*American Mineralogist, Volume 100, pages 1921–1931, 2015*

# Provenance determination of sapphires and rubies using laser-induced breakdown spectroscopy and multivariate analysis

**Kristen A. Kochelek[1], Nancy J. McMillan[1,*], Catherine E. McManus[2] and David L. Daniel[3]**

[1]Department of Geological Sciences, Box 30,001, MSC 3AB, New Mexico State University, Las Cruces, New Mexico 88003-8001, U.S.A.
[2]Materialytics, Inc., P.O. Box 10988, Killeen, Texas 76547-0988, U.S.A.
[3]Department of Economics, Applied Statistics, and International Business, Box 30,001, MSC 3CQ, New Mexico State University, Las Cruces, New Mexico 88003-8001, U.S.A.

## Abstract

Determination of gem provenance is a topic of research in the gemological community for financial, security, and societal reasons. Laser-induced breakdown spectroscopy (LIBS) and multivariate analysis have the potential to revolutionize the field of gem provenance. This study acquired LIBS spectra from 569 rough sapphire and ruby specimens from 21 localities in 11 countries. The spectra were analyzed using the multivariate technique partial least-squares regression (PLSR) in separate algorithms for sapphires and rubies. Each algorithm consists of a series of PLS models. Each model compares the spectra from a locality of interest to the spectra from all other localities in the database. Success rates, as determined by the percent of correct provenance identifications, are 98.9% (sapphire) and 96.0% (ruby) for country of origin and 97.9% (sapphire) and 95.4% (ruby) for deposit of origin. Individual deposits are not recognized by the concentrations of a few elements; rather, the unique compositional signature of each deposit consists of the ratios of many elements, primarily Ca, Zr, Fe, Ba, Mt, Ti, Sr, Si, Cr, H, C, and Li, some of which may reside in inclusions. This work demonstrates that determination of country or deposit of origin may be related to a quantitative measure with a high level of success.

**Keywords:** Ruby, sapphire, provenance, laser-induced breakdown spectroscopy, chemometrics