

Accepted Manuscript

A general framework for ion equilibrium calculations in compacted bentonite

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PII: S0016-7037(16)30647-0

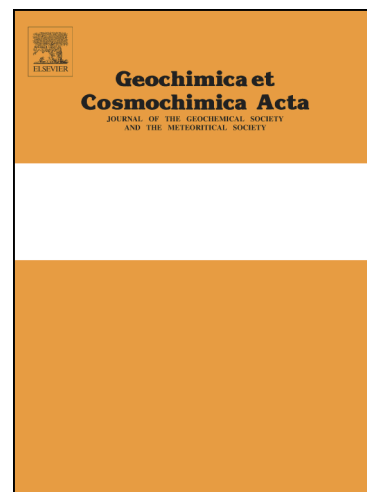
DOI: <http://dx.doi.org/10.1016/j.gca.2016.11.010>

Reference: GCA 10013

To appear in: *Geochimica et Cosmochimica Acta*

Received Date: 2 March 2015

Accepted Date: 5 November 2016



Please cite this article as: Birgersson, M., A general framework for ion equilibrium calculations in compacted bentonite, *Geochimica et Cosmochimica Acta* (2016), doi: <http://dx.doi.org/10.1016/j.gca.2016.11.010>

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1 A general framework for ion equilibrium calculations in
2 compacted bentonite

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5 **Abstract**

6 An approach for treating chemical equilibrium between compacted bentonite
7 and aqueous solutions is presented. The treatment is based on conceptualiz-
8 ing bentonite as a homogeneous mixture of water and montmorillonite, and
9 assumes Gibbs-Donnan membrane equilibrium across interfaces to external
10 solutions. An equation for calculating the electrostatic potential difference
11 between bentonite and external solution (Donnan potential) is derived and
12 solved analytically for some simple systems. The solutions are furthermore
13 analyzed in order to illuminate the general mechanisms of ion equilibrium
14 and their relation to measurable quantities. A method is suggested for es-
15 timating interlayer activity coefficients based on the notion of an interlayer
16 ionic strength. Using this method, several applications of the framework are
17 presented, giving a set of quantitative predictions which may be relatively
18 simply tested experimentally, e.g.: (1) The relative amount of anions enter-
19 ing the bentonite depends approximately on the square-root of the external
20 concentration for a 1:2 salt (e.g. CaCl_2). For a 1:1 salt (e.g. NaCl) the
21 dependence is approximately linear, and for a 1:2 salt (e.g. Na_2SO_4) the
22 dependence is approximately quadratic. (2) Bentonite contains substantially
23 more nitrate as compared to chloride if equilibrated with the two salt so-
24 lutions at equal external concentration. (3) Potassium bentonite generally
25 contains more anions as compared to sodium bentonite if equilibrated at the

Prepared for submission to Elsevier
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November 15, 2016

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