

Electronic Supplementary Information

Unusual chemical transformations of acetone thiosemicarbazone mediated by ruthenium: C-H bond activation, thiolation, and C-N bond cleavage

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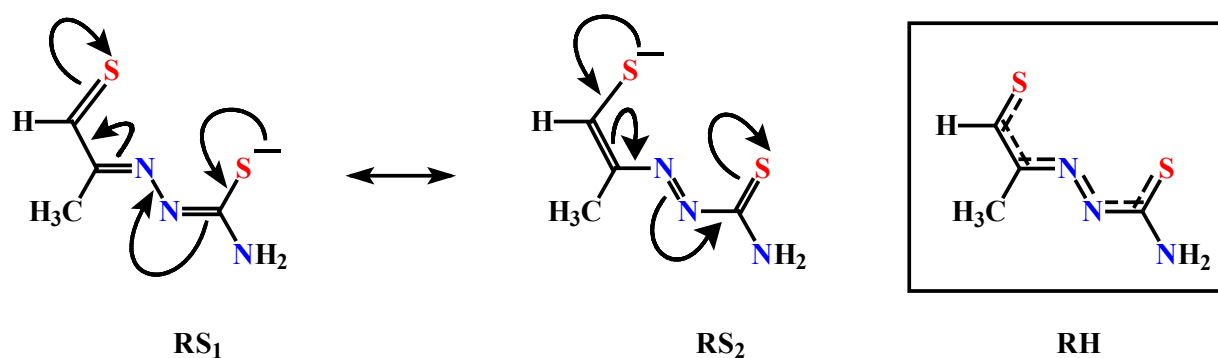


Fig. S1 Possible resonance structures (**RS₁** and **RS₂**) and resonance hybrid (**RH**) for the anionic SNS-coordinated ligand in complex 1.

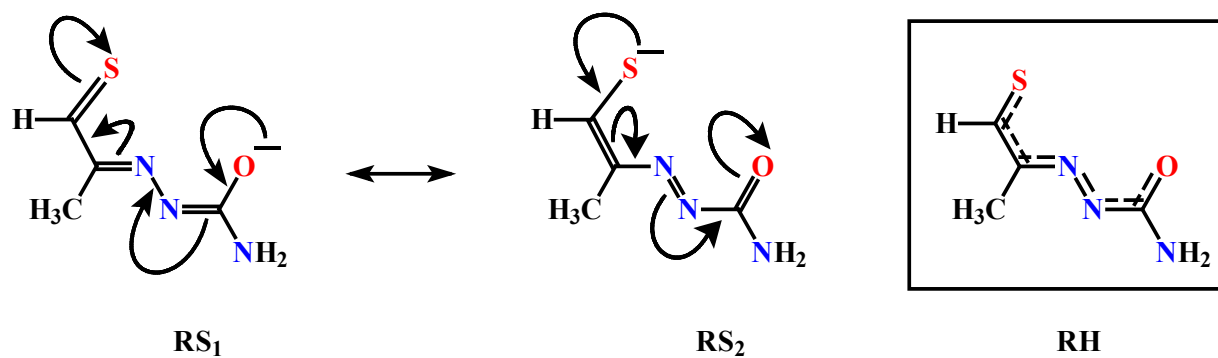


Fig. S2 Possible resonance structures (**RS₁** and **RS₂**) and resonance hybrid (**RH**) for the anionic SNO-coordinated ligand in complex 2.

