ORGANOMETALLICS
Organometallics, 1997, 16(24), 5289-5301, DOI:10.1021/om970837b

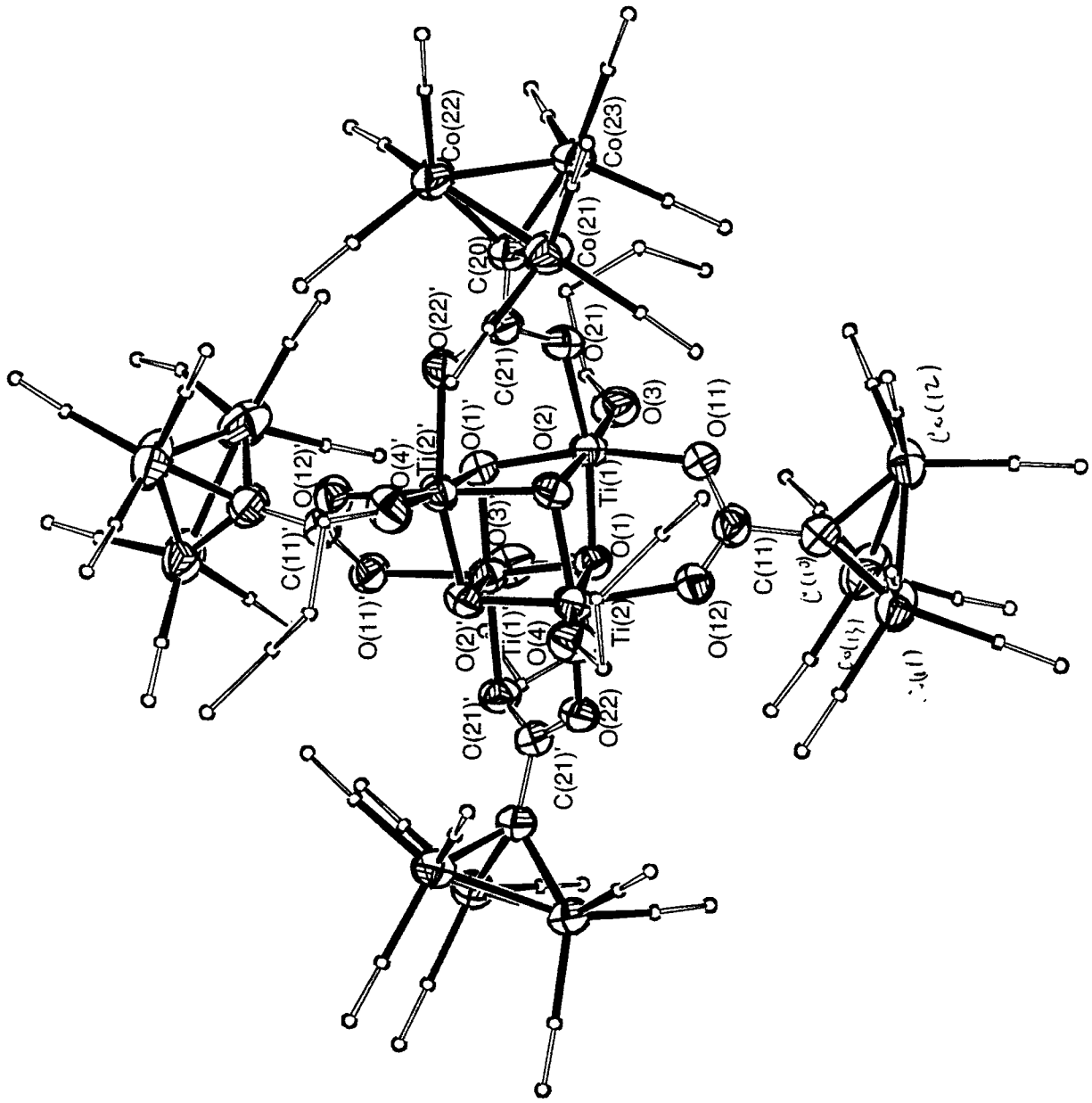
Table 6. Anisotropic displacement parameters ($Å^2$) for $Ti_4O_4(OBu)_4[O_2CCCo_3(CO)_9]_4$.

	U11	U22	U33	U23	U13	U12
Ti(1)	0.0536(6)	0.0653(8)	0.0644(7)	-0.0079(6)	-0.0050(5)	-0.0008(6)
Ti(2)	0.0637(7)	0.0667(8)	0.0573(7)	0.0007(6)	-0.0049(5)	-0.0090(6)
Co(11)	0.1000(13)	0.167(2)	0.113(2)	-0.030(2)	0.0415(12)	-0.0353(14)
Co(12)	0.1035(12)	0.149(2)	0.0865(12)	-0.0347(12)	0.0282(9)	-0.0136(12)
Co(13)	0.0869(14)	0.160(2)	0.169(2)	0.004(2)	0.0181(14)	0.0361(15)
Co(14)	0.150(15)	0.159(14)	0.105(11)	-0.025(10)	0.025(10)	0.052(11)
Co(15)	0.106(10)	0.138(14)	0.162(14)	0.017(11)	0.051(9)	0.008(10)
Co(16)	0.172(26)	0.381(48)	0.153(21)	0.174(30)	0.100(22)	0.175(33)
Co(21)	0.0762(7)	0.1041(9)	0.0888(7)	0.0232(6)	-0.0095(6)	0.0005(6)
Co(22)	0.0609(6)	0.1331(10)	0.0759(7)	0.0084(6)	-0.0051(5)	0.0169(6)
Co(23)	0.0691(6)	0.1219(9)	0.0661(6)	0.0013(6)	-0.0105(5)	-0.0038(6)
O(1)	0.051(2)	0.060(3)	0.065(3)	-0.002(2)	-0.002(2)	0.002(2)
O(2)	0.066(3)	0.063(3)	0.053(2)	0.004(2)	-0.008(2)	-0.001(2)
O(3)	0.082(3)	0.067(3)	0.114(4)	-0.021(3)	-0.009(3)	-0.006(3)
O(4)	0.096(4)	0.070(3)	0.085(3)	0.010(3)	-0.007(3)	-0.027(3)
O(11)	0.059(3)	0.096(4)	0.065(3)	-0.010(2)	0.003(2)	-0.005(3)
O(12)	0.073(3)	0.087(3)	0.061(3)	-0.004(3)	0.005(2)	-0.013(3)
O(21)	0.058(3)	0.082(3)	0.068(3)	-0.009(2)	-0.011(2)	0.001(2)
O(22)	0.063(3)	0.095(3)	0.056(3)	0.000(3)	-0.004(2)	-0.014(2)
C(10)	0.069(4)	0.111(6)	0.079(5)	-0.008(5)	0.005(4)	-0.004(4)
C(11)	0.069(5)	0.091(6)	0.058(4)	0.008(4)	0.005(4)	0.007(4)
C(20)	0.060(4)	0.095(5)	0.064(4)	0.003(4)	-0.006(3)	0.004(4)
C(21)	0.054(4)	0.078(5)	0.062(4)	0.004(4)	-0.001(3)	-0.001(4)
C(111)	0.187(17)	0.224(23)	0.166(17)	-0.013(17)	0.058(13)	-0.048(18)
C(112)	0.110(9)	0.257(18)	0.166(13)	-0.093(12)	0.039(8)	-0.058(10)
C(113)	0.167(14)	0.392(29)	0.242(18)	-0.176(19)	0.107(14)	-0.123(17)
C(121)	0.118(9)	0.212(15)	0.123(9)	-0.034(9)	0.011(7)	-0.028(10)
C(122)	0.190(14)	0.301(22)	0.201(15)	-0.152(16)	0.088(13)	-0.062(14)
C(123)	0.200(17)	0.240(20)	0.091(9)	-0.001(10)	0.003(9)	0.015(14)
C(131)	0.127(11)	0.140(12)	0.191(14)	0.031(10)	0.039(9)	0.033(9)
C(133)	0.147(13)	0.324(26)	0.227(21)	0.043(19)	-0.085(14)	0.025(14)

Table 6. continued page 2

C(211)	0.095(7)	0.132(9)	0.146(9)	0.044(7)	0.009(7)	-0.022(7)
C(212)	0.126(8)	0.099(8)	0.151(10)	0.025(7)	-0.027(7)	0.013(7)
C(213)	0.107(7)	0.156(10)	0.120(8)	0.048(8)	0.000(6)	0.001(7)
C(221)	0.089(7)	0.195(12)	0.115(8)	0.010(8)	-0.007(6)	0.044(7)
C(222)	0.089(7)	0.177(12)	0.140(9)	0.019(8)	0.031(6)	0.005(7)
C(223)	0.110(8)	0.180(12)	0.111(8)	-0.003(8)	0.001(6)	0.038(8)
C(231)	0.143(9)	0.117(9)	0.115(8)	-0.004(7)	0.018(7)	-0.026(7)
C(232)	0.085(6)	0.194(11)	0.076(6)	-0.001(6)	-0.016(5)	-0.007(6)
C(233)	0.095(6)	0.143(9)	0.077(6)	-0.003(5)	-0.003(5)	0.004(6)
O(111)	0.449(27)	0.186(13)	0.235(16)	0.021(12)	0.050(15)	-0.056(15)
O(112)	0.133(7)	0.300(14)	0.214(11)	-0.116(10)	0.016(7)	-0.049(8)
O(113)	0.179(10)	0.529(27)	0.387(20)	-0.249(19)	0.194(13)	-0.135(14)
O(121)	0.158(9)	0.265(13)	0.210(11)	-0.022(9)	0.002(8)	-0.083(9)
O(122)	0.255(14)	0.534(28)	0.319(17)	-0.300(19)	0.176(13)	-0.124(16)
O(123)	0.294(18)	0.349(21)	0.156(10)	0.064(11)	-0.019(10)	0.083(15)
O(131)	0.195(11)	0.143(9)	0.321(16)	0.048(9)	0.066(11)	0.024(8)
O(133)	0.282(19)	0.587(36)	0.298(21)	0.107(22)	-0.177(17)	-0.033(19)
O(211)	0.090(5)	0.208(9)	0.234(10)	0.056(7)	0.046(6)	-0.001(6)
O(212)	0.209(10)	0.109(6)	0.195(9)	-0.006(6)	-0.056(8)	0.004(6)
O(213)	0.173(8)	0.247(11)	0.152(7)	0.112(8)	-0.024(6)	0.022(7)
O(221)	0.114(6)	0.321(13)	0.162(7)	0.064(8)	-0.034(6)	0.083(7)
O(222)	0.174(9)	0.252(13)	0.257(13)	0.068(10)	0.097(9)	-0.008(9)
O(223)	0.239(12)	0.256(12)	0.154(8)	-0.093(8)	-0.019(8)	0.081(9)
O(231)	0.252(12)	0.164(9)	0.212(10)	-0.020(8)	0.056(9)	-0.086(9)
O(232)	0.130(6)	0.290(11)	0.093(5)	0.018(6)	-0.040(5)	0.014(7)
O(233)	0.111(5)	0.200(9)	0.132(6)	-0.014(5)	0.015(5)	0.040(6)
C(31)	0.307(23)	0.128(12)	0.245(19)	0.025(12)	-0.083(17)	-0.079(13)
C(41)	0.254(18)	0.183(13)	0.193(15)	0.108(12)	-0.075(13)	-0.101(13)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$


