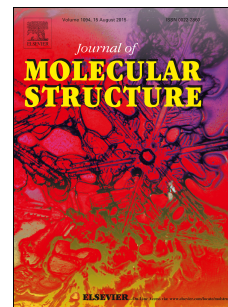


# Accepted Manuscript

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# Uncoordination mode of $\kappa^0$ -Janus scorpionate with La(III) and Ce(III) complexes: Synthesis, characterization, thermolysis and crystal structure determination

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**Abstract:** Reaction of La(III) or Ce(III) nitrates with potassium tris(3-mercapto-4-methyl-1,2,4-triazolyl)borate ( $\text{KTr}^{\text{Me}}$ ) and 1,10-phenanthroline (1:1:1 molar ratio) in water/methanol mixture leads to the formation of  $[\text{Ln}(\text{phen})_2(\text{H}_2\text{O})_2(\text{NO}_3)_2][\text{Tr}^{\text{Me}}]$  complexes ( $\text{Ln} = \text{La}$  (**1**),  $\text{Ce}$  (**2**)) in which the complexes show the uncoordinated binding mode of the scorpionate ligand to the centre metal ion. These complexes have been characterized by IR,  $^1\text{H}$  NMR and X-ray crystallography. Both the complexes exhibit ten coordination number and show multistep decomposition pathways on thermolytic study.

**Keyword:** Janus scorpionate, La(III) and Ce(III), coordination, X-ray crystallography.

## 1. Introduction

Poly(pyrazolyl)borates are well known scorpionate ligands introduced by Trofimenko in mid of 1960 [1]. Since their discovery, the metal complexes formed by these ligands have been reported with almost every metal in the Periodic Table [2]. These ligands have many coordination modes towards the centre metal. In most of the complexes, they coordinate in a facial tripodal fashion with ( $\kappa^3\text{-N,N',N}$ ) mode, but there are some complexes in which these ligands show different hapticity of bi ( $\kappa^2\text{-N, N'}$ ), mono ( $\kappa^1\text{-N}$ ) and even in uncoordinated mode  $\kappa^0$  were also observed [3-4]. Most of poly(pyrazolyl)borate ligands possess only hard nitrogen donor sites and the chemistry of these ligands are well developed in contrast to the hybrid scorpionate which have both hard and soft donor sites. These hybrid ligands have some features of Trofimenko first generation tris(pyrazolyl) borate [5] and Reglinski's soft scorpionate tris(methimazolyl)borate ( $\text{Tm}$ ) [6]. They are known as Janus scorpionate ligands [7-8] and belongs to second generation scorpionate ligands which can bind to the metal through either N or S atoms (**Fig1.1**).

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