Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting information for

Electronic and Molecular Behaviors of a Novel Ionic Paramagnetic Ruthenium (III) Complex

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	Exp.	Cal.[a]	Cal.[b]
Ru-Cl_1	2.363	2.376	2.445
Ru-Cl_2	2.344	2.363	2.439
Ru-P_1	2.408	2.405	2.314
Ru-P_2	2.408	2.405	2.314
Cl_1-Ru-Cl_2	89.634	90.225	90.026
Cl_1-Ru-Cl_{2a}	90.374	89.775	89.974
Cl_1-Ru-P_1	90.284	89.974	90.399
Cl_2-Ru-P_1	90.594	90.983	90.230
Cl_1-Ru-P_{1a}	89.724	90.026	89.601
Cl_2-Ru-P_{1a}	89.414	89.017	89.770
P_1-Ru-P_{1a}	180.0	180.0	180

Table S1: Selected bond lengths [Å] and angles [°] for the Ru (III) complex with Ru (Ⅱ) the optimized geometry values. Cal.[a]: the parameters of the Ru (III) complex, Cal.[b]: the parameters of the Ru (II) complex.

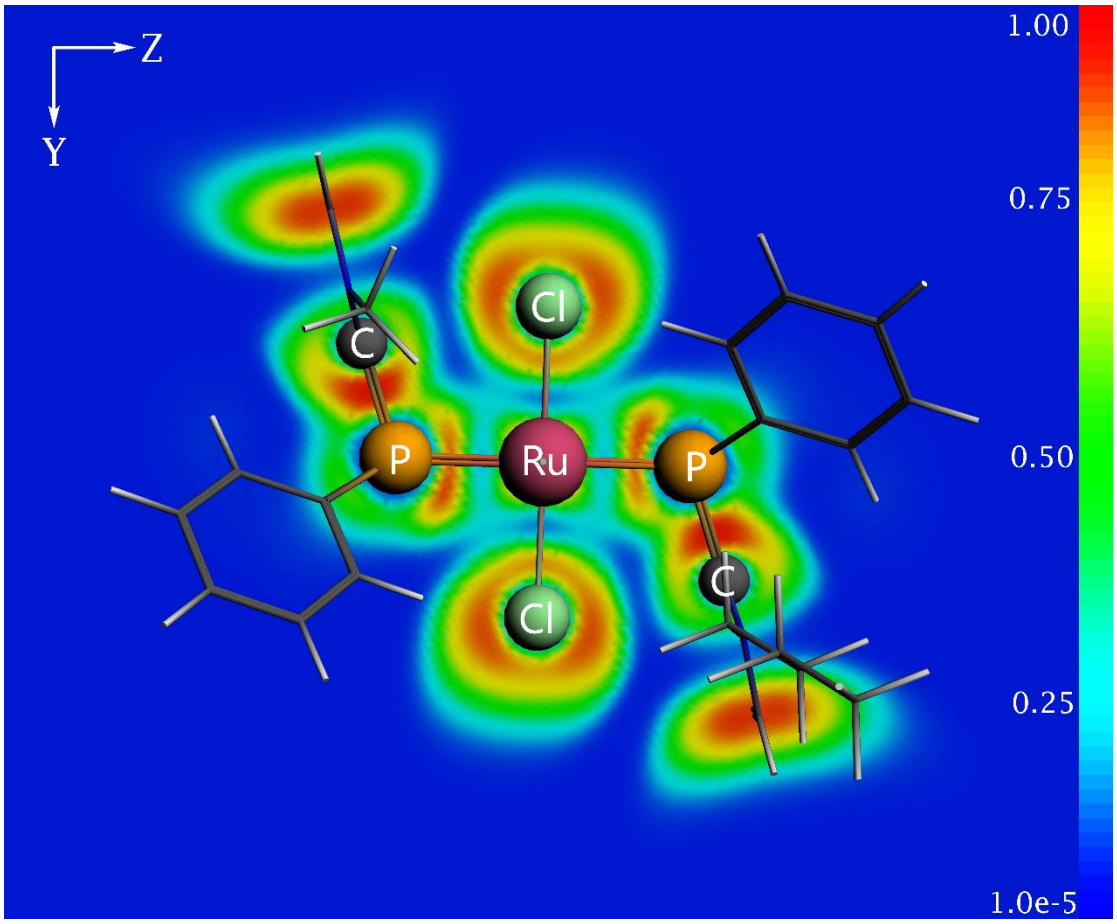

Figure S1. Calculated electron localization function plots for Ru (II) complex (Note: isovalue = 0.03)