Co(22)
Co(23)
Co(21)
C(20)
O(22')
C(21)
O(21)
O(1')
O(2)
O(3)
O(11)
Ti(2)'
O(4')
O(12')
C(11)'
O(11)'
O(2)'
Ti(1)'
O(4)
O(3)'
Ti(1)
O(1)
Ti(2)
O(12)
C(11)
O(21)'
O(22)
C(21)'

EXPERIMENTAL

DATA COLLECTION

A black block-shaped crystal of $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4 \cdot C6H_{14}$ having approximate dimensions of 0.31 x 0.28 x 0.25 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were performed with MoKα radiation (λ = 0.71073 Å) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal, incident beam monochromator.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 25 reflections in the range $26^\circ < 2\theta < 30^\circ$, measured by the computer controlled diagonal slit method of centering. The monoclinic cell parameters and calculated volume are: a = 21.939(2), b = 16.311(2), c = 30.200(3) Å, β = 90.321(8)°, V = 10807(2) $Å^3$. For Z = 4 and F.W. = 2656.76 the calculated density is 1.700 g/cm^3. As a check on crystal quality, an omega/theta profile analysis of reflections was carried out, which showed that Δω and Δθ reached 0.85°, indicating poor crystal quality. From the systematic absences of:

hkl h+k=2n

h0l l=2n

and from subsequent least-squares refinement, the space group was determined to be C2/c (No. 15).

The data were collected at a temperature of 20°C using the ω/2θ scan technique. The scan rate varied from 1.37 to 8.24°/min (in ω). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections where a slow scan rate is used. Data were collected to a maximum 2θ of 45.0°. The

scan range (in degrees) was determined as a function of θ to correct for the separation of the Kα doublet; the scan width was calculated as follows:

$$\omega \text{ scan width} = 0.85 + 0.35 \tan\theta$$

Moving-crystal moving-counter background counts were made by scanning an additional 25% above and below this range. Thus the ratio of peak counting time to background counting time was 2:1. The counter aperture was also adjusted as a function of θ. The horizontal aperture width ranged from 2.4 to 2.8 mm; the vertical aperture was set at 4.0 mm. The diameter of the incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector; the attenuator factor was 19.291.

DATA REDUCTION

A total of 7197 reflections were collected, of which 7035 were unique and not systematically absent. As a check on crystal and electronic stability 3 representative reflections were measured every 180 minutes of X-ray exposure. The slopes of the least-squares lines through plots of intensity versus time were -0.08% per hour which corresponds to a total loss in intensity of 6.9% (when applying the average slope) over 88.3 hours of X-ray exposure. A linear decay correction was applied. The correction factors on I ranged from 1.000 to 1.036 with an average value of 1.017.

Lorentz and polarization corrections were applied to the data. The linear absorption coefficient is 21.55 cm^{-1} for MoKα radiation. An empirical absorption correction based on a series of psi-scans was applied to the data. Relative transmission coefficients ranged from 0.7224 to 0.9986 with an average value of 0.845.

STRUCTURE SOLUTION AND REFINEMENT

The structure was solved by direct methods of the SDP package.[1] Metal atoms

and their coordinating atoms were located from an E-map. The remaining atoms were locatedin succeeding difference Fourier syntheses. Data were then transfered to a SHELXTL environment for further structure solution and refinement.- The molecule was found disordered on two sets of positions as if it rotated around its 2-fold axis for 90 so that every apex atom of a cube-like core (alternating 4 Ti atoms and 4 O atoms) was completely overlapped with diffrent type of atom from the other core, while orientations of two independent dimethylphenoxy ligand groups of a set were different from those on the other set and were not overlapped, which could be seen by overlapping Figure 1 and Figure 2. As for the two independent $[O_2CCCo_3(CO)_9]^-$ groups, oxygen atoms were completely disordered along with the cube-like core, one rotational disorder with an occupancy coefficient for the secondary set of positions (Co(24) - Co(26)) of 0.317(8) after convergence, while other atoms remained intact. It should be pointed out that Ti(1) and O(3), although chemically belonged to different molecules as shown on Figure 1 and Figure 2 respectively, they were located on the same position and refined for X-ray diffraction as a unique mixture of atoms consisting of 50% oxygen and 50% titanium, and so did Ti(2) and O(4), O(1) and Ti(3), and O(2) and Ti(4). Refinement of the hexane solvent molecule with full occupancy yielded too high thermal parameters for carbon atoms, such as 0.45 for Uiso of C(303), moreover, refinement of the group occupancy converged to the wrong direction: larger than 1.0 group occupancy and even higher thermal parameters. In the final refinement the group occupancy was arbitrarily set to 0.5 and bond length restraint was applied. All hydrogen atoms were included in the refinement but restrained to ride on the atom to which they are bonded. The observed criterion of $F^2 > 2\sigma(F^2)$ was used only for calculating conventional R factor and wasnot relavent to the choice of reflections for refinement. The refinement converged to a final value of

R_1 = 0.1149 and wR_2 = 0.2714 for observed unique reflections ($I > 2\sigma(I)$) and R_1 = 0.1882 and wR_2 = 0.3779 for all unique reflections including those with negative intensities. The weighted R-factors, wR, are based on F^2 and conventional R-factors, R, on F, with F set to zero for negative intensities. All reflections, including those with negative intensities, were included in the refinement and the $I > 2\sigma(I)$ criterion was used only for calculating R_1. The maximum and minimum residual electron densities on the final difference Fourier map were 0.721 e/Å^3 and -0.699 e/Å^3, respectively. All e.s.d's were estimated by the use of the full covariance matrix. The cell e.s.d's were included in the estimation of e.s.d's of bond distances and angles. Final atomic coordinates are listed in Table 2. Selected bond distances and angles are given in Table 3.

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(2) SHELXTL Version 5, Siemens Industrial Automation Inc., 1994

Table 1. Crystal data and structure refinement for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$

Empirical formula	$C_{82}\ H_{50}\ Co_{12}\ O_{52}\ Ti_4$
Formula weight	2765.98
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 21.939(2) Å α = 90 deg. b = 16.311(2) Å β = 90.321(8) deg. c = 30.200(3) Å γ = 90 deg.
Volume	10807(2) $Å^3$
Z	4
Density (calculated)	1.700 Mg/m^3
Crystal size	0.31 x 0.28 x 0.25 mm
Wavelength	0.71073 Å
Absorption coefficient	2.155 mm^{-1}
F(000)	5480
Temperature	293(2) K
Diffractometer	CAD4
Theta range for data collection	2.06 to 22.48 deg.
Index ranges	$-23 \le h \le 23$, $-17 \le k \le 0$, $0 \le l \le 32$
Scan type	ω/2θ
Scan rate	1.37 - 8.24°/min (in ω)
Scan width	0.85° + 0.35°tanθ (in ω)
Total data collected	7197
Unique data	7035 [R(int) = 0.0609]
Unique observed data [$I>2\sigma(I)$]	4229

Table 1. continued page 2.

Corrections	Lorentz-polarization linear decay (-6.9%/88.3h) psi-scans absorption (0.9986 - 0.7224 on I)
Refinement method	Full-matrix on F^2 (SHELXL-93)
Data / restraints / parameters	6980 / 5 / 711
Goodness-of-fit on F^2	1.196
Final R indices [$I>2\sigma(I)$]	R_1 = 0.1149, wR_2 = 0.2714
R indices (all data)	R_1 = 0.1882, wR_2 = 0.3779
Largest diff. peak and hole	0.721 and -0.699 e·Å^{-3}

