Stars and stripes: hexatopic tris(3,2 ':6 ',3 "-terpyridine) ligands that unexpectedly form one-dimensional coordination polymers

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The hexatopic ligands 1,3,5-tris(4,2″:6″,4″-terpyridin-4″-yl)benzene (1), 1,3,5-tris(3,2″:6″,3″-terpyridin-4″-yl) benzene (2), 1,3,5-tris{4-(4,2″:6″,4″-terpyridin-4″-yl)phenyl}benzene (3), 1,3,5-tris{4-(3,2″:6″,3″-terpyridin-4″- yl)phenyl}benzene (4) and 1,3,5-trimethyl-2,4,6-tris{4-(3,2″:6″,3″-terpyridin-4″-yl)phenyl}benzene (5) have been prepared and characterized. The single crystal structure of 1ů1.75DMF was determined; 1 exhibits a propeller-shaped geometry with each of the three 4,2″:6″,4″-tpy domains being crystallographically independent. Packing of molecules of 1 is dominated by face-to-face π-stacking interactions which is consistent with the low solubility of 1 in common organic solvents. Reaction of 5 with [Cu(hfacac)2]ůH2O (Hhfacac = 1,1,1,5,5,5-hexafluoropentane-2,4-dione) under conditions of crystal growth by layering resulted in the formation of [Cu3(hfacac)6(5)]nů2.8nC7H8ů0.4nCHCl3. Single-crystal X-ray diffraction reveals an unusual 1D-coordination polymer consisting of a series of alternating single and double loops. Each of the three crystallographically independent Cu atoms is octahedrally sited with cis-arrangements two N-donors from two different ligands 1 and, therefore, cis-arrangements of coordinated [hfacac]− ligands; this observation is unusual among compounds in the Cambridge Structural Database containing {Cu(hfacac)2- N2} coordination units in which the two N-donors are in a non-chelating ligand.
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