Gesteuerte Kristallisation des Gadolinium(III)-Komplexes von Diethylentriaminpentaacetat: Monomere und dimere Struktur

Controlled Crystallization of the Gadolinium(III) Complex of Diethylenetriamine-Pentaacetate: Monomeric and Dimeric Structure

Robert Ruloff*, Thomas Gelbrich, Eberhard Hoyer, Joachim Sieler, Lothar Beyer

Universität Leipzig, Institut für Anorganische Chemie, Talstr. 35, D-04103 Leipzig

Z. Naturforsch. **53 b,** 955–959 (1998); eingegangen am 29. Mai 1998

Gadolinium(III) Chelates, Diethylenetriamine-Pentaacetate Complexes, Coordinated Water, Solid State Structures, Magnetic Resonance Imaging

We present the preparation and X-ray crystal structures of two gadolinium(III) complexes of the ligand diethylenetriamine pentaacetic acid (H_5dtpa). With two equivalents of guanidinium (gu^+) per equivalent of complex we obtained the dimer $(gu)_4[Gd_2(dtpa)_2]\cdot(gu)HCO_3$, and with one equivalent of aminoguanidinium (agu^+) the monomer $(agu)[Gd(Hdtpa)(H_2O)]\cdot 2H_2O$, both with the metal atoms in a coordination number of 9. The dimer contains no coordinated water molecule. The monomer is present as two crystallographically independent complexes hydrogen-bridged via carboxylate oxygen atoms (O···O 2.48 Å; O-H···O 172°) and with $Gd\text{-}O_{coord.\ water}$ distances of 2.418(4) and 2.423(4) Å, respectively.

* Sonderdruckanforderungen an Dr. R. Ruloff.