Table 2. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$

	x	y	z	U_{eq}(Å^2)[a]
Ti(1)	0.9356(2)	0.0553(2)	0.75445(13)	0.0448(10)[b]
Ti(2)	0.9940(2)	0.1887(2)	0.70321(13)	0.0476(10)[b]
O(1)	0.9369(2)	0.1842(3)	0.7540(2)	0.0648(13)[b]
O(2)	0.9940(2)	0.0541(3)	0.7043(2)	0.0698(14)[b]
Ti(3)	0.9369(2)	0.1842(3)	0.7540(2)	0.0648(13)[b]
Ti(4)	0.9940(2)	0.0541(3)	0.7043(2)	0.0698(14)[b]
O(3)	0.9356(2)	0.0553(2)	0.75445(13)	0.0448(10)[b]
O(4)	0.9940(2)	0.1887(2)	0.70321(13)	0.0476(10)[b]
Co(11)	0.82849(13)	0.1284(2)	0.57578(9)	0.0886(9)
Co(12)	0.76483(13)	0.2001(2)	0.63012(11)	0.1090(11)
Co(13)	0.76380(13)	0.0490(2)	0.62633(10)	0.1013(10)
Co(21)	1.1539(2)	0.1579(3)	0.56456(13)	0.090(2)[c]
Co(22)	1.1956(2)	0.0335(2)	0.5985(2)	0.088(2)[c]
Co(23)	1.2303(2)	0.1692(3)	0.6237(2)	0.079(2)[c]
Co(24)	1.2321(4)	0.0645(5)	0.6267(3)	0.072(4)[d]
Co(25)	1.1586(4)	0.0751(7)	0.5664(3)	0.095(5)[d]
Co(26)	1.2009(5)	0.2005(5)	0.5983(3)	0.072(3)[d]
O(11A)	0.8709(8)	0.0747(10)	0.7070(6)	0.049(5)[b]
O(11B)	0.9216(8)	0.1639(10)	0.6639(6)	0.047(5)[b]
O(12A)	0.8712(11)	0.1703(15)	0.7056(8)	0.084(7)[b]
O(12B)	0.9186(13)	0.0756(15)	0.6629(8)	0.091(8)[b]
O(21A)	1.0589(8)	0.1680(10)	0.6553(6)	0.048(5)[b]
O(21B)	1.1193(8)	0.0824(10)	0.6932(6)	0.042(4)[b]
O(22A)	1.1202(11)	0.1615(15)	0.6924(8)	0.080(7)[b]
O(22B)	1.0611(12)	0.0715(14)	0.6548(8)	0.087(8)[b]
C(10)	0.8278(7)	0.1221(10)	0.6376(6)	0.072(4)
C(11)	0.8758(7)	0.1221(10)	0.6711(5)	0.057(4)
C(20)	1.1529(7)	0.1188(10)	0.6240(5)	0.070(4)
C(21)	1.1083(7)	0.1195(11)	0.6606(6)	0.063(5)
O(31)	0.9243(7)	-0.0534(10)	0.7601(6)	0.044(4)[b,e]
O(41)	0.9873(7)	0.2978(10)	0.6918(5)	0.043(4)[b,e]

Table 2. continued page 2.

O(51)	0.9238(11)	0.2942(16)	0.7600(8)	0.090(7)[b,e]
O(61)	0.9845(11)	-0.0595(15)	0.6918(8)	0.085(7)[b,e]
C(31)	0.9265(12)	-0.1358(17)	0.7742(9)	0.049(7)[b,e]
C(32)	0.9042(15)	-0.1910(22)	0.7425(12)	0.066(9)[b,e]
C(33)	0.9083(17)	-0.2750(24)	0.7531(13)	0.088(11)[b,e]
C(34)	0.9283(18)	-0.2913(28)	0.7956(14)	0.100(12)[b,e]
C(35)	0.9468(15)	-0.2410(20)	0.8249(11)	0.069(9)[b,e]
C(36)	0.9467(15)	-0.1545(21)	0.8123(11)	0.072(9)[b,e]
C(37)	0.8785(20)	-0.1620(26)	0.6988(13)	0.098(12)[b,e]
C(38)	0.9671(21)	-0.0975(28)	0.8444(16)	0.103(14)[b,e]
C(41)	0.9725(12)	0.3805(17)	0.6849(9)	0.048(6)[b,e]
C(42)	1.0084(14)	0.4198(20)	0.6570(11)	0.064(8)[b,e]
C(43)	0.9915(20)	0.5062(27)	0.6487(15)	0.105(13)[b,e]
C(44)	0.9499(23)	0.5404(33)	0.6713(16)	0.125(16)[b,e]
C(45)	0.9171(18)	0.5012(25)	0.7044(14)	0.093(11)[b,e]
C(46)	0.9271(15)	0.4178(19)	0.7098(11)	0.058(8)[b,e]
C(47)	1.0575(18)	0.3818(26)	0.6281(13)	0.096(12)[b,e]
C(48)	0.8879(15)	0.3675(21)	0.7433(11)	0.069(9)[b,e]
C(51)	0.9237(15)	0.3762(22)	0.7732(12)	0.072(9)[b,e]
C(52)	0.9122(20)	0.4265(30)	0.7439(16)	0.100(13)[b,e]
C(53)	0.9116(25)	0.5110(37)	0.7552(21)	0.144(19)[b,e]
C(54)	0.9329(28)	0.5320(43)	0.7924(23)	0.164(23)[b,e]
C(55)	0.9485(27)	0.4770(41)	0.8238(22)	0.156(21)[b,e]
C(56)	0.9444(30)	0.3911(43)	0.8145(23)	0.165(22)[b,e]
C(57)	0.8821(27)	0.4078(34)	0.7017(17)	0.140(19)[b,e]
C(58)	0.9620(23)	0.3319(32)	0.8480(17)	0.128(17)[b,e]
C(61)	0.9689(17)	-0.1395(23)	0.6846(12)	0.080(10)[b,e]
C(62)	0.9996(29)	-0.1721(43)	0.6507(21)	0.153(21)[b,e]
C(63)	0.9837(37)	-0.2585(53)	0.6375(26)	0.210(31)[b,e]
C(64)	0.9329(48)	-0.3057(68)	0.6576(34)	0.279(45)[b,e]
C(65)	0.9151(29)	-0.2568(43)	0.6997(23)	0.167(23)[b,e]
C(66)	0.9233(22)	-0.1770(29)	0.7093(16)	0.100(13)[b,e]
C(67)	1.0483(46)	-0.1167(59)	0.6273(34)	0.273(50)[b,e]
C(68)	0.8919(21)	-0.1286(30)	0.7403(16)	0.115(14)[b,e]

Table 2. continued page 3.

C(111)	0.7800(14)	0.1374(18)	0.5292(9)	0.140(10)
C(112)	0.8831(14)	0.2046(20)	0.5676(10)	0.155(11)
C(113)	0.8785(11)	0.0454(15)	0.5605(8)	0.111(7)
C(121)	0.6951(15)	0.2232(24)	0.6000(10)	0.170(13)
C(122)	0.7473(13)	0.2177(20)	0.6850(11)	0.151(11)
C(123)	0.8042(12)	0.2985(16)	0.6237(12)	0.156(13)
C(131)	0.6984(17)	0.0308(21)	0.5925(11)	0.163(12)
C(132)	0.7375(14)	0.0285(21)	0.6802(11)	0.161(13)
C(133)	0.8019(13)	-0.0472(16)	0.6202(11)	0.142(11)
C(211)	1.1975(13)	0.1249(21)	0.5152(9)	0.152(11)
C(212)	1.0787(16)	0.1263(24)	0.5495(10)	0.168(13)
C(213)	1.1478(17)	0.2678(17)	0.5629(10)	0.158(14)
C(221)	1.2751(16)	0.0146(16)	0.5762(12)	0.201(18)
C(222)	1.2057(10)	-0.0297(13)	0.6477(9)	0.113(9)
C(223)	1.1429(17)	-0.0283(16)	0.5660(12)	0.147(12)
C(231)	1.2114(10)	0.2647(13)	0.6496(9)	0.111(8)
C(232)	1.2894(13)	0.1993(17)	0.5827(11)	0.163(13)
C(233)	1.2654(10)	0.1195(16)	0.6679(10)	0.116(8)
O(111)	0.7477(13)	0.1419(19)	0.4998(8)	0.231(14)
O(112)	0.9200(14)	0.2555(17)	0.5646(11)	0.272(17)
O(113)	0.9115(9)	-0.0052(13)	0.5535(7)	0.170(8)
O(121)	0.6528(12)	0.2323(24)	0.5784(11)	0.293(19)
O(122)	0.7369(13)	0.2273(20)	0.7237(8)	0.243(14)
O(123)	0.8284(13)	0.3554(13)	0.6199(12)	0.238(14)
O(131)	0.6574(13)	0.0226(21)	0.5691(11)	0.278(18)
O(132)	0.7245(16)	0.0130(19)	0.7154(9)	0.272(18)
O(133)	0.8275(12)	-0.1063(13)	0.6180(10)	0.206(11)
O(211)	1.2266(9)	0.1179(14)	0.4847(6)	0.173(9)
O(212)	1.0284(11)	0.1179(19)	0.5437(9)	0.216(12)
O(213)	1.1474(14)	0.3295(15)	0.5565(9)	0.221(13)
O(221)	1.3151(12)	0.0053(13)	0.5533(10)	0.249(15)
O(222)	1.2022(9)	-0.0738(10)	0.6745(7)	0.152(8)
O(223)	1.1132(19)	-0.0695(22)	0.5478(9)	0.177(17)[c]

Table 2. continued page 4.

O(231)	1.2056(8)	0.3169(10)	0.6726(7)	0.150(7)
O(232)	1.3277(9)	0.2116(11)	0.5602(8)	0.193(11)
O(233)	1.2880(11)	0.1022(18)	0.6990(8)	0.201(11)
O(253)	1.1696(46)	-0.1023(66)	0.5692(35)	0.229(39)[d,e]
C(301)	-0.0059(36)	0.4739(10)	0.0208(7)	0.207(31)[b,e]
C(302)	0.0007(33)	0.3825(5)	0.0093(16)	0.191(27)[b,e]
C(303)	-0.0155(44)	0.3299(23)	0.0499(23)	0.298(49)[b,e]

[a] $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

[b] Group occupancy is 0.5

[c] Group occupancy is 0.682(8)

[d] Group occupancy is 0.317(8)

[e] Atom was refined isotropically.

Table 3. Selected bond lengths (Å) and angles (deg) for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$.

