Mineral Identification by Elemental Composition:
A New Tool with PDF-4 Databases

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Summary

Many minerals have characteristic elemental profiles that can often distinguish the mineral from others by their composition differences. In Release 2016 ICDD PDF-4 databases 20,670 unique compositions have been identified out of 44,341 mineral and mineral related entries. For many common mineral classes such as garnets, kaolin and olivine, there are multiple distinct compositions but they fall within well-defined composition ranges. The ICDD has developed a microanalysis tool to help scientists identify minerals from a micro-XRF or a microprobe analysis. In all PDF-4 databases all entries have their chemical formula expressed in atomic and weight percent. This data can be data mined and ICDD has developed algorithms that are analogous to the search/match processes used for powder diffraction identification. Data can be input as either the element or common oxide.

To test the algorithm and graphics interfaces we compared results from the microanalysis module to the published data from the Smithsonian Microbeam reference mineral collection. The software correctly identified 18/22 minerals by the highest merit score in the algorithm. In the other 4 cases, the correct mineral was among the top candidates but another isoelemental mineral was selected. In 12 cases the identification not only identified the right mineral but also matched total composition (mass balance) within 96 to 100% on real specimens. This new analysis module is scheduled to be released with all 2017 PDF databases.
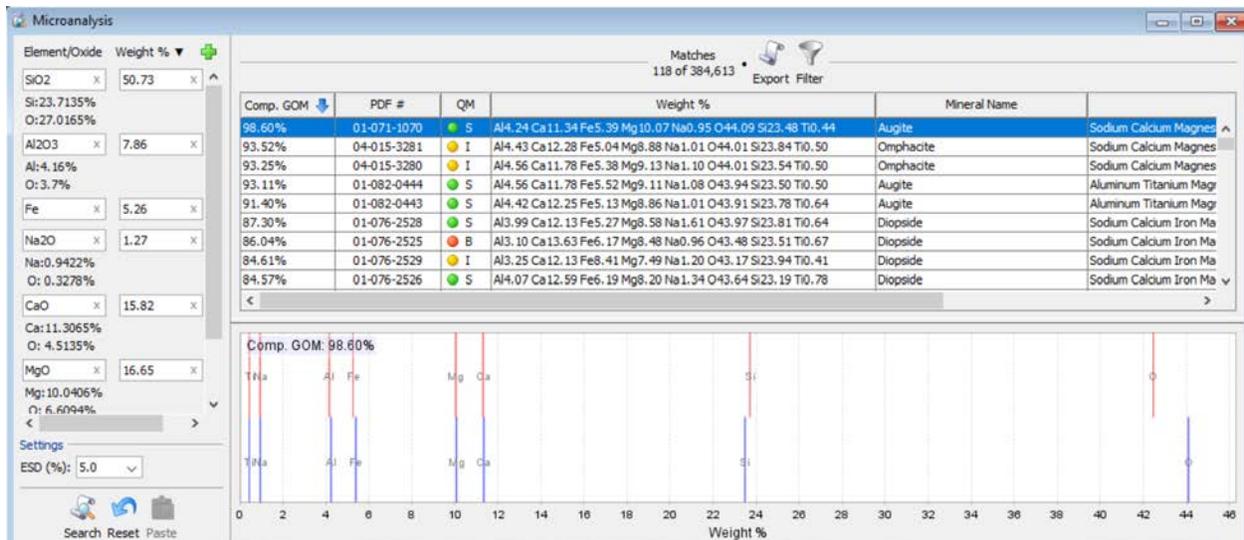
Figure 1. Identification of Augite, NMNH R6600, from input Smithsonian Microbeam reference data. The red is the experimental composition profile compared to the reference in blue. In this case both experiment and reference were different specimens from Kakanui, New Zealand.