

Publication

4'-(Pyrimidin-5-yl)- and 4'-(2-methylpyrimidin-5-yl)-4,2':6',4''-terpyridines: Selective coordination to zinc(II) through the 4,2':6',4''-terpyridine domain

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)**ID** 2615894**Author(s)** Klein, Y. M.; Constable, E. C.; Housecroft, C. E.; Zampese, J. A.**Author(s) at UniBasel** [Housecroft, Catherine](#) ; [Constable, Edwin Charles](#) ; [Zampese, Jennifer Ann](#) ; [Klein, Maximilian](#) ;**Year** 2014**Title** 4'-(Pyrimidin-5-yl)- and 4'-(2-methylpyrimidin-5-yl)-4,2':6',4''-terpyridines: Selective coordination to zinc(II) through the 4,2':6',4''-terpyridine domain**Journal** Polyhedron**Volume** 81**Pages / Article-Number** 98-104**Keywords** 4,2':6',4''-Terpyridine, Zinc, Structure, Coordination polymer, X-ray diffraction

The preparation and characterization of the compounds 4'-(pyrimidin-5-yl)-4,2':6',4''-terpyridine (3) and 4'-(2-methylpyrimidin-5-yl)-4,2':6',4''-terpyridine (4) are described. Preferential coordination through the terminal pyridine donors of the tpy domain is observed when 3 and 4 are treated with ZnCl₂ or ZnI₂. The 1-dimensional coordination polymers [{ZnCl₂(3)}_n], [{ZnI₂(3)}_n] and [{ZnI₂(4)·MeOH}_n] have been structurally characterized by single crystal X-ray crystallography. [{ZnI₂(3)}_n] is helical and crystallizes with both P- and M-helices in the lattice; the packing of P- and M-chains involves discrete tetradecar π -stacking domains involving 4,2'':6'',4''-tpy units. The introduction of the 2-methyl substituent on going from 3 to 4 has only a small effect on the structure of [{ZnI₂(L)}_n] (L = 3 or 4). The two coordination polymer chains assemble through face-to-face π -interactions into sheets with the pyrimidin-5-yl units projecting outwards. The presence of the 2-methyl substituents in 4 forces the sheets in [{ZnI₂(4)·MeOH}_n] further apart compared to those in [{ZnI₂(3)}_n], leading to the accommodation of MeOH molecules in cavities between the sheets.

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