Ti(1)-Ti(1)#1	2.839(8)	Co(21)-C(20)	1.91(2)
Ti(1)-Ti(2)#1	2.955(5)	Co(21)-C(211)	1.86(3)
Ti(1)-Ti(2)	2.965(5)	Co(21)-C(212)	1.78(3)
Ti(1)-O(1)	2.103(5)	Co(21)-C(213)	1.80(3)
Ti(1)-O(2)	1.990(6)	Co(22)-Co(23)	2.460(6)
Ti(1)-O(2)#1	1.978(7)	Co(22)-C(20)	1.85(2)
Ti(1)-O(11A)	2.04(2)	Co(22)-C(221)	1.90(3)
Ti(1)-O(21B)#1	2.04(2)	Co(22)-C(222)	1.82(3)
Ti(1)-O(31)	1.80(2)	Co(22)-C(223)	1.82(4)
Ti(2)-Ti(2)#1	2.837(8)	Co(23)-C(20)	1.89(2)
Ti(2)-O(1)	1.987(6)	Co(23)-C(231)	1.79(2)
Ti(2)-O(1)#1	1.988(6)	Co(23)-C(232)	1.86(3)
Ti(2)-O(2)	2.196(6)	Co(23)-C(233)	1.74(3)
Ti(2)-O(11B)	2.02(2)	O(11A)-C(11)	1.34(2)
Ti(2)-O(21A)	2.06(2)	O(11B)-C(11)	1.24(2)
Ti(2)-O(41)	1.82(2)	O(21A)-C(21)	1.35(2)
Co(11)-Co(12)	2.456(4)	O(21B)-C(21)	1.18(2)
Co(11)-Co(13)	2.459(4)	C(10)-C(11)	1.45(2)
Co(11)-C(10)	1.87(2)	C(20)-C(21)	1.48(2)
Co(11)-C(111)	1.77(3)	O(31)-C(31)	1.41(3)
Co(11)-C(112)	1.74(3)	O(41)-C(41)	1.40(3)
Co(11)-C(113)	1.81(2)	C(31)-C(32)	1.40(4)
Co(12)-Co(13)	2.466(5)	C(31)-C(36)	1.27(4)
Co(12)-C(10)	1.89(2)	C(32)-C(33)	1.41(5)
Co(12)-C(121)	1.81(3)	C(32)-C(37)	1.51(5)
Co(12)-C(122)	1.73(3)	C(33)-C(34)	1.38(5)
Co(12)-C(123)	1.83(3)	C(34)-C(35)	1.27(5)
Co(13)-C(10)	1.87(2)	C(35)-C(36)	1.46(5)
Co(13)-C(131)	1.78(4)	C(36)-C(38)	1.42(5)
Co(13)-C(132)	1.76(3)	C(41)-C(42)	1.32(4)
Co(13)-C(133)	1.79(3)	C(41)-C(46)	1.39(4)
Co(21)-Co(22)	2.448(6)	C(42)-C(43)	1.48(5)
Co(21)-Co(23)	2.449(7)	C(42)-C(47)	1.52(5)

Table 3. continued page 2.

C(43)-C(44)	1.27(6)	C(132)-O(132)	1.13(3)
C(44)-C(45)	1.39(6)	C(133)-O(133)	1.12(3)
C(45)-C(46)	1.39(5)	C(211)-O(211)	1.13(3)
C(46)-C(48)	1.57(5)	C(212)-O(212)	1.12(3)
C(111)-O(111)	1.13(3)	C(213)-O(213)	1.03(3)
C(112)-O(112)	1.17(3)	C(221)-O(221)	1.13(3)
C(113)-O(113)	1.12(2)	C(222)-O(222)	1.09(2)
C(121)-O(121)	1.14(3)	C(223)-O(223)	1.08(4)
C(122)-O(122)	1.20(3)	C(231)-O(231)	1.11(2)
C(123)-O(123)	1.08(3)	C(232)-O(232)	1.10(2)
C(131)-O(131)	1.15(3)	C(233)-O(233)	1.10(3)

O(1)-Ti(1)-O(2)#1	90.2(2)	C(10)-Co(12)-C(123)	104.9(9)
O(1)-Ti(1)-O(2)	89.8(2)	C(121)-Co(12)-C(122)	104.7(14)
O(1)-Ti(1)-O(11A)	81.3(5)	C(121)-Co(12)-C(123)	99(2)
O(1)-Ti(1)-O(21B)#1	78.3(5)	C(122)-Co(12)-C(123)	94(2)
O(1)-Ti(1)-O(31)	171.1(6)	Co(11)-Co(13)-Co(12)	59.84(12)
O(2)-Ti(1)-O(2)#1	88.7(3)	C(10)-Co(13)-C(132)	101.7(11)
O(2)-Ti(1)-O(11A)	85.2(5)	C(10)-Co(13)-C(131)	144.2(12)
O(2)#1-Ti(1)-O(11A)	169.5(5)	C(10)-Co(13)-C(133)	103.1(10)
O(2)-Ti(1)-O(21B)#1	167.7(5)	C(131)-Co(13)-C(132)	103(2)
O(2)#1-Ti(1)-O(21B)#1	88.6(6)	C(131)-Co(13)-C(133)	100(2)
O(2)-Ti(1)-O(31)	98.8(6)	C(132)-Co(13)-C(133)	95(2)
O(2)-Ti(1)-O(31)#1	92.2(6)	Co(22)-Co(21)-Co(23)	60.3(2)
Co(12)-Co(11)-Co(13)	60.23(13)	C(20)-Co(21)-C(211)	131.9(11)
C(10)-Co(11)-C(111)	142.4(11)	C(20)-Co(21)-C(212)	97.4(11)
C(10)-Co(11)-C(112)	100.9(11)	C(20)-Co(21)-C(213)	111.0(11)
C(10)-Co(11)-C(113)	102.9(10)	C(211)-Co(21)-C(212)	101.1(14)
C(111)-Co(11)-C(112)	104(2)	C(211)-Co(21)-C(213)	107.7(13)
C(111)-Co(11)-C(113)	102.9(12)	C(212)-Co(21)-C(213)	102(2)
C(112)-Co(11)-C(113)	94.5(13)	Co(21)-Co(22)-Co(23)	59.9(2)
Co(11)-Co(12)-Co(13)	59.93(12)	C(20)-Co(22)-C(221)	137.6(11)
C(10)-Co(12)-C(121)	144.4(13)	C(20)-Co(22)-C(222)	98.3(8)
C(10)-Co(12)-C(122)	99.5(11)	C(20)-Co(22)-C(223)	108.7(12)

Table 3. continued page 3.

C(221)-Co(22)-C(222)	95.2(12)	Co(23)-C(20)-C(21)	126.8(13)
C(221)-Co(22)-C(223)	108(2)	O(21A)-C(21)-O(21B)	124(2)
C(222)-Co(22)-C(223)	101.6(13)	O(21A)-C(21)-C(20)	117(2)
Co(21)-Co(23)-Co(22)	59.8(2)	O(21B)-C(21)-C(20)	119(2)
C(20)-Co(23)-C(231)	99.6(8)	Ti(1)-O(31)-C(31)	165(2)
C(20)-Co(23)-C(232)	138.4(11)	Ti(2)-O(41)-C(41)	171(2)
C(20)-Co(23)-C(233)	100.8(9)	O(31)-C(31)-C(32)	113(3)
C(231)-Co(23)-C(232)	103.0(11)	O(31)-C(31)-C(36)	121(3)
C(231)-Co(23)-C(233)	99.9(13)	O(41)-C(41)-C(42)	115(2)
C(232)-Co(23)-C(233)	109.0(14)	O(41)-C(41)-C(46)	120(2)
Ti(1)-O(11A)-C(11)	127.0(13)	Co(11)-C(111)-O(111)	178(3)
Ti(2)-O(11B)-C(11)	130.2(14)	Co(11)-C(112)-O(112)	176(3)
Ti(2)-O(21A)-C(21)	124.7(13)	Co(11)-C(113)-O(113)	176(3)
Ti(1)#1-O(21B)-C(21)	129.6(14)	Co(12)-C(121)-O(121)	174(3)
Co(11)-C(10)-Co(12)	81.6(7)	Co(12)-C(122)-O(122)	177(3)
Co(11)-C(10)-Co(13)	82.2(7)	Co(12)-C(123)-O(123)	179(3)
Co(11)-C(10)-C(11)	133.2(12)	Co(13)-C(131)-O(131)	176(4)
Co(12)-C(10)-Co(13)	81.9(7)	Co(13)-C(132)-O(132)	175(4)
Co(12)-C(10)-C(11)	127.5(12)	Co(13)-C(133)-O(133)	177(3)
Co(13)-C(10)-C(11)	131.6(13)	Co(21)-C(211)-O(211)	169(3)
O(11A)-C(11)-O(11B)	122(2)	Co(21)-C(212)-O(212)	168(4)
O(11A)-C(11)-C(10)	120(2)	Co(21)-C(213)-O(213)	170(3)
O(11B)-C(11)-C(10)	118(2)	Co(22)-C(221)-O(221)	163(4)
Co(21)-C(20)-Co(22)	81.4(6)	Co(22)-C(222)-O(222)	167(3)
Co(21)-C(20)-Co(23)	80.5(6)	Co(23)-C(231)-O(231)	166(3)
Co(21)-C(20)-C(21)	135.3(13)	Co(23)-C(232)-O(232)	173(3)
Co(22)-C(20)-Co(23)	82.4(6)	Co(23)-C(233)-O(233)	167(3)
Co(22)-C(20)-C(21)	131.0(12)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+3/2

Table 4. Full list of Bond lengths (Å)
for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$

