

The title compound (I) crystallizes in the orthorhombic space group  $P2_12_12$  ( $a=10.7028 \text{ \AA}$ ,  $b=12.8508 \text{ \AA}$ ,  $c=6.5844 \text{ \AA}$ ,  $V=905.62 \text{ \AA}^3$ ) at 298 K (phase I). The Ti complex resides on a two-fold axis with  $Z'=0.5$ . Complex (I) undergoes two sharp enantiotropic phase transitions upon cooling. The first transformation occurs at 293 K to yield a unit cell with a doubled  $c$  axis ( $a=10.5539 \text{ \AA}$ ,  $b=12.8757 \text{ \AA}$ ,  $c=13.0817 \text{ \AA}$ ,  $V=1777.66 \text{ \AA}^3$ ) at 175 K and the orthorhombic space group  $P2_12_12_1$  (phase II). The doubling of the unit cell volume results in the addition of a translational component to the two-fold rotational symmetry in the  $c$  direction, and now the complex is in a general position. The second transition takes place at 147 K to convert the single crystal into a merohedrally twinned crystal with two monoclinic components of half the size ( $a=10.5529 \text{ \AA}$ ,  $b=12.7403 \text{ \AA}$ ,  $c=6.5486 \text{ \AA}$ ,  $\beta=92.327^\circ$ ,  $V=879.71 \text{ \AA}^3$ ) at 100 K) in the monoclinic space group  $P2_1$  (phase III). The Ti complex remains in a general position. The concomitant phase transition and twinning necessarily result in the loss of symmetry along the  $a$  and  $c$  axes and can be thought of as taking the  $b$  axis in phase II and "pulling" (shifting) it in the positive direction to generate the twinning in phase III (see diagram). The unique angle widens as the temperature is lowered. The variable temperature study of the selected crystal was conducted in an automated mode on a Bruker SMART APEX2 diffractometer with Cu  $K\alpha$  radiation while the exact transition temperatures were manually pinpointed with Mo  $K\alpha$  radiation. The molecular symmetry evaluations and exact refinement procedures are also discussed.

Keywords: Polymorphism, Twinning, Solid phase transitions

### P09.01.01

*Acta Cryst.* (2008). A64, C474

#### Knowledge-based design of host-guest interactions in wheel-and-axle inorganic diols

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We are interested in the design of hybrid organic-inorganic wheel-and-axle systems (waad) with flexible dynamic frameworks that can create pores "on demand" to accommodate small guest molecules [1-3]. A reversible dynamic reorganization between the waad non-solvate and solvate phases requires two conditions: (i) a low cost structural rearrangement between two states represented by the initial close (self-mediated) and the final open (guest-mediated) host frameworks, (ii) an easily accessible migration path for the outgoing and incoming guest molecules. Palladium complexes of triarylcarbinol ligands have shown suitable structural requisites to give reversible host-guest properties [2, 3]. New iminic ligands designed on this basis result very promising promoters of potentially bistable supramolecular architectures based on metallo-organic supramolecular building units as wide as 40 Å (Figure).

#### References

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Keywords: host-guest complexes, supramolecular assemblies, crystal engineering

### P09.01.02

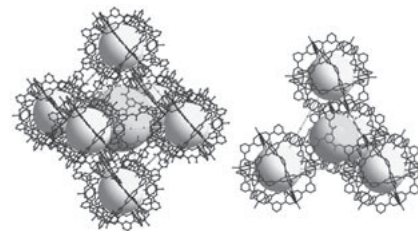
*Acta Cryst.* (2008). A64, C474

#### A designed metal-organic framework based on a metal-organic polyhedron

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Metal-organic frameworks (MOFs) based on metal-organic polyhedra (MOPs) might provide efficient ways for the construction of designed porous MOFs, because MOPs themselves have their inherent cavities. We have prepared a (3,24)-connected MOF,  $[Zn_{24}(L)_8(H_2O)_{24}]_n$ , using a  $C_3$  symmetric tritopic ligand, 5,5',5''-[1,3,5-benzenetriyltris(carbonylimino)]tris-1,3-benzenedicarboxylic acid (H6L). The carboxylate groups of 1,3-benzenedicarboxylate unit of the ligand can be combined with  $Zn^{2+}$  ion to form paddle wheel secondary building units,  $Zn_2(COO)_4$ , which produce an edge-directed corner-linked metal-organic cuboctahedron (MOC). The planar  $C_3$  symmetric tritopic character of the ligand can force all of the resulting MOCs to a triangular arrangement for a cubic close packing (CCP) arrangement at all 24 edges of the cuboctahedron. This CCP arrangement of the MOCs led to additional superoctahedral and supertetrahedral cavities. Though the (3,24)-connected MOF represents the highest connected network topology presently known for frameworks corresponds to ~71% of the total crystal volume.



Keywords: metal-organic framework, metal-organic polyhedra, metal-organic cuboctahedron

### P09.01.03

*Acta Cryst.* (2008). A64, C474-475

#### Properties of metal-organometallic frameworks derived from facially $\eta^6$ metalated terephthalates

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Interest in the design and synthesis of metal-organometallic