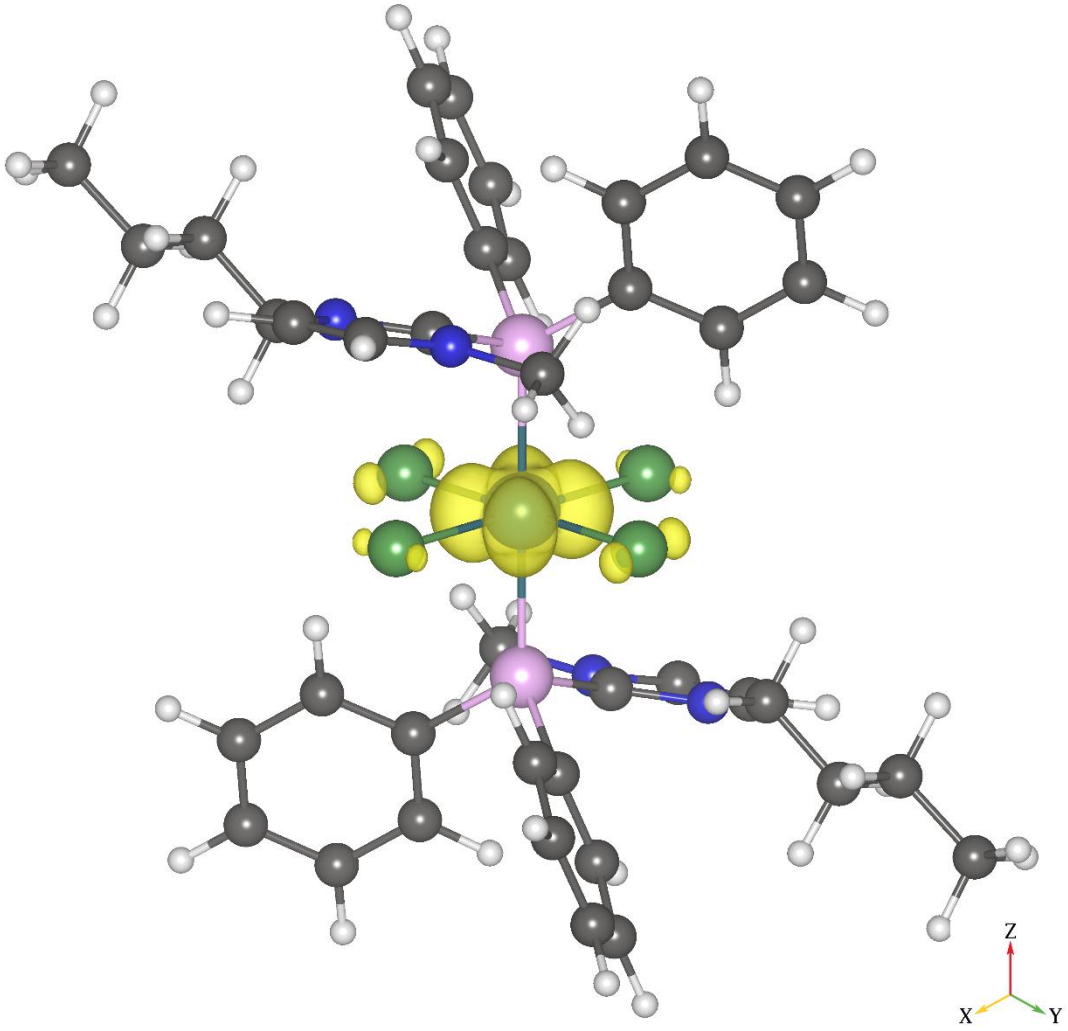

Figure S2. The spin-polarized distribution of the Ru (III) complex (Note isosurface level = 0.007)

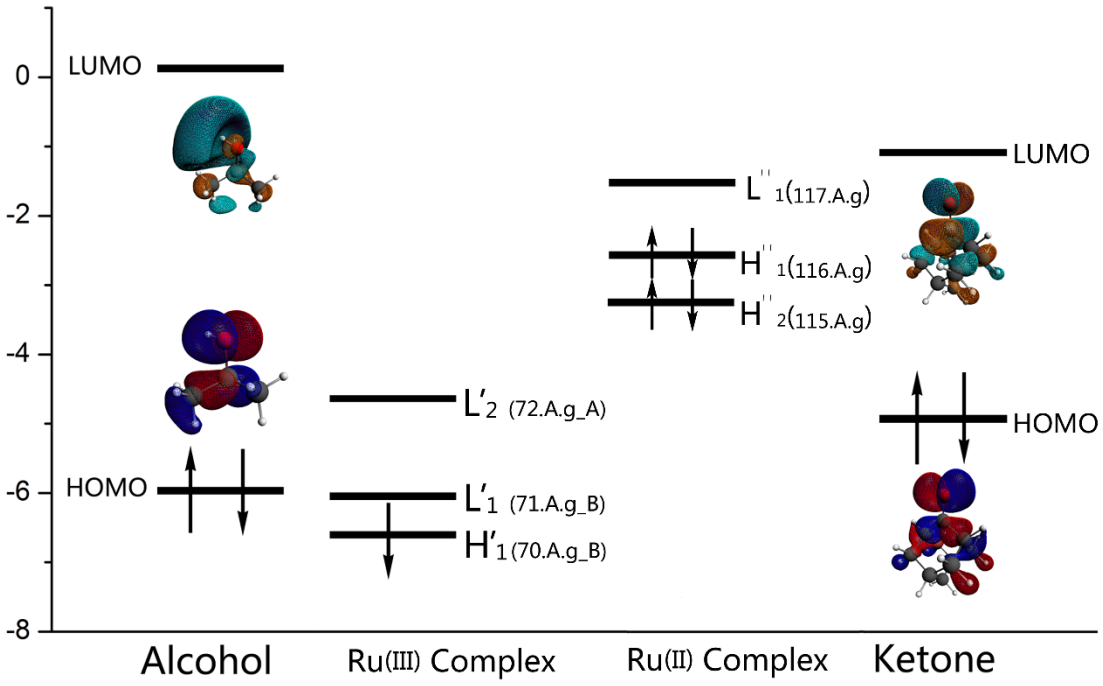

Figure S3. The relative position and interaction of the frontier orbitals (FMOs) of the Ru (III) complex, the Ru (II) complex, Ketone (2-adamantanone) and Alcohol (2-propanol).