derivable by following the tree from top to bottom: E.g. pegmatite if $Li < 324$, leucogranite if $Li \geq 324$ and $Be < 21$ and $P \geq 112$, spodumene pegmatite if $Li \geq 324$ and $Be \geq 21$ and $Co \geq 0.22$ and $Fe_wt < 2.2$ and $Zn \geq 172$, ...
- One of the great advantages of CARTs is that they can handle missing data. This is done by creating **surrogates** for the corresponding predictors. For example, in the above set of rules, e.g. if no Co content is available, the rule "Ba < 2.242 to the left" can be used instead of the division rule "Co < 0.215 to the left". The accuracy decreases by these surrogates, because they are formed based on correlations to the actual division.

Conclusion

- Muscovite geochemistry can be used to distinguish pegmatite categories of the Austroalpine Unit Pegmatite Province.
- CARTs seem suitable for this purpose because they cope with missing data in classification and provide results that are easy to interpret.
- On the other hand, these trees suffer from strong variance - they are not stable. A different training dataset yields a different tree. This can be handled with methods like "bagging" or "random forests". However, these methods need more data preparation (e.g. handling of missing data) and the results cannot be visualized in simple graphs.
- As with geochemical discrimination diagrams one may not forget the "garbage in garbage out"-principle when using data mining and machine learning methods.
- Possible application: Since muscovite - unlike spodumene - is easy to identify in the field even by non-experts, this method allows for a fast and easy prospecting of spodumene bearing pegmatite in larger pegmatite fields.
- This method identified several pegmatite bodies and areas within the Austroalpine Unit, where spodumene is likely to occur. These areas are shown in Fig. 1.

¹⁾ Geological Survey of Austria, Neulinggasse 38, 1030 Vienna

²⁾ Lehrstuhl für Geologie und Lagerstättenlehre, Peter-Tunner-Straße 5, 8700 Leoben