Goldschmidt 2024 Abstract
https://doi.org/10.46427/gold2024.24178

Gas-phase reactions involved in radioxenon detection after an underground nuclear explosion

BERNARD BOURDON[1] AND STEPHAN STEINMANN[2]

[1]Laboratoire de Géologie de Lyon, ENS de Lyon, Université Lyon I, CNRS
[2]ENS de Lyon

Presenting Author: bernard.bourdon@ens-lyon.fr

Following an underground nuclear explosion, a magma pool is created underground initially in equilibrium with a vapor phase that occupies the nuclear cavity. Subsequently, radioactive xenon produced by fission can migrate through the rock column, be detected at the surface and used as a tool in proliferation monitoring. Establishing the relative proportions of Xe isotopes can inform the processes that have taken place, including the rate of cooling.

The radioactive precursors of the radioxenon (^{131}Xe, ^{133}Xe and ^{135}Xe) are moderately volatile elements [1] that can condense at rates dependent on the cooling rate inside the nuclear cavity. There is thus a potential competition between the radioactive decay leading to Xe and the rates of vapor-liquid reactions. In particular, reactions in the gas phase compete with the rates of radioactive decay of nuclides, yielding ultimately radioxenon.

In order to design a comprehensive model of these processes, one needs to estimate the reaction rates of Xe precursors (Sb, Sn, Te, I) and their speciation in the gas phase. For this purpose, we have investigated using DFT methods the rates of the reaction $Sn+O_2$ ->SnO+O. These simulations allow the identification of a transition state and the activation energy can be calculated. The forward rate of the reaction is estimated using transition state theory and compares well with experimental data from the literature [2-3]. Having validated this theoretical approach, it is possible to extend it to other relevant reactions where no experimental data exist.

[1] Bourdon B. Pili E. (2023) J. Environ. Radioact. 107125 [2] Takahashi K. et al. (2001) Phys. Chem. Chem. Phys. 3, 4296-4300 [3] Fontijn A. Bajaj P.N. (1996) J. Phys. Chem. 100, 7085-7089.