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Dissolved State of Radon Atom with Cluster Molecules of Solvent

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Radon is a rare gas element which has only radioactive isotopes. It is supposed to be an important and useful element because we could find anywhere on the earth and we might utilize for medical use in cancer therapy. There are several measurements available such as an ionization chamber measurement and a track counter method. We can also measure the radon concentration in solution by using liquid scintillation counting which needs an extraction process into organic solvent while the element has a notable water solubility compared to the other rare gas elements.

However, dissolved state of radon atom in water is not well known thus far. In order to clarify the state, the interaction between radon atom and water molecules needs to be investigated.

In this study, we assume the interaction of a rare gas atom trapped inside a cluster of molecules in liquid, that were theoretically proposed in 2001[1] to estimate the enthalpy change due to their association based on a theoretical calculation. Besides, we performed measurement of distribution ratios of radon between mixed solutions of ethanol in water and dodecane to investigate the radon dissolution on cluster formation to be related to the concentration of alcohol in water.

For Ne, Ar, Kr, Xe, and Rn atoms into a cluster consisting of 20 H₂O molecules, complexation energies were estimated by the DFT method (wB97XD/Aug-cc-pVDZ) with the BSSE correction. Since the calculated complexation energies and the solution enthalpies[2,3] showed a strong correlation, we have found that rare gas and water clustering is an important factor in the dissolution.

The performed experiments in this study also demonstrated that suppressed is the transfer of radon into the mixed solution in the concentration where the interaction of H₂O and ethanol makes a layer structure[4,5] rather than an cluster structure.

In conclusion, both of theoretical and experimental approaches to solution of rare gas atoms in water suggest a possible association with a cluster consisting of H₂O molecules. The results will give one important information on the cluster formation of molecules.

references

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Primary authors: Mr YAMADA, Norihiro (Kanazawa University); Mr SHIN, Yuki (Kanazawa University); Mr KAWASAKI, Kohei (Kanazawa University); Dr IDA, Tomonori (Kanazawa University); YOKOYAMA, Akihiko (Kanazawa University)

Presenter: YOKOYAMA, Akihiko (Kanazawa University)

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