Supplementary Material (ESI) for Chemical Communications

Supplementary information for

Self-assembly of heterodinuclear triple-stranded helicates: control by coordination number and charge

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Comments on CHECKCIF:

In the structures **3**, **5b**, and **7** the non-bonded parts of the ligands show higher thermal displacement parameters than the bonded ones (PLAT222, PLAT220). Furthermore all free refined hydrogen positions show shortened X-H distances (PLAT352, PLAT354), but we don't like to fix them to expected values with the relative "hard" restraint DFIX.

Concerning the very poor analysis of **4**: The diffracting power of the crystals was poor due to a huge amount of disordered solvents and to the size of the investigated crystals. The three non-coordinated DMFs were refined with geometrical restraints (SAME from the coordinated one) and one common isotropic thermal parameter. One methanol is refined with split positions using same isotropic thermal parameters (EADP) and geometrical restraints (SADI) There are some close contacts between the hydrogen positions, but no better way of refinement was found. The structure still has big voids, but no chemically meaningful electron density could be located in these regions.