Reactions of Dinuclear Rhenium Carboxylate Compounds with Purine Dinucleotides

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Dinuclear metal carboxylate complexes of rhodium, ruthenium, and rhenium are promising metallopharmaceutical compounds. These metal-metal bonded complexes covalently bind to purine DNA nucleobases, and the binding has been proposed as a source of their anticancer activity. This investigation focuses on the formation of dinuclear rhenium:purine dinucleotide complexes and aims to elucidate the coordination mode of the metal complexes to purine dideoxynucleotides. In consecutive studies, $Re_2(O_2CCH_3)_2Cl_4 \cdot 2H_2O$ was reacted with 2'-deoxyguanylyl(3'→5')-2'-deoxyguanosine (dGpG) and 2'-deoxyadenylyl(3'→5')-2'-deoxyguanosine (dApG) in H_2O and D_2O. The pH of the solutions were recorded and manipulated to optimize product formation and stability. The reactions were monitored by ^1H NMR spectroscopy, MALDI-TOF and ES mass spectrometry to confirm metal binding. These spectra show novel dirhenium metal:DNA complexes. The potential products were evaluated using geometry optimization with density functional theory at the appropriate level in order to predict probable product structures that agree with the experimental results. The results of the experimental and theoretical studies will be discussed.