Ti(1)-Ti(1)#1	2.839(8)	Co(11)-Co(13)	2.459(4)
Ti(1)-Ti(2)#1	2.955(5)	Co(11)-C(10)	1.87(2)
Ti(1)-Ti(2)	2.965(5)	Co(11)-C(111)	1.77(3)
Ti(1)-O(1)	2.103(5)	Co(11)-C(112)	1.74(3)
Ti(1)-O(2)	1.990(6)	Co(11)-C(113)	1.81(2)
Ti(1)-O(2)#1	1.978(7)	Co(12)-Co(13)	2.466(5)
Ti(1)-O(11A)	2.04(2)	Co(12)-C(10)	1.89(2)
Ti(1)-O(21B)#1	2.04(2)	Co(12)-C(121)	1.81(3)
Ti(1)-O(31)	1.80(2)	Co(12)-C(122)	1.73(3)
Ti(2)-Ti(2)#1	2.837(8)	Co(12)-C(123)	1.83(3)
Ti(2)-O(1)	1.987(6)	Co(13)-C(10)	1.87(2)
Ti(2)-O(1)#1	1.988(6)	Co(13)-C(131)	1.78(4)
Ti(2)-O(2)	2.196(6)	Co(13)-C(132)	1.76(3)
Ti(2)-O(11B)	2.02(2)	Co(13)-C(133)	1.79(3)
Ti(2)-O(21A)	2.06(2)	Co(21)-Co(22)	2.448(6)
Ti(2)-O(41)	1.82(2)	Co(21)-Co(23)	2.449(7)
Ti(3)-Ti(3)#1	2.780(9)	Co(21)-C(20)	1.91(2)
Ti(3)-Ti(4)	2.889(6)	Co(21)-C(211)	1.86(3)
Ti(3)-Ti(4)#1	2.892(7)	Co(21)-C(212)	1.78(3)
Ti(3)-O(3)	2.103(5)	Co(21)-C(213)	1.80(3)
Ti(3)-O(4)	1.987(6)	Co(22)-Co(23)	2.460(6)
Ti(3)-O(4)#1	1.988(6)	Co(22)-C(20)	1.85(2)
Ti(3)-O(12A)	2.06(2)	Co(22)-C(221)	1.90(3)
Ti(3)-O(22A)#1	2.09(2)	Co(22)-C(222)	1.82(3)
Ti(3)-O(51)	1.83(3)	Co(22)-C(223)	1.82(4)
Ti(4)-Ti(4)#1	2.773(10)	Co(23)-C(20)	1.89(2)
Ti(4)-O(3)	1.990(6)	Co(23)-C(231)	1.79(2)
Ti(4)-O(3)#1	1.978(7)	Co(23)-C(232)	1.86(3)
Ti(4)-O(4)	2.196(6)	Co(23)-C(233)	1.74(3)
Ti(4)-O(12B)	2.10(3)	Co(24)-Co(25)	2.43(2)
Ti(4)-O(22B)	2.12(2)	Co(24)-Co(26)	2.474(13)
Ti(4)-O(61)	1.90(3)	Co(24)-C(20)	1.95(2)
Co(11)-Co(12)	2.456(4)	Co(24)-C(221)	1.97(3)

Table 4. continued page 2.

Co(24)-C(222)	1.76(2)	C(41)-C(46)	1.39(4)
Co(24)-C(233)	1.69(3)	C(42)-C(43)	1.48(5)
Co(25)-Co(26)	2.441(13)	C(42)-C(47)	1.52(5)
Co(25)-C(20)	1.88(2)	C(43)-C(44)	1.27(6)
Co(25)-C(211)	1.95(3)	C(44)-C(45)	1.39(6)
Co(25)-C(212)	2.01(4)	C(45)-C(46)	1.39(5)
Co(25)-C(223)	1.72(3)	C(46)-C(48)	1.57(5)
Co(26)-C(20)	1.87(2)	C(51)-C(52)	1.23(5)
Co(26)-C(213)	1.92(4)	C(51)-C(56)	1.35(7)
Co(26)-C(231)	1.88(3)	C(52)-C(53)	1.42(6)
Co(26)-C(232)	2.00(3)	C(52)-C(57)	1.47(6)
O(11A)-C(11)	1.34(2)	C(53)-C(54)	1.26(7)
O(11B)-C(11)	1.24(2)	C(54)-C(55)	1.35(7)
O(12A)-C(11)	1.31(3)	C(55)-C(56)	1.43(8)
O(12B)-C(11)	1.23(3)	C(56)-C(58)	1.45(7)
O(21A)-C(21)	1.35(2)	C(61)-C(62)	1.34(6)
O(21B)-C(21)	1.18(2)	C(61)-C(66)	1.39(5)
O(22A)-C(21)	1.21(3)	C(62)-C(63)	1.50(9)
O(22B)-C(21)	1.31(3)	C(62)-C(67)	1.57(10)
C(10)-C(11)	1.45(2)	C(63)-C(64)	1.49(11)
C(20)-C(21)	1.48(2)	C(64)-C(65)	1.55(10)
O(31)-C(31)	1.41(3)	C(65)-C(66)	1.35(7)
O(41)-C(41)	1.40(3)	C(66)-C(68)	1.41(6)
O(51)-C(51)	1.40(4)	C(111)-O(111)	1.13(3)
O(61)-C(61)	1.37(4)	C(112)-O(112)	1.17(3)
C(31)-C(32)	1.40(4)	C(113)-O(113)	1.12(2)
C(31)-C(36)	1.27(4)	C(121)-O(121)	1.14(3)
C(32)-C(33)	1.41(5)	C(122)-O(122)	1.20(3)
C(32)-C(37)	1.51(5)	C(123)-O(123)	1.08(3)
C(33)-C(34)	1.38(5)	C(131)-O(131)	1.15(3)
C(34)-C(35)	1.27(5)	C(132)-O(132)	1.13(3)
C(35)-C(36)	1.46(5)	C(133)-O(133)	1.12(3)
C(36)-C(38)	1.42(5)	C(211)-O(211)	1.13(3)
C(41)-C(42)	1.32(4)	C(212)-O(212)	1.12(3)

Table 4. continued page 3.

C(213)-O(213)	1.03(3)	C(232)-O(232)	1.10(2)
C(221)-O(221)	1.13(3)	C(233)-O(233)	1.10(3)
C(222)-O(222)	1.09(2)	C(301)-C(301)#2	1.541(5)
C(223)-O(223)	1.08(4)	C(301)-C(302)	1.539(5)
C(223)-O(253)	1.35(10)	C(302)-C(303)	1.540(5)
C(231)-O(231)	1.11(2)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+3/2 #2 -x,-y+1,-z

Table 5. Full list of bond angles (deg)
for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$

O(1)-Ti(1)-O(2)#1	90.2(2)	O(3)-Ti(3)-O(22A)#1	79.0(7)
O(1)-Ti(1)-O(2)	89.8(2)	O(3)-Ti(3)-O(51)	168.4(8)
O(1)-Ti(1)-O(11A)	81.3(5)	O(4)-Ti(3)-O(4)#1	91.1(3)
O(1)-Ti(1)-O(21B)#1	78.3(5)	O(4)-Ti(3)-O(12A)	84.1(7)
O(1)-Ti(1)-O(31)	171.1(6)	O(4)#1-Ti(3)-O(12A)	173.5(7)
O(2)-Ti(1)-O(2)#1	88.7(3)	O(4)-Ti(3)-O(22A)#1	171.8(7)
O(2)-Ti(1)-O(11A)	85.2(5)	O(4)#1-Ti(3)-O(22A)#1	87.8(8)
O(2)#1-Ti(1)-O(11A)	169.5(5)	O(4)-Ti(3)-O(51)	98.1(8)
O(2)-Ti(1)-O(21B)#1	167.7(5)	O(4)#1-Ti(3)-O(51)	91.1(8)
O(2)#1-Ti(1)-O(21B)#1	88.6(6)	O(12A)-Ti(3)-O(22A)#1	96.3(10)
O(2)-Ti(1)-O(31)	98.8(6)	O(12A)-Ti(3)-O(51)	93.9(10)
O(2)-Ti(1)-O(31)#1	92.2(6)	O(22A)-Ti(3)-O(51)#1	90.1(10)
O(11A)-Ti(1)-O(21B)#1	95.6(7)	O(3)-Ti(4)-O(3)#1	91.3(3)
O(11A)-Ti(1)-O(31)	97.1(7)	O(3)#1-Ti(4)-O(4)	90.0(2)
O(21B)-Ti(1)-O(31)#1	93.3(7)	O(3)-Ti(4)-O(4)	90.1(2)
O(1)-Ti(2)-O(1)#1	88.8(3)	O(3)#1-Ti(4)-O(12B)	169.6(7)
O(1)-Ti(2)-O(2)	87.2(2)	O(3)-Ti(4)-O(12B)	86.7(7)
O(1)#1-Ti(2)-O(2)	87.3(2)	O(3)#1-Ti(4)-O(22B)	84.3(8)
O(1)-Ti(2)-O(11B)	87.1(5)	O(3)-Ti(4)-O(22B)	170.7(8)
O(1)#1-Ti(2)-O(11B)	165.8(5)	O(3)#1-Ti(4)-O(61)	102.6(8)
O(1)-Ti(2)-O(21A)	167.3(5)	O(3)-Ti(4)-O(61)	95.2(8)
O(1)#1-Ti(2)-O(21A)	85.6(6)	O(4)-Ti(4)-O(12B)	79.9(7)
O(1)-Ti(2)-O(41)	97.5(6)	O(4)-Ti(4)-O(22B)	81.7(6)
O(1)-Ti(2)-O(41)#1	102.7(6)	O(4)-Ti(4)-O(61)	166.2(8)
O(2)-Ti(2)-O(11B)	78.9(5)	O(12B)-Ti(4)-O(22B)	96.1(10)
O(2)-Ti(2)-O(21A)	81.2(5)	O(12B)-Ti(4)-O(61)	87.7(10)
O(2)-Ti(2)-O(41)	168.9(6)	O(22B)-Ti(4)-O(61)	93.8(10)
O(11B)-Ti(2)-O(21A)	95.7(7)	Co(12)-Co(11)-Co(13)	60.23(13)
O(11B)-Ti(2)-O(41)	91.3(7)	Co(12)-Co(11)-C(10)	49.6(5)
O(21A)-Ti(2)-O(41)	94.8(7)	Co(12)-Co(11)-C(111)	98.6(9)
O(3)-Ti(3)-O(4)	92.9(2)	Co(12)-Co(11)-C(112)	98.6(11)
O(3)-Ti(3)-O(4)#1	92.5(2)	Co(12)-Co(11)-C(113)	151.2(8)
O(3)-Ti(3)-O(12A)	83.4(7)	Co(13)-Co(11)-C(10)	49.0(5)

Table 5. continued page 2.

