The Way of Crystal of [cpMe$_4$SiMe$_2$N(t-Bu)]TiCl$_2$ from Disoder thru Modulation to Twinning

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Constrained geometry catalysts based on *ansa*-{(*tert*-butylamido-κ*N*)dimethyl(η^5-2,3,4,5-tetramethylcyclopentadienyl)silane} dichlorotitanium (IV) (**1**) allowed for a large scale production of new polymers and copolymers of specific properties [1] The structure of compound **1** was investigated by X-ray diffraction a [2,3], however the geometrical parameters were not published in full.

From our reinvestigation [4] follows that the *tert*-butyl moiety is disordered in two positions over mirror operation of Pnma space group at room temperature. The new measurement of **1** at low temperatures revealed two phase transitions by reordering t-Bu moiety. The results of first one can be described in supercel 4**a**,**b**,**c** (**1**b), and space group Pna2$_1$, the second one (**1**c) as 3**a**,**b**,**c** and P2$_1$/n11 pseudomeroedricaly twinned into the lattice symmetry mmm. Whole pathway can be unified by applying the modulation concept, superspace group Pnma(a00)0s0 with two q-vectors (1/4,0,0) and (1/3,0,0) for **1**b and **1**c, respectively, affording unique opportunity to test various models (commensurate versus incommensurate etc.).

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