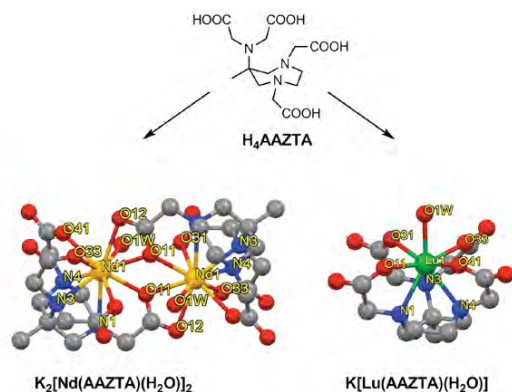


be explained by the different coordination geometry of $[\text{Ln}(\text{AAZTA})]^-$ complexes formed by the smaller and larger Ln(III)-ions.



Scheme 1. Structures of H_4AAZTA ligand, $\text{K}_2[\text{Nd}(\text{AAZTA})(\text{H}_2\text{O})]_2$ and $\text{K}[\text{Lu}(\text{AAZTA})(\text{H}_2\text{O})]$ complexes

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Keywords: lanthanides, square antiprism, dodecahedron

MS36-O3

Mixed ligand Ni Werner complexes: enhanced selectivity and hydrogen bonding frameworks

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A mixed-ligand approach in the synthesis of Werner complexes with central nickel metal and thiocyanate anions with ligands of different aromatic or hydrogen bonding functionalities formed structural intricacy. In the selectivity of xylene isomers, differentiation showed that meta xylene was favoured over the other isomers, ortho xylene (ox), para xylene (px) and ethylbenzene (eb) in the co-ordination with the host $\text{Ni}(\text{NCS})_2(\text{isoquinoline})_2(4\text{-phenylpyridine})_2$.¹ The arrangement of the rigid isoquinoline² and the flexible 4-phenylpyridine ligands in trans positions gave the host flexibility to pack meta xylene more intimately than the other isomers. The outcome of the selectivity, $\text{mx} > \text{eb} > \text{ox} > \text{px}$, was confirmed by Hirshfeld surface analysis and void spacing determinations. The ‘tunability’ of the crystal structures arises from the transformation of the nature and size of the inclusion cavities.³ Attractive functionality using hydrogen bonding of the ligands was reflected in the structure of the complex, $\text{Ni}(\text{NCS})_2(\text{nicotinamide})_2(\text{isonicotinamide})_2$. Close packing in the crystal was realised. The complex arrangement of the host showed hydrogen bonding in different directions with amide bonding between the functional groups of the ligands and sulphur of the neighbouring host anion. The use of nickel as the metal centre gives the advantage of geometries not easily accessible in organic structures.

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Keywords: inclusion compound, selectivity, mixed ligand