Co(13)-Co(11)-C(111)	101.0(10)	C(10)-Co(13)-C(131)	144.2(12)
Co(13)-Co(11)-C(112)	149.6(10)	C(10)-Co(13)-C(133)	103.1(10)
Co(13)-Co(11)-C(113)	96.7(7)	C(131)-Co(13)-C(132)	103(2)
C(10)-Co(11)-C(111)	142.4(11)	C(131)-Co(13)-C(133)	100(2)
C(10)-Co(11)-C(112)	100.9(11)	C(132)-Co(13)-C(133)	95(2)
C(10)-Co(11)-C(113)	102.9(10)	Co(22)-Co(21)-Co(23)	60.3(2)
C(111)-Co(11)-C(112)	104(2)	Co(22)-Co(21)-C(20)	48.3(5)
C(111)-Co(11)-C(113)	102.9(12)	Co(22)-Co(21)-C(211)	84.4(10)
C(112)-Co(11)-C(113)	94.5(13)	Co(22)-Co(21)-C(212)	102.2(12)
Co(11)-Co(12)-Co(13)	59.93(12)	Co(22)-Co(21)-C(213)	149.9(13)
Co(11)-Co(12)-C(10)	48.8(5)	Co(23)-Co(21)-C(20)	49.4(5)
Co(11)-Co(12)-C(121)	104.2(10)	Co(23)-Co(21)-C(211)	104.7(9)
Co(11)-Co(12)-C(122)	148.3(9)	Co(23)-Co(21)-C(212)	146.7(10)
Co(11)-Co(12)-C(123)	94.4(9)	Co(23)-Co(21)-C(213)	89.7(13)
Co(13)-Co(12)-C(10)	48.7(5)	C(20)-Co(21)-C(211)	131.9(11)
Co(13)-Co(12)-C(121)	100.2(12)	C(20)-Co(21)-C(212)	97.4(11)
Co(13)-Co(12)-C(122)	102.1(11)	C(20)-Co(21)-C(213)	111.0(11)
Co(13)-Co(12)-C(123)	150.9(8)	C(211)-Co(21)-C(212)	101.1(14)
C(10)-Co(12)-C(121)	144.4(13)	C(211)-Co(21)-C(213)	107.7(13)
C(10)-Co(12)-C(122)	99.5(11)	C(212)-Co(21)-C(213)	102(2)
C(10)-Co(12)-C(123)	104.9(9)	Co(21)-Co(22)-Co(23)	59.9(2)
C(121)-Co(12)-C(122)	104.7(14)	Co(21)-Co(22)-C(20)	50.3(5)
C(121)-Co(12)-C(123)	99(2)	Co(21)-Co(22)-C(221)	109.2(8)
C(122)-Co(12)-C(123)	94(2)	Co(21)-Co(22)-C(222)	148.6(7)
Co(11)-Co(13)-Co(12)	59.84(12)	Co(21)-Co(22)-C(223)	89.9(11)
Co(11)-Co(13)-C(10)	48.9(5)	Co(23)-Co(22)-C(20)	49.4(5)
Co(11)-Co(13)-C(131)	101.4(11)	Co(23)-Co(22)-C(221)	88.5(11)
Co(11)-Co(13)-C(132)	150.1(10)	Co(23)-Co(22)-C(222)	102.7(9)
Co(11)-Co(13)-C(133)	97.3(9)	Co(23)-Co(22)-C(223)	149.4(11)
Co(12)-Co(13)-C(10)	49.4(5)	C(20)-Co(22)-C(221)	137.6(11)
Co(12)-Co(13)-C(131)	101.6(11)	C(20)-Co(22)-C(222)	98.3(8)
Co(12)-Co(13)-C(132)	98.6(11)	C(20)-Co(22)-C(223)	108.7(12)
Co(12)-Co(13)-C(133)	151.3(9)	C(221)-Co(22)-C(222)	95.2(12)
C(10)-Co(13)-C(132)	101.7(11)	C(221)-Co(22)-C(223)	108(2)

Table 5. continued page 3.

C(222)-Co(22)-C(223)	101.6(13)	Co(24)-Co(25)-C(212)	142.7(11)
Co(21)-Co(23)-Co(22)	59.8(2)	Co(24)-Co(25)-C(223)	94(2)
Co(21)-Co(23)-C(20)	50.1(5)	Co(26)-Co(25)-C(20)	49.2(5)
Co(21)-Co(23)-C(231)	103.0(9)	Co(26)-Co(25)-C(211)	78.3(10)
Co(21)-Co(23)-C(232)	90.7(11)	Co(26)-Co(25)-C(212)	94.7(12)
Co(21)-Co(23)-C(233)	145.4(9)	Co(26)-Co(25)-C(223)	154(2)
Co(22)-Co(23)-C(20)	48.1(5)	C(20)-Co(25)-C(211)	127.4(12)
Co(22)-Co(23)-C(231)	147.7(7)	C(20)-Co(25)-C(212)	90.9(12)
Co(22)-Co(23)-C(232)	104.3(8)	C(20)-Co(25)-C(223)	111.3(13)
Co(22)-Co(23)-C(233)	87.3(10)	C(211)-Co(25)-C(212)	90.6(14)
C(20)-Co(23)-C(231)	99.6(8)	C(211)-Co(25)-C(223)	119.4(14)
C(20)-Co(23)-C(232)	138.4(11)	C(212)-Co(25)-C(223)	103(2)
C(20)-Co(23)-C(233)	100.8(9)	Co(24)-Co(26)-Co(25)	59.3(4)
C(231)-Co(23)-C(232)	103.0(11)	Co(24)-Co(26)-C(20)	51.1(6)
C(231)-Co(23)-C(233)	99.9(13)	Co(24)-Co(26)-C(213)	150.6(12)
C(232)-Co(23)-C(233)	109.0(14)	Co(24)-Co(26)-C(231)	100.4(10)
Co(25)-Co(24)-Co(26)	59.7(4)	Co(24)-Co(26)-C(232)	78.8(10)
Co(25)-Co(24)-C(20)	49.4(6)	Co(25)-Co(26)-C(20)	49.7(6)
Co(25)-Co(24)-C(221)	76.6(13)	Co(25)-Co(26)-C(213)	91.8(12)
Co(25)-Co(24)-C(222)	96.5(11)	Co(25)-Co(26)-C(231)	146.6(8)
Co(25)-Co(24)-C(233)	142.4(10)	Co(25)-Co(26)-C(232)	105.4(8)
Co(26)-Co(24)-C(20)	48.2(5)	C(20)-Co(26)-C(213)	107.3(12)
Co(26)-Co(24)-C(221)	103.5(9)	C(20)-Co(26)-C(231)	96.9(9)
Co(26)-Co(24)-C(222)	144.6(9)	C(20)-Co(26)-C(232)	129.8(12)
Co(26)-Co(24)-C(233)	84.1(10)	C(213)-Co(26)-C(231)	102.2(12)
C(20)-Co(24)-C(221)	125.7(14)	C(213)-Co(26)-C(232)	117.5(14)
C(20)-Co(24)-C(222)	96.6(9)	C(231)-Co(26)-C(232)	94.9(12)
C(20)-Co(24)-C(233)	99.8(10)	Ti(1)-O(11A)-C(11)	127.0(13)
C(221)-Co(24)-C(222)	94.5(11)	Ti(2)-O(11B)-C(11)	130.2(14)
C(221)-Co(24)-C(233)	126(2)	Ti(3)-O(12A)-C(11)	125(2)
C(222)-Co(24)-C(233)	109.8(14)	Ti(4)-O(12B)-C(11)	126(2)
Co(24)-Co(25)-Co(26)	61.0(4)	Ti(2)-O(21A)-C(21)	124.7(13)
Co(24)-Co(25)-C(20)	51.9(6)	Ti(1)#1-O(21B)-C(21)	129.6(14)
Co(24)-Co(25)-C(211)	109.5(9)	Ti(3)#1-O(22A)-C(21)	126(2)

Table 5. continued page 4.

Ti(4)-O(22B)-C(21)	123(2)	Ti(4)-O(61)-C(61)	172(2)
Co(11)-C(10)-Co(12)	81.6(7)	O(31)-C(31)-C(32)	113(3)
Co(11)-C(10)-Co(13)	82.2(7)	O(31)-C(31)-C(36)	121(3)
Co(11)-C(10)-C(11)	133.2(12)	C(32)-C(31)-C(36)	126(3)
Co(12)-C(10)-Co(13)	81.9(7)	C(31)-C(32)-C(33)	117(3)
Co(12)-C(10)-C(11)	127.5(12)	C(31)-C(32)-C(37)	122(3)
Co(13)-C(10)-C(11)	131.6(13)	C(33)-C(32)-C(37)	122(3)
O(11A)-C(11)-O(11B)	122(2)	C(32)-C(33)-C(34)	115(4)
O(11A)-C(11)-C(10)	120(2)	C(33)-C(34)-C(35)	129(4)
O(11B)-C(11)-C(10)	118(2)	C(34)-C(35)-C(36)	116(4)
O(12A)-C(11)-C(10)	120(2)	C(31)-C(36)-C(35)	118(3)
O(12A)-C(11)-O(12B)	126(2)	C(31)-C(36)-C(38)	125(4)
O(12B)-C(11)-C(10)	114(2)	C(35)-C(36)-C(38)	117(3)
Co(21)-C(20)-Co(22)	81.4(6)	O(41)-C(41)-C(42)	115(2)
Co(21)-C(20)-Co(23)	80.5(6)	O(41)-C(41)-C(46)	120(2)
Co(21)-C(20)-C(21)	135.3(13)	C(42)-C(41)-C(46)	124(3)
Co(22)-C(20)-Co(23)	82.4(6)	C(41)-C(42)-C(43)	115(3)
Co(22)-C(20)-C(21)	131.0(12)	C(41)-C(42)-C(47)	126(3)
Co(23)-C(20)-C(21)	126.8(13)	C(43)-C(42)-C(47)	118(3)
Co(24)-C(20)-Co(25)	78.7(7)	C(42)-C(43)-C(44)	121(5)
Co(24)-C(20)-Co(26)	80.7(7)	C(43)-C(44)-C(45)	124(5)
Co(24)-C(20)-C(21)	124.4(13)	C(44)-C(45)-C(46)	117(4)
Co(25)-C(20)-Co(26)	81.1(7)	C(41)-C(46)-C(45)	119(3)
Co(25)-C(20)-C(21)	137.7(13)	C(41)-C(46)-C(48)	121(3)
Co(26)-C(20)-C(21)	132.9(13)	C(45)-C(46)-C(48)	120(3)
O(21A)-C(21)-O(21B)	124(2)	O(51)-C(51)-C(52)	116(4)
O(21A)-C(21)-C(20)	117(2)	O(51)-C(51)-C(56)	116(4)
O(21B)-C(21)-C(20)	119(2)	C(52)-C(51)-C(56)	128(5)
O(22A)-C(21)-O(22B)	128(2)	C(51)-C(52)-C(53)	119(5)
O(22A)-C(21)-C(20)	117(2)	C(51)-C(52)-C(57)	125(5)
O(22B)-C(21)-C(20)	115(2)	C(53)-C(52)-C(57)	114(5)
Ti(1)-O(31)-C(31)	165(2)	C(52)-C(53)-C(54)	118(6)
Ti(2)-O(41)-C(41)	171(2)	C(53)-C(54)-C(55)	123(7)
Ti(3)-O(51)-C(51)	166(2)	C(54)-C(55)-C(56)	120(7)

