

THEORETICAL INVESTIGATION ON HOMOLEPTIC YTTRIUM TRI-GUANIDINATES:

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The electronic and molecular structures of the homoleptic yttrium tris-guanidinate complexes $Y[(N^iPr)_2CNR_1R_2]_3$, [$R_1=R_2=Me, Et$ and iPr] have been investigated employing DFT calculations in order to understand the structures, bonding and energies of the interactions between yttrium metal and a guanidinate ligands. The effect of the substitution on nitrogen position of guanidinate on these complexes has been also investigated employing DFT and TDDFT calculations for 6 kinds of models obtained by alternative substitution of alkyl on nitrogen of guanidinate ligands. The results reveal that the substitution position plays a crucial role in the geometry structure by affecting the torsion angle and the HOMO-LUMO transitions. The energy decomposition analysis indicates a majority of ionic bonding in all systems; the exception is in the model4 ($Y[(N^iPr)_2CN^cR_1R_2]_3$; $R=Et, R_1=R_2=H$) which present a significant degree of covalency.

