Supplementary Material (ESI) for PCCP
This journal is © the Owner Societies 2009

Ligand Dynamics on the Surface of Zirconium Oxo Clusters

Electronic supplementary information

Table 1. Crystal data and structure refinement for $Zr_4O_2(OMc)_{12} \cdot C_6H_6$.

Empirical formula	$C_{54}H_{66}O_{26}Zr_4$
Formula weight	1495.95
Temperature	173(2) K
Wavelength	71.073 pm
Crystal system, space group	triclinic, P-1
Unit cell dimensions	a = 1115.5(1) pm α = 76.062(2) deg.
	b = 1184.5(1) pm ß = 85.173(2) deg.
	c = 12.049(1) pm γ = 85.040(2) deg.
Volume	1536.0(2) 10^6 pm^3
Z, Calculated density	1, 1.617 g/cm^3
Absorption coefficient	0.741 mm^{-1}
Crystal size	0.40 x 0.32 x 0.24 mm
Theta range for data collection	2.47–26.37°
Reflections collected / unique	9283 / 6195 [R(int) = 0.0132]
Max. and min. transmission	0.8421 and 0.7558
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6195 / 0 / 397
Goodness-of-fit on F^2	1.058
Final R indices [I>2σ(I)]	R_1 = 0.029, wR_2 = 0.071
R indices (all data)	R_1 = 0.035, wR_2 = 0.074
Largest diff. peak and hole	0.618 and -0.391 $e \cdot A^3$

Table 2. Selected bond lengths [pm] and angles [deg]

Zr(1)-O(25)*	207.3(2)
Zr(1)-O(25)	208.6(2)
Zr(1)-O(19)	213.8(2)
Zr(1)-O(13)	216.6(2)
Zr(1)-O(7)	217.4(2)
Zr(1)-O(1)	217.5(2)
Zr(1)-O(24)	220.5(2)
Zr(2)-O(25)	205.3(2)
Zr(2)-O(32)	214.5(2)
Zr(2)-O(15)	217.8(2)
Zr(2)-O(9)	218.0(2)
Zr(2)-O(28)	223.2(2)
Zr(2)-O(37)	223.7(2)
Zr(2)-O(3)	224.6(2)
Zr(2)-O(26)	228.8(2)
O(25)*-Zr(1)-O(25)	74.72(7)
O(25)*-Zr(1)-O(19)	86.24(7)
O(25)-Zr(1)-O(19)	147.19(7)
O(25)*-Zr(1)-O(13)	121.71(7)
O(25)-Zr(1)-O(13)	78.89(7)
O(19)-Zr(1)-O(13)	133.80(7)
O(25)*-Zr(1)-O(7)	59.47(8)
O(25)-Zr(1)-O(7)	105.81(8)
O(19)-Zr(1)-O(7)	83.07(8)
O(13)-Zr(1)-O(7)	77.83(8)
O(25)*-Zr(1)-O(1)	84.26(7)
O(25)-Zr(1)-O(1)	76.56(7)
O(19)-Zr(1)-O(1)	75.12(7)
O(13)-Zr(1)-O(1)	137.36(7)
O(7)-Zr(1)-O(1)	76.08(8)
O(25)*-Zr(1)-O(24)	86.88(7)

O(25)-Zr(1)-O(24)	128.25(7)
O(19)-Zr(1)-O(24)	75.72(7)
O(13)-Zr(1)-O(24)	70.64(7)
O(7)-Zr(1)-O(24)	107.25(8)
O(1)-Zr(1)-O(24)	149.98(7)
O(25)-Zr(2)-O(32)	93.17(7)
O(25)-Zr(2)-O(15)	82.36(7)
O(32)-Zr(2)-O(15)	144.07(7)
O(25)-Zr(2)-O(9)	93.59(8)
O(32)-Zr(2)-O(9)	142.93(8)
O(15)-Zr(2)-O(9)	72.99(8)
O(25)-Zr(2)-O(28)	152.68(7)
O(32)-Zr(2)-O(28)	92.85(7)
O(15)-Zr(2)-O(28)	77.21(7)
O(9)-Zr(2)-O(28)	97.52(8)
O(25)-Zr(2)-O(37)	80.97(7)
O(32)-Zr(2)-O(37)	73.31(7)
O(15)-Zr(2)-O(37)	70.77(7)
O(9)-Zr(2)-O(37)	143.76(8)
O(28)-Zr(2)-O(37)	75.32(7)
O(25)-Zr(2)-O(3)	76.18(6)
O(32)-Zr(2)-O(3)	72.72(7)
O(15)-Zr(2)-O(3)	138.74(7)
O(9)-Zr(2)-O(3)	73.66(8)
O(28)-Zr(2)-O(3)	130.93(7)
O(37)-Zr(2)-O(3)	137.49(7)
O(25)-Zr(2)-O(26)	149.95(7)
O(32)-Zr(2)-O(26)	78.82(8)
O(15)-Zr(2)-O(26)	120.70(7)
O(9)-Zr(2)-O(26)	77.24(8)
O(28)-Zr(2)-O(26)	57.32(7)
O(37)-Zr(2)-O(26)	122.94(7)
O(3)-Zr(2)-O(26)	73.78(7)
Zr(2)-O(25)-Zr(1)*	130.69(8)

This journal is © the Owner Societies 2009

Zr(2)-O(25)-Zr(1)	122.11(8)
Zr(1)*-O(25)-Zr(1)	105.28(7)

Symmetry transformation used to generate equivalent atoms (*): -x+1,-y,-z