

H/D isotopic fractionation between minerals and water, as predicted by first-principles calculations

M. MEHEUT^{1*}, M. LAZZERI², E. BALAN^{2,3}
AND F. MAURI²

¹LMTG, Université Paul Sabatier, Toulouse, France

(*correspondence: meheut@lmtg.obs-mip.fr)

²IMPMC, Université Paris VI, Paris, France

³IRD –UMR CEREGE, Aix en Provence, France

Hydrogen isotopic compositions are a tool of primary importance to quantify fluid-rock interactions in geothermal systems [1]. Precise knowledge of the equilibrium constant for hydrogen fractionation and of its temperature dependence is therefore essential to an accurate use of this tool. However, there are major discrepancies between published values of fractionation factors for various hydrous mineral-water systems, such as lizardite-water ([2], and references therein).

To resolve these discrepancies, theoretical approaches represent a fully independent way to obtain fractionation factors at equilibrium. In this work, hydrogen fractionation factors between selected hydrous minerals (brucite, kaolinite, lizardite and gibbsite), and perfect water gas (corresponding to vapor at null density) have been computed from first-principles quantum-mechanical calculations [3]. These calculations confirm the experimental or natural calibrations by Xu & Zheng [4] and Horita *et al.* [5] (brucite-water), Gilg & Sheppard [6] (kaolinite-water), Wenner & Taylor [7] (lizardite-water), and in some extents Vitali *et al.* [8] (gibbsite-water) as representative of equilibrium fractionations. Application of a system-independent and relatively simple correction to our calculations permits to reach a global agreement with all these natural or experimental estimates, and to propose a calibration curve valid for any temperatures in these systems.

Besides, internal isotopic fractionation of hydrogen between inner-surface and inner hydroxyl groups has been computed for kaolinite and lizardite minerals. The obtained fractionation is large, of opposite sign for the two systems (respectively -23‰ and +63‰ at 25°C) and is linear in T^{-2} , making it a potentially good geothermometer.

[1] Savin & Lee (1988) *RMG* **19**, 189–223. [2] Vennemann & O'Neil (1996) *GCA* **60**, 2437–2451. [3] Meheut *et al.* (2010) *GCA*, accepted. [4] Horita *et al.* (2002) *GCA* **66**, 3769–3788. [5] Xu & Zheng (1999) *GCA* **63**, 2009–2018. [6] Gilg & Sheppard (1996) *GCA* **60**, 529–533. [7] Wenner & Taylor (1973) *AJS* **273**, 207–239. [8] Vitali *et al.* (2001) *GCA* **65**, 1391–1398.

Generation of integrated geochemical-geological predictive model of porphyry-Cu potential, Chahargonbad District, Iran

A. MEHRABI* AND R. DERAKHSHANI

Department of Geology, Shahid Bahonar University, Kerman, Iran (*correspondence: alimehrabi225@yahoo.com, reza_1217@yahoo.com)

Geochemical surveys are essential in most modern mineral explorations. Since Au and Cu are, respectively, pathfinder and indicator for porphyry copper deposits [1], in this paper, a geochemical potential map of Chahargonbad area is prepared by analysing stream sediment geochemical data of those elements, including elementary statistics of the raw geochemical data, mean, maximum, minimum, standard deviation and skewness of \log_e -transformed data and finally providing histograms of \log_e -transformed data. Moreover, using the advantages of the fuzzy logic theory, a geologically-constrained predictive porphyry-Cu potential map is prepared. For this purpose, specific relations of known porphyry-Cu deposits and structural features in the Chahargonbad area, that is provided by weights of evidence modelling, maps of fuzzy membership values for hydrothermal alteration units, lithologic formations, batholithic pluton margins, pluton centroids and faults-fractures are prepared. Porphyry-Cu potential zones are delineated by using the fuzzy gamma operator to combine the mentioned evidential layers. The results of the study show that the area could be divided into four areas: good potential (0.43%), moderate potential (0.82%), weak potential (19.76%) and non-potential for porphyry-Cu deposits (78.99%). A good spatial coincidence is obtained by comparing the geochemical anomaly maps with the porphyry-Cu potential map obtained via the fuzzy logic method.

[1] Carranza (2008) *Geochemical Anomaly & Mineral Prospectivity Mapping in GIS*. Amsterdam: Elsevier.