Coordination-based spherical assemblies have developed to an elegant and useful pillar of modern supramolecular chemistry. Nanosized spheres are prepared by the combination of multi-topic ligands (linkers) and metals (nodes) under thermodynamic control. The rich variety of available organic ligands and versatile coordination geometry of transition metals allowed preparation of nanospheres in many different geometric shapes (cube, octahedron, cuboctahedron, tetrahedron) and sizes (1-10 nm). The characteristic shapes, interior cavities, porosities and sizes are distinct features of nanospheres that differentiate them from molecular substances. These characteristics have been utilized in many fascinating applications including separation, catalysis, light harvesting, host-guest chemistry and more. Recently, coordination-based spherical assemblies got increasing interest in the bio medicinal field. Although bio medicinal application of coordination-based self-assemblies is in its infancy, many preliminary studies presented the potential of nanospheres as drug delivery vehicles or as cytotoxic drugs for cancer treatment with non-classical activity mechanisms of toxicity and distributions in comparison to molecular complexes. To improve the application scope of nanospheres further, novel assemblies, host-guest chemistry and multi-functional features are highly desirable and subject of this thesis.