

21世紀の Goldschmidt 的地球化学: 分子地球化学 Molecular Geochemistry as a Future Topic in Geochemistry

高橋 嘉夫^{1*}
TAKAHASHI, Yoshio^{1*}

¹ 東京大学大学院理学系研究科地球惑星科学専攻

¹Department of Earth and Planetary Science, Graduate School of Science, The University of Tokyo

Professor V. M. Goldschmidt is a father of geochemistry. He wrote in 1954 that *geochemistry is the study of the distribution and amounts*. Based on this concept, he discussed (i) substitution of trace elements into major element within a certain crystal, (ii) reaction of metal ions with the ligands in water in terms of ion potential ($= z/r$; z : charge; r : ionic radius), and (iii) classification of all the elements in the periodic table in terms of chemical bonding nature such as ionic, covalent, and metallic bonding. Using X-ray emission spectroscopy, which was the state-of-the-art method at that time, he determined abundances of trace elements in various geochemical samples.

However, his discussion on the distribution of these elements *on the basis of the properties of their atoms and ions* could not be proved by any methods, since it was difficult at that time to clarify the chemical species (bonding nature and structure) of trace elements. At present, on the other hand, we can determine the neighboring atom and interatomic distance of trace elements in various samples by advanced speciation methods such as by X-ray absorption fine structure (XAFS) spectroscopy. As shown in our recent studies, abundances and isotopic compositions of various elements in natural samples strongly depend on the chemical state of various elements in nature. This fact shows that we can predict behaviors and isotopic fractionation of various elements based on physico-chemical properties. This field can be called as "Molecular Geochemistry". This field includes (i) identification of organic polymolecules in nature which can be used for the paleoenvironment reconstruction, (ii) isotopomers of various molecules, and (iii) fundamental understanding of isotopic fractionation such as mass-independent fractionation. Thus, I propose "Molecular Geochemistry" as an important future topic of geochemistry, which cannot be conducted by researchers in other fields in earth and planetary sciences and must be conducted by Prof. Goldschmidt if he could use the methods to reveal the atomic- and molecular-level information in geochemical samples.

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