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Straight versus branched chain substituents in 4'-(butoxyphenyl)-3,2':6',3"-terpyridines: Effects on (4,4) coordination network assemblies

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The preparation and characterization of the isomers rac-4'-(4-butan-2-yloxyphenyl)-3,2':6',3"-terpyridine (rac-2), 4'-(2-methylpropoxyphenyl)-3,2':6',3"-terpyridine (3) and 4'-(tert-butoxyphenyl)-3,2':6',3"-terpyridine (4) are reported. The compounds react with Co(NCS)₂ under conditions of crystal growth at room temperature to give single crystals of [Co(rac-2)₂(NCS)₂] · CHCl₃]_n, [Co(3)₂(NCS)₂]_n and [Co(4)₂(NCS)₂] · CHCl₃]_n which possess (4,4) networks with the Co centers acting as 4-connecting nodes. Powder X-ray diffraction (PXRD) was used to confirm that the crystals chosen for single crystal X-ray diffraction were representative of the bulk samples. The detailed structures of the three networks have been compared with that of the previously reported [Co(1)₂(NCS)₂] · 4CHCl₃]_n in which 1 is 4'-(butoxyphenyl)-3,2':6',3"-terpyridine. Whereas the switch from 1 with the straight-chain butoxy substituent to rac-2, 3 and 4 with branched chains causes significant structural perturbation, changes in the spatial properties of the branched substituents are accommodated with subtle conformational changes in the 3,2':6',3"-tpy domain

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