## **Supplementary information for:**

## Tuning the size of supramolecular $M_4L_4$ tetrahedra by ligand connectivity

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Representations of the containers  $[(L^1)_4 Ti_4]^{8-}$  and  $[(L^2)_4 Ti_4]^{8-}$  showing a compressed structure of  $[(L^1)_4 Ti_4]^{8-}$  and the expanded structure of  $[(L^2)_4 Ti_4]^{8-}$ .



The blue line shows that the ligand  $L^1$  points inwards. Therefore, the cavity of the tetrahedron is small. The average Ti-N distance of the complex  $[(L^1)_4 Ti_4]^{8-}$  is 9.51 Å.



The red line shows that ligand  $L^2$  is nearly planar. The average Ti-N distance of the complex  $[(L^2)_4 Ti_4]^{8-1}$  is 10.37 Å which is 0.86 Å larger than the Ti-N distance of the tetrahrdron with ligand  $L^1$ .



ESI MS in methanol of  $Na_8[(1)_4Ti_4]$ 



Relevant parts of the ESI MS spectrum of  $Na_8[(2)_4Ti_4]$ . (The sample was directly sprayed from deuterated solvents in order to guarantee that the species detected by NMR and MS are the same).

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