6–3 Understanding Hydrated Radium at the Molecular Level

— The Advent of Molecular-Level Research on Radium 125 Years After the Discovery of the Element —

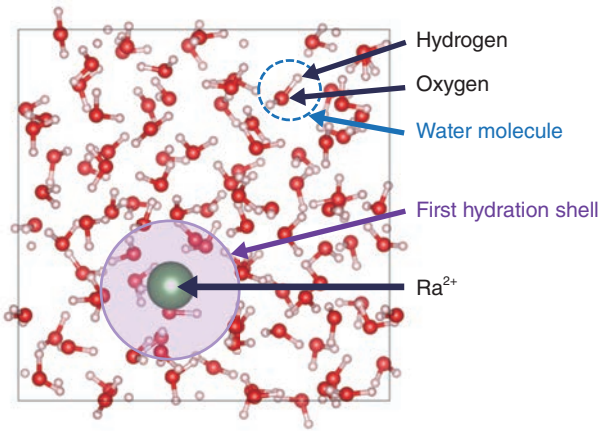

Fig.1 Snapshot of hydrated Ra^{2+} simulation
Dynamics of one Ra^{2+} and 100 water molecules was calculated for 60 ps. Analysis of the result yielded the data provided in Table 1.

Table 1 Comparison of experiment and simulation results
The experimental coordination numbers and distances between Ra^{2+} and oxygen atoms in the first hydration shell were close to the simulated values.

Methods	Coordination number	Distance (Å)
Experiments	9.2 ± 1.9	2.87 ± 0.06
Simulations	8.4	2.88

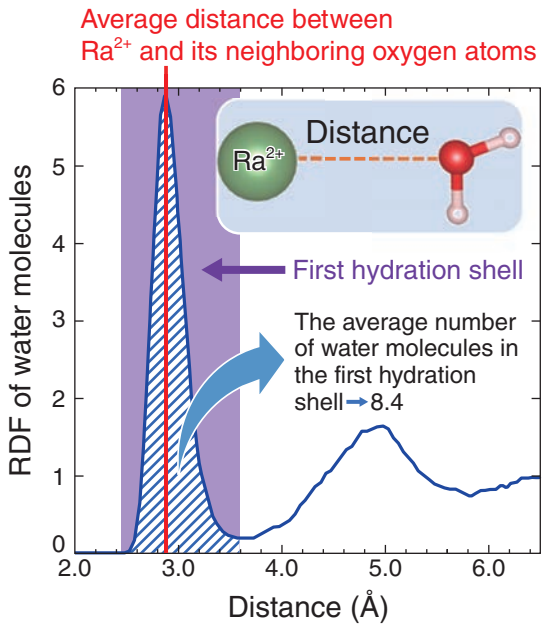

Fig.2 Distribution of water molecules hydrating Ra^{2+}
This radial distribution function (RDF) was obtained via simulation by averaging the distances between Ra^{2+} and oxygen atoms in all structures. The average number of water molecules in the first hydration shell was obtained by summing the shaded areas.

Radium (Ra), discovered by Marie and Pierre Curie in 1898, is now attracting attention in diverse fields such as medicine and earth sciences; meanwhile, environmental pollution by Ra is becoming a concern. However, details of Ra chemical reactions in living organisms and environment remain unknown. Since these reactions primarily occur in water, the structure of Ra dissolved in water (i.e., hydrated Ra^{2+}) is the most fundamental and important information. However, since Ra is a radioactive element without a stable isotope, and radon, a gaseous radioactive element, is produced by Ra decay, there is high risk of internal exposure during its study, and a high level of safety control is required for Ra experimentation. Therefore, >100 years after the discovery, no experiments at the molecular level have been conducted on this element.

In this study, we developed a container that prevents radon leakage and established a method to safely prepare, transport, and measure high-concentration Ra samples. Then, using SPring-8, we successfully performed the first molecular-level measurement of hydrated Ra^{2+}. In addition, *ab initio* molecular dynamics simulations were performed using a supercomputer (Fig.1). The results (Fig.2) successfully reproduced the experimental results (Table 1). A more detailed analysis of the simulation results and comparison with barium (Ba), an element similar to Ra, revealed that the average residence time of water molecules in the first hydration sphere of Ra^{2+} (38 ps) is shorter than Ba^{2+} (98 ps), indicating that Ra^{2+} has a weak binding with the hydrating water molecules. The results indicate that the hydration structure of Ra^{2+} can be changed more easily than Ba^{2+}, suggesting that compared to other alkaline earth metals, Ra^{2+} is more likely to leave water and be incorporated into the solid phase in living organisms and the environment.

To summarize, in this study, we established a method for studying Ra chemistry at the molecular level using synchrotron radiation experiments and simulations. In the future, this method is expected to be applied to study more complex chemical reactions and may help us understand the mechanisms of cancer drugs; additionally, it is expected to make possible novel drug development, improved soil age estimation techniques, and resolution of environmental concerns and other important social problems.

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Reference

Yamaguchi, A. et al., Extended X-Ray Absorption Fine Structure Spectroscopy Measurements and *Ab Initio* Molecular Dynamics Simulations Reveal the Hydration Structure of the Radium (II) Ion, iScience, vol.25, issue 8, 2022, 104763, 12p.