Jarv's guide to expanding Mono/Bis/Tris to Tetrakis & on and on. (Actually, I just looked up the names - officially it is: Bis, Tris, Tetrakis, Pentakis, Hexakis ; Table 2 here: <http://www.chemistry.wustl.edu/~edudev/LabTutorials/naming_coord_comp.html> )

\* Start with the Tris forcefield: <https://github.com/jarvist/CoarseGrainPCBM/blob/master/GromacsForcefield/T/TRIS-PCBM.top>

This is in a .TOPology file; which is the full force field specification.

and a collection of Tris molecules (1000 in this case):-

<https://github.com/jarvist/CoarseGrainPCBM/blob/master/GromacsForcefield/T/TRIS-PCBM.pdb>

\* Edit the PDB file down to a single molecule (i.e. delete 999\*4 lines, for each of the pseudo atoms)

\* Check that it displays OK in Pymol & that you have a single molecule, in a big box (see the unit cell).

\* Copy TRIS-PCBM.top --> TETRAKIS\_PCBM.top

\* Add an additional sidechain to the topology; this will require making additions to [atoms], [bonds], [exclusions] and [angles] . The gromacs manual is the best reference for this file; there's a whole chapter on Topologies.

 - you'll need to think about what combination of right angles you want to build a structured tetra...

\* Add an additional sidechain to the PDB file, put it somewhere within the box a way away from the molecule already there.

\* Do a steepest descent minimisation, which will require something like:

> grompp -f steep.mdp -p TETRAKIS\_PCBM.top -c TETRAKIS-PCBM.pdb

> mdrun

You should then have a confout.gro with a relaxed structure, and should be able to view the trajectory to watch it 'fix' your geometry.

\* Take the fixed single-molecule tetrakis, and build up a big box of solvent with it. This used to be (Gromacs versions 4.X) the 'genbox' command, which I now think is now part of their super tool 'gmx insert-molecules'.

\* Take this big box of solvent (well, OK - 1000 molecules at first!) and setup a job ('grompp') for first minimisation (to get rid of bad contacts), and then MD, to equilibriate with a barostat & probably an elevated temperature if the MD FF is stable, to equilibrate a box.

There's probably loads of small steps that I've missed out there; hopefully this is somewhat useful though.