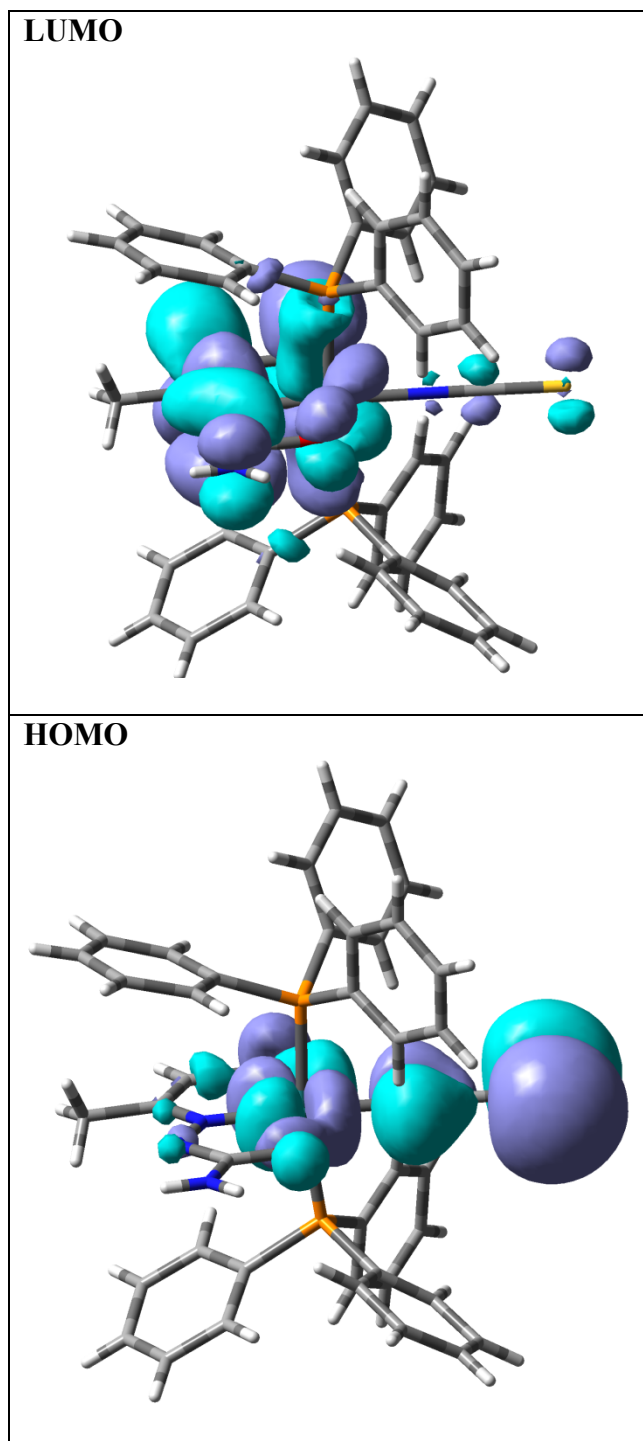


Fig. S3 Contour plots of the HOMO and LUMO of complex **2**.

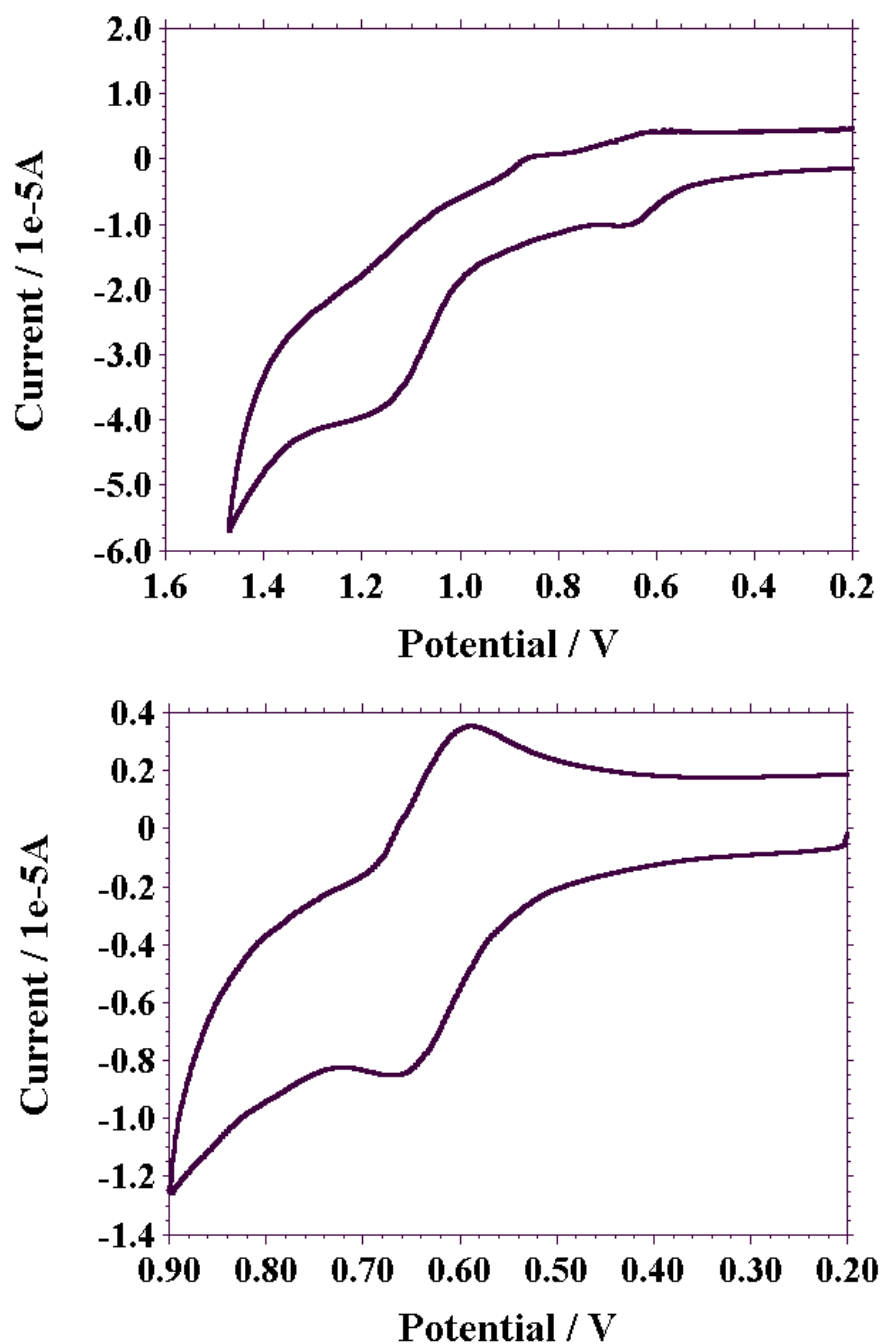


Fig. S4 Cyclic voltammograms of complex **1** in acetonitrile solution (0.1 M TBHP) at a scan rate of 50 mVs⁻¹. Both the oxidative responses are shown on top, and only the first oxidation is shown at the bottom as a segmented scan.