

## ELECTRONIC STRUCTURE OF THE GROUND AND EXCITED STATES OF $\text{RhO}^{2+}$ : ITS ROLE IN THE C-H BOND ACTIVATION OF METHANE

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In this project, we have studied the electronic structure of  $\text{RhO}^{2+}$  using high level quantum mechanical calculations. Multireference method (MRCI) has been employed in combination with large basis sets to construct the potential energy profiles of the ground and excited states of  $\text{RhO}^{2+}$  with different spin multiplicities. Spectroscopic constants have been tabulated for 20 states along with the spin-orbit calculation for a few low-lying states. The ground state of  $\text{RhO}^{2+}$  is  $^2\Pi$  followed by  $^4\Delta$  and  $^2\Delta$ . The equilibrium bond lengths for these states are between 1.594-1.752 Å and the electronic structure is in situ  $\text{Rh}^{4+}\text{O}^{2-}$  that corresponds to an oxo moiety. The next state is  $^6\Sigma^+$  with an equilibrium bond length of 2.161 Å and possesses an in situ electronic structure of  $\text{Rh}^{3+}\text{O}^-$  that corresponds to oxyl character with one unpaired electron on oxygen. Further investigation reveals that  $^6\Sigma^+$ , which is 19.6 kcal/mol higher in energy than the  $^2\Pi$  (ground state), has the potency to activate C-H bond of methane with higher efficiency. Finally, from the spin-orbit calculations, the ground state of  $\text{RhO}^{2+}$  is assigned  $^2\Pi_{1/2}$  followed by the state  $^4\Delta_{7/2}$ . In future, this project is going to probe the effect of ligands in the electronic structure of  $\text{RhO}^{2+}$ .