Table 5. continued page 5.

C(51)-C(56)-C(55)	112(6)	Co(13)-C(131)-O(131)	176(4)
C(51)-C(56)-C(58)	128(6)	Co(13)-C(132)-O(132)	175(4)
C(55)-C(56)-C(58)	120(6)	Co(13)-C(133)-O(133)	177(3)
O(61)-C(61)-C(62)	112(4)	Co(21)-C(211)-O(211)	169(3)
O(61)-C(61)-C(66)	121(4)	Co(25)-C(211)-O(211)	149(3)
C(61)-C(62)-C(63)	117(6)	Co(21)-C(212)-O(212)	168(4)
C(61)-C(62)-C(67)	118(7)	Co(25)-C(212)-O(212)	148(4)
C(62)-C(61)-C(66)	127(5)	Co(21)-C(213)-O(213)	170(3)
C(63)-C(62)-C(67)	125(7)	Co(26)-C(213)-O(213)	132(4)
C(62)-C(63)-C(64)	123(8)	Co(22)-C(221)-O(221)	163(4)
C(63)-C(64)-C(65)	105(9)	Co(24)-C(221)-O(221)	155(4)
C(64)-C(65)-C(66)	130(8)	Co(22)-C(222)-O(222)	167(3)
C(61)-C(66)-C(65)	114(5)	Co(24)-C(222)-O(222)	150(3)
C(61)-C(66)-C(68)	118(4)	Co(23)-C(231)-O(231)	166(3)
C(65)-C(66)-C(68)	128(5)	Co(26)-C(231)-O(231)	158(3)
Co(11)-C(111)-O(111)	178(3)	Co(23)-C(232)-O(232)	173(3)
Co(11)-C(112)-O(112)	176(3)	Co(26)-C(232)-O(232)	153(3)
Co(11)-C(113)-O(113)	176(3)	Co(23)-C(233)-O(233)	167(3)
Co(12)-C(121)-O(121)	174(3)	Co(24)-C(233)-O(233)	133(3)
Co(12)-C(122)-O(122)	177(3)	C(301)#2-C(301)-C(302)	109.5(5)
Co(12)-C(123)-O(123)	179(3)	C(301)-C(302)-C(303)	109.7(5)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y,-z+3/2 #2 -x,-y+1,-z

Table 6. Anisotropic displacement parameters ($Å^2$) for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4.C_6H_{14}$.[a]

	U11	U22	U33	U23	U13	U12
Ti(1)	0.055(2)	0.023(2)	0.057(3)	0.000(2)	0.015(2)	-0.003(2)
Ti(2)	0.048(2)	0.030(2)	0.065(3)	-0.002(2)	0.018(2)	0.001(2)
O(1)	0.072(3)	0.050(3)	0.073(3)	-0.003(2)	0.014(2)	0.002(2)
O(2)	0.067(3)	0.060(3)	0.083(4)	0.007(2)	0.026(3)	0.004(2)
Ti(3)	0.072(3)	0.050(3)	0.073(3)	-0.003(2)	0.014(2)	0.002(2)
Ti(4)	0.067(3)	0.060(3)	0.083(4)	0.007(2)	0.026(3)	0.004(2)
O(3)	0.055(2)	0.023(2)	0.057(3)	0.000(2)	0.015(2)	-0.003(2)
O(4)	0.048(2)	0.030(2)	0.065(3)	-0.002(2)	0.018(2)	0.001(2)
Co(11)	0.096(2)	0.089(2)	0.080(2)	0.0025(15)	0.0002(14)	0.005(2)
Co(12)	0.085(2)	0.119(3)	0.123(3)	-0.016(2)	-0.003(2)	0.037(2)
Co(13)	0.081(2)	0.120(2)	0.103(2)	-0.009(2)	0.000(2)	-0.025(2)
Co(21)	0.086(3)	0.101(4)	0.084(3)	0.012(2)	0.035(2)	0.001(2)
Co(22)	0.098(4)	0.065(2)	0.101(4)	-0.007(3)	0.051(4)	0.004(2)
Co(23)	0.066(3)	0.071(3)	0.101(4)	-0.004(3)	0.033(3)	-0.006(2)
Co(24)	0.068(6)	0.069(6)	0.081(7)	0.002(5)	0.040(5)	0.014(5)
Co(25)	0.093(7)	0.122(12)	0.070(6)	-0.021(6)	0.040(5)	-0.028(7)
Co(26)	0.077(7)	0.064(5)	0.075(7)	0.011(4)	0.033(5)	0.001(4)
O(11A)	0.050(11)	0.038(10)	0.058(13)	0.010(9)	0.010(9)	-0.011(8)
O(11B)	0.047(12)	0.031(10)	0.063(13)	0.016(9)	0.008(9)	-0.003(9)
O(12A)	0.080(16)	0.085(17)	0.087(18)	-0.007(14)	0.012(13)	-0.017(13)
O(12B)	0.122(22)	0.075(17)	0.077(17)	-0.013(13)	0.015(15)	-0.022(16)
O(21A)	0.045(11)	0.030(10)	0.072(13)	0.008(8)	0.035(9)	0.005(8)
O(21B)	0.062(12)	0.030(10)	0.033(11)	0.016(8)	0.013(9)	0.006(9)
O(22A)	0.090(18)	0.072(17)	0.078(18)	0.020(14)	0.023(14)	-0.015(14)
O(22B)	0.115(21)	0.069(16)	0.076(17)	-0.005(12)	0.053(15)	0.028(15)
C(10)	0.063(10)	0.067(11)	0.084(12)	0.000(9)	0.002(9)	-0.002(9)
C(11)	0.062(10)	0.054(9)	0.056(10)	-0.015(9)	0.002(8)	0.023(10)
C(20)	0.068(10)	0.070(10)	0.072(10)	0.004(9)	0.032(8)	-0.007(9)
C(21)	0.053(10)	0.051(10)	0.086(13)	-0.018(11)	0.023(9)	-0.022(10)
C(111)	0.162(26)	0.149(24)	0.109(20)	-0.046(19)	-0.003(18)	0.008(20)
C(112)	0.148(25)	0.161(27)	0.156(26)	0.022(21)	0.036(20)	-0.051(21)

Table 6. continued page 2.

C(113)	0.115(18)	0.098(17)	0.121(19)	-0.022(14)	0.040(15)	0.003(14)
C(121)	0.133(25)	0.262(40)	0.114(22)	-0.014(23)	-0.023(19)	0.046(26)
C(122)	0.140(24)	0.168(27)	0.147(27)	0.007(22)	0.030(21)	0.053(20)
C(123)	0.106(19)	0.072(16)	0.292(41)	-0.051(22)	0.014(22)	0.022(15)
C(131)	0.176(32)	0.178(30)	0.136(26)	-0.019(22)	-0.011(23)	-0.021(25)
C(132)	0.152(25)	0.196(31)	0.137(26)	-0.028(22)	0.066(21)	-0.075(22)
C(133)	0.130(22)	0.074(17)	0.222(33)	0.024(19)	0.020(21)	-0.016(16)
C(211)	0.131(22)	0.222(34)	0.104(19)	0.004(22)	0.026(17)	-0.030(22)
C(212)	0.122(23)	0.247(40)	0.135(24)	0.017(24)	-0.020(20)	-0.030(28)
C(213)	0.250(35)	0.089(18)	0.137(23)	0.012(17)	0.119(23)	0.039(23)
C(221)	0.232(34)	0.105(20)	0.267(39)	0.067(22)	0.188(32)	0.067(21)
C(222)	0.103(16)	0.063(14)	0.174(25)	0.014(14)	0.068(16)	0.023(12)
C(223)	0.187(30)	0.088(18)	0.167(28)	-0.029(19)	0.080(23)	-0.040(20)
C(231)	0.090(15)	0.065(13)	0.180(25)	-0.005(15)	0.054(15)	-0.006(12)
C(232)	0.152(24)	0.131(23)	0.207(30)	-0.048(20)	0.107(24)	-0.047(19)
C(233)	0.069(14)	0.116(19)	0.163(25)	0.026(20)	-0.005(15)	-0.009(14)
O(111)	0.248(27)	0.313(34)	0.130(17)	-0.019(20)	-0.083(18)	0.079(24)
O(112)	0.282(32)	0.185(24)	0.353(39)	-0.010(24)	0.158(29)	-0.113(23)
O(113)	0.157(17)	0.151(17)	0.203(21)	-0.002(15)	0.078(15)	0.052(14)
O(121)	0.152(21)	0.426(49)	0.299(36)	-0.032(32)	-0.081(23)	0.155(27)
O(122)	0.255(30)	0.334(38)	0.140(20)	-0.039(22)	0.059(20)	0.054(25)
O(123)	0.227(26)	0.071(13)	0.416(42)	-0.013(19)	0.019(26)	-0.007(15)
O(131)	0.206(26)	0.327(39)	0.298(36)	-0.006(28)	-0.154(27)	-0.094(25)
O(132)	0.374(40)	0.273(31)	0.169(23)	-0.040(21)	0.126(25)	-0.199(29)
O(133)	0.213(24)	0.091(15)	0.315(32)	0.017(18)	0.024(22)	-0.015(15)
O(211)	0.185(18)	0.245(24)	0.090(12)	-0.023(14)	0.075(12)	-0.022(16)
O(212)	0.119(16)	0.300(34)	0.228(25)	-0.004(22)	-0.031(18)	-0.026(21)
O(213)	0.317(33)	0.119(17)	0.229(26)	0.051(18)	0.113(23)	0.055(21)
O(221)	0.240(25)	0.136(17)	0.374(36)	0.022(19)	0.226(27)	0.051(16)
O(222)	0.157(16)	0.084(12)	0.216(21)	0.046(12)	0.069(15)	0.034(11)
O(223)	0.291(45)	0.144(26)	0.097(19)	-0.025(17)	0.015(22)	-0.118(30)
O(231)	0.146(15)	0.090(12)	0.214(20)	-0.056(12)	0.056(14)	-0.022(11)

