

Hydration number: Crucial role in nuclear magnetic relaxivity of Gd(III) chelate-based nanoparticles

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Abstract

© 2017 The Author(s). Today, nanostructure-based contrast agents (CA) are emerging in the field of magnetic resonance imaging (MRI). Their sensitivity is reported as greatly improved in comparison to commercially used chelate-based ones. The present work is aimed at revealing the factors governing the efficiency of longitudinal magnetic relaxivity (r_1) in aqueous colloids of core-shell Gd(III)-based nanoparticles. We report for the first time on hydration number (q) of gadolinium(III) as a substantial factor in controlling r_1 values of polyelectrolyte-stabilized nanoparticles built from water insoluble complexes of Gd(III). The use of specific complex structure enables to reveal the impact of the inner-sphere hydration number on both r_1 values for the Gd(III)-based nanoparticles and the photophysical properties of their luminescent Tb(III) and Eu(III) counterparts. The low hydration of TTA-based Gd(III) complexes ($q \approx 1$) agrees well with the poor relaxivity values ($r_1 = 2.82 \text{ mM}^{-1} \text{ s}^{-1}$ and $r_2 = 3.95 \text{ mM}^{-1} \text{ s}^{-1}$), while these values tend to increase substantially ($r_1 = 12.41 \text{ mM}^{-1} \text{ s}^{-1}$, $r_2 = 14.36 \text{ mM}^{-1} \text{ s}^{-1}$) for aqueous Gd(III)-based colloids, when macrocyclic 1,3-diketonate is applied as the ligand ($q \approx 3$). The regularities obtained in this work are fundamental in understanding the efficiency of MRI probes in the fast growing field of nanoparticulate contrast agents.

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