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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