

Toward a unified method for the quantification of volatiles in magmas via FTIR

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Fourier Transform Infrared (FTIR) spectroscopy is a common tool used to quantify dissolved volatiles in melts. The use of this method for the analysis of melt inclusions in particular is crucial to understanding a multitude of volcanic and geochemical processes such as magma storage, crystallization, and degassing. Despite the ubiquitous nature of this technique in the literature, standard methods for the retrieval of dissolved volatile concentrations from IR spectral data are poorly defined and often rely on hand-drawn or assumed straight-line-fit background curves that introduce significant error and variation within data sets. Propogated errors from differences in “acceptable” background curves for a single IR spectrum drawn by a set of individuals (or even by a single individual at different times) can equate to variation in final retrieved volatile concentrations on the order of wt%. In an effort to reconcile this problem, we are developing a simple software package capable of retrieving dissolved volatile concentrations (i.e. H₂O, OH, CO₂, and CO₃) from FTIR spectra based on a set of standard peak fitting algorithms. By using spectroscopic first principles to define a volatile-free background spectra, peak heights, and ultimately volatile concentrations, we can eliminate variations between individual researchers that stem from the subjectivity in choosing a “good” background spectrum. In addition, the automation of this procedure by computer eliminates internal variation within data sets and expedites the process of analyzing large data sets.

Our software tool, currently in the early stages of development, will allow for the creation of volatile-free background spectra based on a curve fit to the user-input FTIR data. Subsequently, a calculation of peak heights and ultimately volatile concentrations (based on the Beer-Lambert law, given sample thickness, density, and absorption coefficient) can be performed. Our goal is to make the tool as transparent as possible in order that the user has more control over and understanding of the data transformations being performed. The program, written in Python and released under the Gnu Public License (GPLv3), is currently in alpha. We are now seeking input on the overall design, desired features, and back-end theory/computation.

REE content of phosphogypsum from Romania

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Phosphogypsum is a technogenic product remaining after the extraction of phosphoric acid from raw phosphate, mainly apatite. The original phosphate rock contains large amounts of REE, mainly replacing Ca from apatite or included in other phosphate structures. About 70% of the REE contents are stacked in the phosphogypsum obtained after sulfuric attack of the raw phosphate and much less in the case of hydrochloric attack. In Romania, the sulfuric attack through the hemidihydrate (HDH) or dihydrate (DH) procedures was extensively used to obtain phosphoric acid at Turnu Măgurele (TM), Valea Călugărească (VC), Năvodari (N) and Bacău (B).

Inductively coupled plasma - atomic emission spectrometry (ICP-AES) analyses performed on selected samples of phosphogypsum from the four deposits showed that the contents in the main REE (cerium, erbium, neodymium, thorium, ytterbium) are specific for the phosphogypsum issued from the processing of sedimentary raw phosphates. The contents are given in the table.

Occ.	Ce (ppm)	Er (ppm)	La (ppm)	Nd (ppm)	Th (ppm)	Yb (ppm)
TM	29,1 - 663,1	0,9 - 11,7	22,7 - 469,0	21,1 - 260,5	0,3 - 20,8	1,1 - 6,8
VC	30,2 - 454,2	0,8 - 7,3	35,7 - 322,5	22,3 - 188,2	0,0 - 12,8	1,6 - 5,0
N	3,9 - 165,0	1,8 - 7,7	14,5 - 135,6	3,8 - 90,6	0,8 - 6,5	1,8 - 6,1
B	19,3 - 174,8	13,1 - 18,8	36,2 - 134,2	24,5 - 104,5	1,7 - 5,2	1,9 - 6,6