Supporting Information

Title: Structural Motifs in (*t*-butoxy)Zirconium Phosphinates, Arsinates and Phosphates

Authors: K. C. Kumara Swamy, Michael Veith, Volker Huch, and Sanjay Mathur

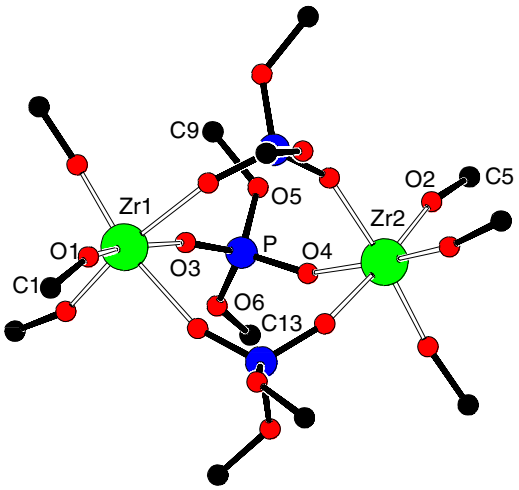

Figure 5. A Platon drawing of Zr_2(O-*t*-Bu)$_5$(HO-*t*-Bu)(μ,μ'-O_2P(O-*t*-Bu)$_2$)$_3$ (**7**); terminal atoms of the *t*-butoxy groups and the hydrogen atoms are not shown for clarity.

Crystal data for **7**: $C_{96}H_{218}O_{36}P_6Zr_4$, M = 2499.40, Trigonal, Space group $P\bar{3}$, *a* = 19.244(3) , *b* = 19.244(3), *c* = 14.978(3) Å, α = β = 90, γ = 120°, *V* = 4803.7(14) Å^3, *Z* = 1 (full molecule), D(calc) = 0.864 Mgm^{-3}, μ = 0.307 mm^{-1}, Data/ restraints/ parameters 4943/ 0/ 225, *S* (on F^2) 1.114, R1 [I > 2σ(I)] = 0.0737, wR2 (all data) = 0.2384, Largest diff. peak and hole 0.461/ -0.361eÅ^{-3}. The hydrogen atom of the hydroxyl group could not be located, but it is probably located on one of the *t*-butoxy groups of Zr(2) (based on bond parameters). Selected bond parameters: Zr(1)- O(1) 1.964(4), Zr(1) – O(3) 2.239(4), Zr(2) – O(2) 2.012(5), Zr(2) – O(4) 2.148(4). O(1) – Zr(1) – O(1') 98.33(17); O(1) – Zr(1) – O(3') 87.92(17); O(1) – Zr(1) - O(3'') 90.72(17), O(1) – Zr(1) – O(3) 168.10(17), O(3) – Zr(1) – O(3') 81.85(15), O(2) – Zr(2) – O(2') 95.5(3), O(2) – Zr(2) - O(4) 87.0(2), O(2) – Zr(2) – O(4') 174.1(2), O(2) – Zr(2) – O(4'') 89.6(2), O(4) – Zr(2) – O(4') 87.67(16). Symmetry relationship: (i) -y+1, x-y, z; (ii) -x+y+1, -x+1, z.