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Awal Noor, Sadaf Qayyum

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Mono-Guanidinate Complexes of Scandium and Lanthanum: Solvated Alkali Metal Halides versus Size of Lanthanide

Awal Noor,^{*,[a,b]} and Sadaf Qayyum^[a]

[a] Lehrstuhl Anorganische Chemie II-Katalysatordesign, Universität Bayreuth, 95440 Bayreuth (Germany).

E-mail: awal.noor@uni-bayreuth.de

[b] Department of Chemistry, COMSATS Institute of Information Technology, Abbottabad Pakistan.

ABSTRACT: The reaction of lithium guanidinate, $\text{Li}[\text{Pr}^i_2\text{NC}(\text{NAr})_2]$ (**1**, Ar = 2,6-diisopropylphenyl) with $[\text{ScCl}_3]$ at 80 °C for eight days and $[\text{LaBr}_3]$ at 50 °C overnight, in THF yields the mono-guanidinate complexes $[\text{Sc}(\text{Pr}^i_2\text{NC}(\text{NAr})_2(\text{Cl})(\mu\text{-Cl})(\text{LiCl}\text{-thf}_2)]$ (**2**) and $[\text{La}(\text{Pr}^i_2\text{NC}(\text{NAr})_2(\mu\text{-Br})_2(\text{LiBr}\text{-thf})_2(\text{LiBr}\text{-thf}_2)]$ (**3**). X-ray analysis shows that due to the varying sizes of the central metal atoms, one or three solvated Li salts are coordinated to Sc or La, respectively. In dinuclear compound **2**, Sc is five coordinate and has a square pyramidal geometry while in compound **3**, La shows a distorted octahedral coordination.

Keywords: Guanidinate / Lanthanum / Lithium / N-Ligands / Scandium

Over the past several years, chemistry of metal complexes employing guanidinate ligands has been actively studied. They have shown various coordination modes depending on the nature and steric bulk of the substituents and the metal centre involved.^[1-7] The coordination chemistry of guanidines and closely related amidinate ligands continues to be a popular area of research.^[8] The steric bulk controls the stoichiometry of ligands to the central metal atom. Jones et al used very bulky ligands to stabilize a number of metal complexes in M^I oxidation state.^[9-11] Later, we reported quintuply bonded Cr^I guanidinate complexes.^[12,13] Lanthanides are known for their high electrophilicity and their tendency to form high coordination numbers. We were interested to explore the behavior of bulky and electron rich guanidine $\text{ArNC}(\text{Pr}^i_2)\text{N}(\text{H})\text{Ar}$ (Ar = 2,6-diisopropylphenyl)^[14] towards Sc and La, which have different ionic radii.

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