A Self-assembled Palladium Nano-cage of the Type M₂L₄ that Accommodates D-Leucine

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Abstract: In supramolecular assemblies such as nanoscopic cages and capsules, metal ions often act as glue for the spontaneous but directed assembly of organic building blocks. In some instances, coordinatively labile sites of metal centers provide a platform for direct binding to guest species through some weak interactions. In the system presented herein, two Pd(II) ions are bound by four monodentate ligands to give stable Pd_2L_4 type assembly. The two Pd(II) centers are directly linked by the semi rigid ligand that contains a long central base and two pyridyl donors linked by methylene groups $[N^2, N^6$ -bis ((pyridin-4-yl) methyl) naphthalene-2, 6-dicarboxamide]. The assembly was characterised by ¹H-NMR study and ESI-MS. Theoretical calculations were performed to obtain energy minimised structure using density functional theory, HR-TEM measurements were used to obtain size and shape information. The size of the assembly obtained experimentally is consistent with the information obtained from DFT calculations. Furthermore 1D/2D NMR and ESI-MS data indicate the utility of the assembly as a host for D-Leucine.

References: 1. Inorg. Chem. 2012, 51, 9574–9576. 2. J. Am. Chem. Soc. 2010, 132, 9973–9975. 3. Chem. Rev. 2011, 111, 6810.