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Nanotubular Cyclodextrin Dimers

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Cyclodextrins are macrocyclic oligosaccharides which have found numerous applications in supramolecular chemistry. When combined with transition metals, they may lead to large assemblies suitable for the formation and study of unusual host-guest complexes.

In this work, we present the synthesis and structural characterization of two new CD dimers. The latter were obtained by reaction of the sulfur-capped CD 6^{A} , 6^{B} , 6^{D} , 6^{E} -tetradeoxy- 6^{A} , 6^{B} -(μ_{2} -sulfido)- 6^{D} , 6^{E} -(μ_{2} -sulfido)- 2^{A} , 2^{B} , 2^{C} , 2^{D} , 2^{E} , 2^{F} , 3^{A} , 3^{B} , 3^{C} , 3^{D} , 3^{E} , 3^{F} -tetradeca-O-meth-

yl-α-CD with K₂PtCl₄ and K₂PdCl₄, respectively.

The two complexes are isostructural, with P1 space group and $a = 14.3341(11)\text{Å}, b = 16.4120(14)\text{Å}, c = 17.3817(19), \alpha =$ 74.814(7)°, $\beta = 82.380(7)$ °, $\gamma = 64.190(3)$ ° for the Pt complex and a = 14.5623(3) Å, b = 16.5684(3) Å, $c = 17.4742(3)^{\circ}$, $\alpha = 16.5684(3)$ Å, $\alpha = 17.4742(3)^{\circ}$ 99.0740(10)°, $\beta = 97.3390(10)$ °, $\gamma = 116.0200(10)$ for the Pd

The X-ray analyses reveal a nanotubular structure for both complexes (length ca. 18 Å). In both of them, the two metal centres adopt a square planar coordination geometry. All CD moieties exhibit a regular torus shape.

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Molecular conformation and crystal packing studies on η^3 - η^5 Ni complexes of N-heterocyclic carbenes

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Metal complexes of N-heterocyclic carbenes have been widely used and studied in solution especially due to their activity in catalysis [1]. Here, we will present a solid state study based on newly determined structures of several Nickel complexes of N-heterocyclic complexes of the type $[Ni(\eta^3-\eta^5)(Im)X]$, $(\eta^3-\eta^5)=C_3H_5$, C_5H_5 , C_9H_7 , Im=imidazol-2-ylidenes and X= Im, Cl, Br, I. Molecular conformation and crystal packing efficiency in these complexes will be analyzed taking into account both the π and σ ligands size, conformation and degree of substitution. Studies will be extended from neutral to cationic complexes and the effect of the counter ion will also be taken into account. Data retrieved in the Cambridge Crystallographic Database will also be used and compared.







[1] Synthesis, Structure and Solution Dynamics of Allyl Nickel Complexes of N-Heterocyclic Carbenes Leonel C. Silva, Pedro T. Gomes, Luis F. Veiros, M. Teresa Duarte, Sofia I. Pascu, José R. Ascenso, and Alberto R. Dias, accepted to Organometallics