Binding of Zwitterionic Ruthenium(III) Complexes with Cucurbit[7]urils in Solution

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Paramagnetic ruthenium(III) compounds have been investigated as anticancer metallodrugs in past two decades.[1] In this work, we analyze a new class of zwitterionic paramagnetic Ru-based complexes containing cyclohexyl or adamantyl anchors. The ultimate goal of this study is to clarify their binding with cucurbit[7]uril (CB7) cavitand in solution.

The structures of Ru coordination compounds and their Rh analogs were characterized by 1D and 2D NMR experiments including temperature-dependent measurements to break the total NMR shift down to the orbital and hyperfine contribution.[2] The experimental observations were complemented by the relativistic density functional theory (DFT) calculations to investigate the host-guest behavior and effect of paramagnetic center on the NMR chemical shifts of CB7 cavitand.[3]

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References:

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