

¹⁷O NMR Study On Water Exchange Of Paramagnetic Contrast Agents

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목적(Purpose): The water exchange rate between bulk water and bound water is an important parameter in deciding the efficiency of paramagnetic contrast agents. In this study, we measured and determined the water exchange rates of various Gd-chelates using oxygen-17 NMR technique.

대상 및 방법(Materials and Method): The samples (Gd-DTPA, Gd-DTPA-BMA, Gd-DOTA, Gd-EOB-DTPA) were prepared by mixing 5% ¹⁷O enriched water (Isotech, USA). The pH was adjusted to physiological value (pH = 7.0) by buffer solution. Variable temperature ¹⁷O NMR measurements were performed at 14.1 Tesla using Bruker-600 (81.3 MHz ¹⁷O resonance frequency). Bruker VT-1000 temperature control units were used to stabilize the temperature. The samples were sealed in glass spheres, fitting into 10 mm NMR tubes, in order to eliminate susceptibility corrections to the chemical shift. The ¹⁷O spin-spin relaxations (T₂) were measured using CPMG pulse sequence. To estimate the water exchange rate (τ_m), the variable temperature T₂ relaxation data were fitted into the Solomon-Bloembergen equations using least-square fit algorithm.

결과(Results): The determined water exchange rates at 300K are: 0.42 μ s (Gd-DTPA), 1.99 μ s (Gd-DTPA-BMA), 0.27 μ s (Gd-DOTA), and 0.11 μ s (Gd-EOB-DTPA) respectively. Gd-DTPA-BMA showed slowest water exchange whereas Gd-EOB-DTPA had fastest exchange rate. In addition, the water exchange rates (τ_m) of all samples showed exponential temperature dependence with different decay constant.

결론(Conclusion): Using oxygen-17 NMR technique, the water exchange rate of paramagnetic agent, which has dual importance in investigating the detailed mechanism of relaxation enhance effect of the agent and in designing new contrast agent, could be determined with precision.