

Thermodynamics of the solid solution - Aqueous solution system (Ba,Sr,Ra)SO₄ + H₂O: I. The effect of strontium content on radium uptake by barite

V.L. Vinograd, D.A. Kulik, F. Brandt, M. Klinkenberg, J. Weber, B. Winkler, D. Bosbach

PII: S0883-2927(17)30359-1

DOI: [10.1016/j.apgeochem.2017.11.009](https://doi.org/10.1016/j.apgeochem.2017.11.009)

Reference: AG 3991

To appear in: *Applied Geochemistry*

Received Date: 10 August 2017

Revised Date: 27 October 2017

Accepted Date: 23 November 2017

Please cite this article as: Vinograd, V.L., Kulik, D.A., Brandt, F., Klinkenberg, M., Weber, J., Winkler, B., Bosbach, D., Thermodynamics of the solid solution - Aqueous solution system (Ba,Sr,Ra)SO₄ + H₂O: I. The effect of strontium content on radium uptake by barite, *Applied Geochemistry* (2017), doi: 10.1016/j.apgeochem.2017.11.009.

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4 Vinograd, V.L.¹, Kulik, D.A.², Brandt, F.¹, Klinkenberg, M.¹, Weber, J.³, Winkler, B.⁴,
5 Bosbach, D.¹

6 ¹*Institute of Energy and Climate Research (IEK-6) – Nuclear Waste Management and Reactor*
7 *Safety, Research Centre Jülich GmbH, 52425 Jülich, Germany*

8 ²*Paul Scherrer Institut, Laboratory for Waste Management, 5232 Villigen PSI, Switzerland*

9 ³*Chemical Science Division, Oak Ridge National Laboratory, TN 37830, USA*

10 ⁴*Goethe University, Frankfurt, Germany*

14 Abstract

15 Thermodynamic properties of mixing in the ternary (Ba,Sr,Ra)SO₄ solid solution are determined
16 using first principles based total energy calculations and Monte Carlo simulations. Two levels of
17 theory, which correspond to the regular mixing and the generalized Ising model, are considered.
18 The results show that the regular mixing parameters increase along the row of Ba-Ra, Ba-Sr and
19 Sr-Ra binary systems proportionally to the squared difference of molar volumes of the end-
20 members. The magnitudes of pairwise interactions similarly increase along the same row,
21 manifesting a tendency to short-range ordering (SRO). In the (Ba,Sr)SO₄ system the SRO effect
22 is approximately equivalent to a 40% decrease in the value of the regular mixing parameter. The
23 ternary solid solution is well described as a regular mixture with the binary parameters $W_{\text{BaRa}} =$

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