

Chemical and isotopic investigation of urbanized streams in Daejeon, South Korea

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The chemical and strontium isotopic compositions (⁸⁷Sr/⁸⁶Sr) in three streams (Gap, Yudeung, and Daejeon streams) passing through Daejeon, one of the metropolitan cities in South Korea, were measured to identify contaminant sources impacted on water quality of each stream, with seasonal variation. The dissolved ion concentrations mostly represented spatio-temporal variation. The water samples in the middle reaches of Daejeon stream and of the Geum River (DS-M and GR-M, respectively) had the high proportion of both Cl⁻ and SO₄²⁻ relative to those of other streams (i.e. Gap and Yudeung streams); i.e. GR-M and DS-M showed (Ca, Na)-HCO₃-SO₄ and Ca-HCO₃-SO₄ water types, respectively, whereas both GS and YS represented Ca-HCO₃. Furthermore, NO₃⁻ concentration of DS-M was also markedly high, indicating anthropogenic inputs. It is considered that high contribution of anthropogenic inputs observed in DS-M was diluted not by mixing with Yudeung stream but by groundwater developed within the catchments.

Although three streams were covered with similar lithology, ⁸⁷Sr/⁸⁶Sr ratios in DS-M clearly were discriminated from those in other water samples, due to potential anthropogenic inputs. However, considering ⁸⁷Sr/⁸⁶Sr for fertilizers and powder detergents, anthropogenic inputs in DS-M were hardly originated from these compounds. Presumably, the water quality of DS-M is likely to be strongly affected by atmospheric and paved road dust in the urban when taking into account higher Cl⁻, SO₄²⁻ and NO₃⁻ concentration in DS-M.

Minerals affect the interconversion between alkanes and alkenes in hydrothermal systems

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Alkane-alkene equilibrium in water can be reached under hydrothermal conditions (1), however the mechanisms governing this equilibrium are unknown. Much of what we use to predict reaction products and mechanisms are based on classical organic chemistry experiments done at ambient temperatures and pressures, but this knowledge-base may not adequately predict the behavior of organic molecules at high temperatures and pressures. Therefore, the extreme temperature and pressure conditions of hydrothermal systems leave much room for mechanistic exploration.

Trans-1, 2-dimethylcyclohexane was chosen to probe the mechanisms of alkane-alkene interconversions at high temperatures and pressures because the stereochemistry of the conversion products may reveal mechanistic information about the reaction. For example, if in the presence of minerals, the *cis*-isomer of the alkane is formed in higher abundance than without minerals, then it is likely that the alkene is reacting at the surface of the mineral rather than in solution.

Experiments were performed in a cold seal vessel, at 300 °C and 100 MPa, using gold capsules containing the *trans*-alkane, water, and various individual minerals (pyrite, pyrrhotite, magnetite, hematite, and corundum). We also conducted mineral free control experiments. After 24 hours, products included the *cis*- isomer (*cis*-1, 2-dimethylcyclohexane), the alkene (1, 2-dimethylcyclohexene), and xylene isomers. The specific proportions of products and conversion rates depend on the mineral present. In control experiments, without mineral, the major product is *o*-xylene. In contrast, when minerals are present, the major product is the *cis*-alkane. We propose that the first step in this reaction is oxidation of the *trans*-alkane to the alkene, which then can be further oxidized to xylene or reduced back to the alkane. Predominant conversion to the *cis*-isomer in the presence of minerals suggests that the reduction reactions occur on the mineral surface. Different minerals also affect the amount of conversion and relative abundance of the other reaction products, suggesting that the structure and chemical composition of the mineral has an effect on the reaction mechanism.

[1] Seewald (1994) *Nature* **370**, 285–287.