Table 6. continued page 3.

O(232)	0.181(18)	0.141(15)	0.259(24)	-0.041(15)	0.170(19)	-0.072(14)
O(233)	0.164(20)	0.282(32)	0.158(21)	0.004(20)	-0.042(16)	-0.003(20)

[a] The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

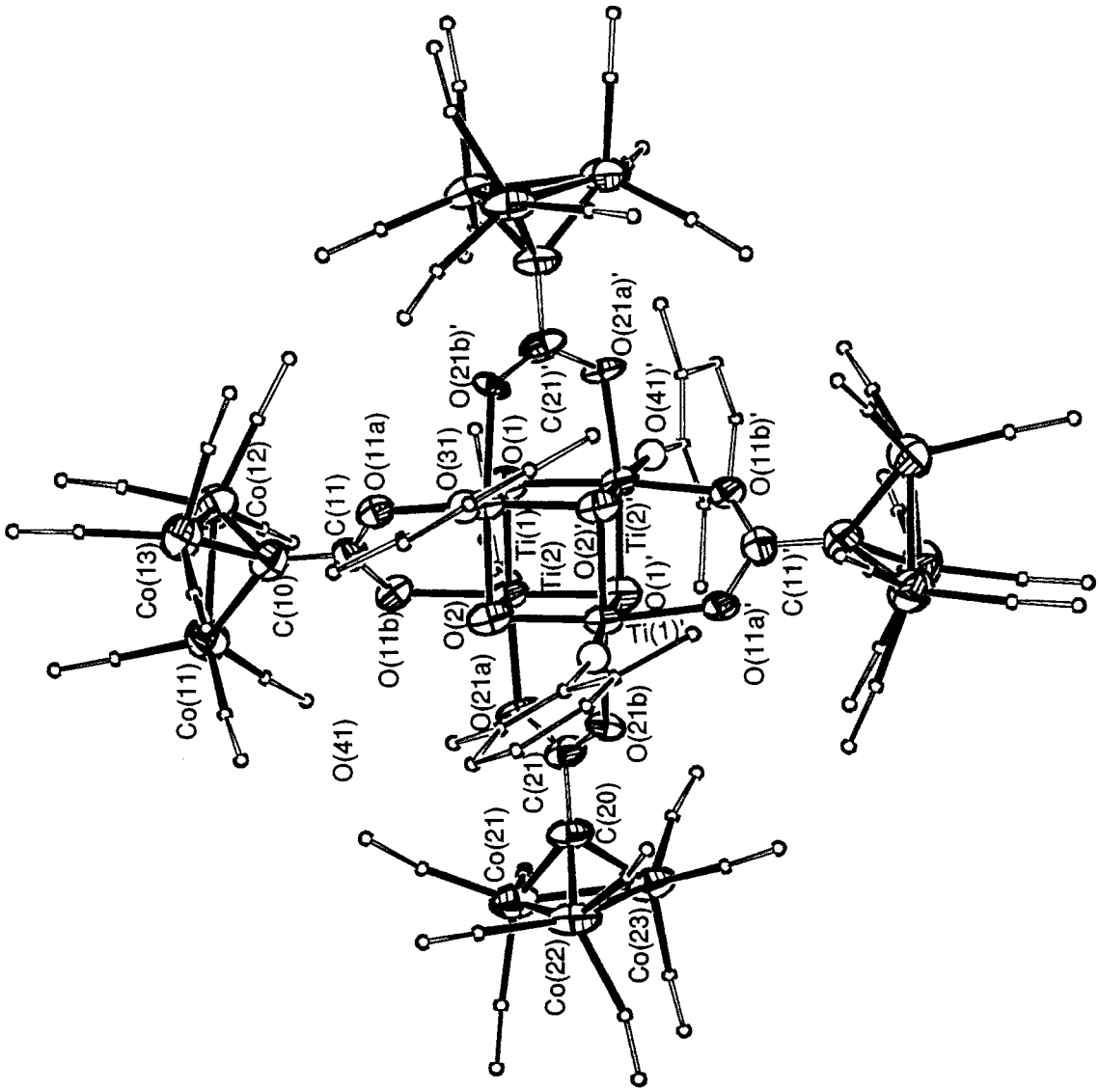
Table 7. Hydrogen coordinates and isotropic displacement parameters U_{iso} for $Ti_4O_4(Me_2PhO)_4[O_2CCCo_3(CO)_9]_4 \cdot C_6H_{14}$.

	x	y	z	U_{iso}(Å^2)[a]
H(33)	0.8982(17)	-0.3162(24)	0.7331(13)	0.105
H(34)	0.9282(18)	-0.3462(28)	0.8039(14)	0.120
H(35)	0.9598(15)	-0.2583(20)	0.8527(11)	0.083
H(37A)	0.8654(20)	-0.2084(26)	0.6817(13)	0.147
H(37B)	0.9093(20)	-0.1325(26)	0.6829(13)	0.147
H(37C)	0.8443(20)	-0.1265(26)	0.7041(13)	0.147
H(38A)	0.9802(21)	-0.1263(28)	0.8705(16)	0.154
H(38B)	0.9344(21)	-0.0610(28)	0.8519(16)	0.154
H(38C)	1.0006(21)	-0.0665(28)	0.8328(16)	0.154
H(43)	1.0115(20)	0.5357(27)	0.6268(15)	0.126
H(44)	0.9408(23)	0.5950(33)	0.6653(16)	0.150
H(45)	0.8897(18)	0.5296(25)	0.7221(14)	0.111
H(47A)	1.0769(18)	0.4239(26)	0.6110(13)	0.144
H(47B)	1.0393(18)	0.3423(26)	0.6085(13)	0.144
H(47C)	1.0873(18)	0.3552(26)	0.6465(13)	0.144
H(48A)	0.8590(15)	0.4032(21)	0.7573(11)	0.104
H(48B)	0.9140(15)	0.3437(21)	0.7655(11)	0.104
H(48C)	0.8665(15)	0.3248(21)	0.7279(11)	0.104
H(53)	0.8959(25)	0.5499(37)	0.7357(21)	0.172
H(54)	0.9381(28)	0.5875(43)	0.7984(23)	0.197
H(55)	0.9619(27)	0.4948(41)	0.8515(22)	0.187
H(57A)	0.8787(27)	0.4570(34)	0.6844(17)	0.210
H(57B)	0.8422(27)	0.3860(34)	0.7071(17)	0.210
H(57C)	0.9058(27)	0.3681(34)	0.6858(17)	0.210
H(58A)	0.9750(23)	0.3602(32)	0.8743(17)	0.192
H(58B)	0.9948(23)	0.2987(32)	0.8372(17)	0.192
H(58C)	0.9277(23)	0.2976(32)	0.8549(17)	0.192
H(63)	1.0068(37)	-0.2837(53)	0.6157(26)	0.252
H(64)	0.9155(48)	-0.3541(68)	0.6472(34)	0.334
H(65)	0.8959(29)	-0.2873(43)	0.7216(23)	0.200

Table 7. continued page 2.

H(67A)	1.0681(46)	-0.1475(59)	0.6044(34)	0.410
H(67B)	1.0781(46)	-0.0989(59)	0.6486(34)	0.410
H(67C)	1.0286(46)	-0.0697(59)	0.6145(34)	0.410
H(68A)	0.9071(21)	-0.0734(30)	0.7392(16)	0.173
H(68B)	0.8981(21)	-0.1506(30)	0.7694(16)	0.173
H(68C)	0.8492(21)	-0.1287(30)	0.7333(16)	0.173
H(30A)	0.0231(36)	0.4885(10)	0.0439(7)	0.249
H(30B)	-0.0466(36)	0.4845(10)	0.0317(7)	0.249
H(30C)	0.0423(33)	0.3711(5)	0.0003(16)	0.230
H(30D)	-0.0262(33)	0.3688(5)	-0.0152(16)	0.230
H(30E)	-0.0102(44)	0.2730(23)	0.0429(23)	0.447
H(30F)	-0.0571(44)	0.3398(23)	0.0580(23)	0.447
H(30G)	0.0108(44)	0.3443(23)	0.0742(23)	0.447

[a] Occupancy coefficiencies for hudrogen atoms are 0.5.



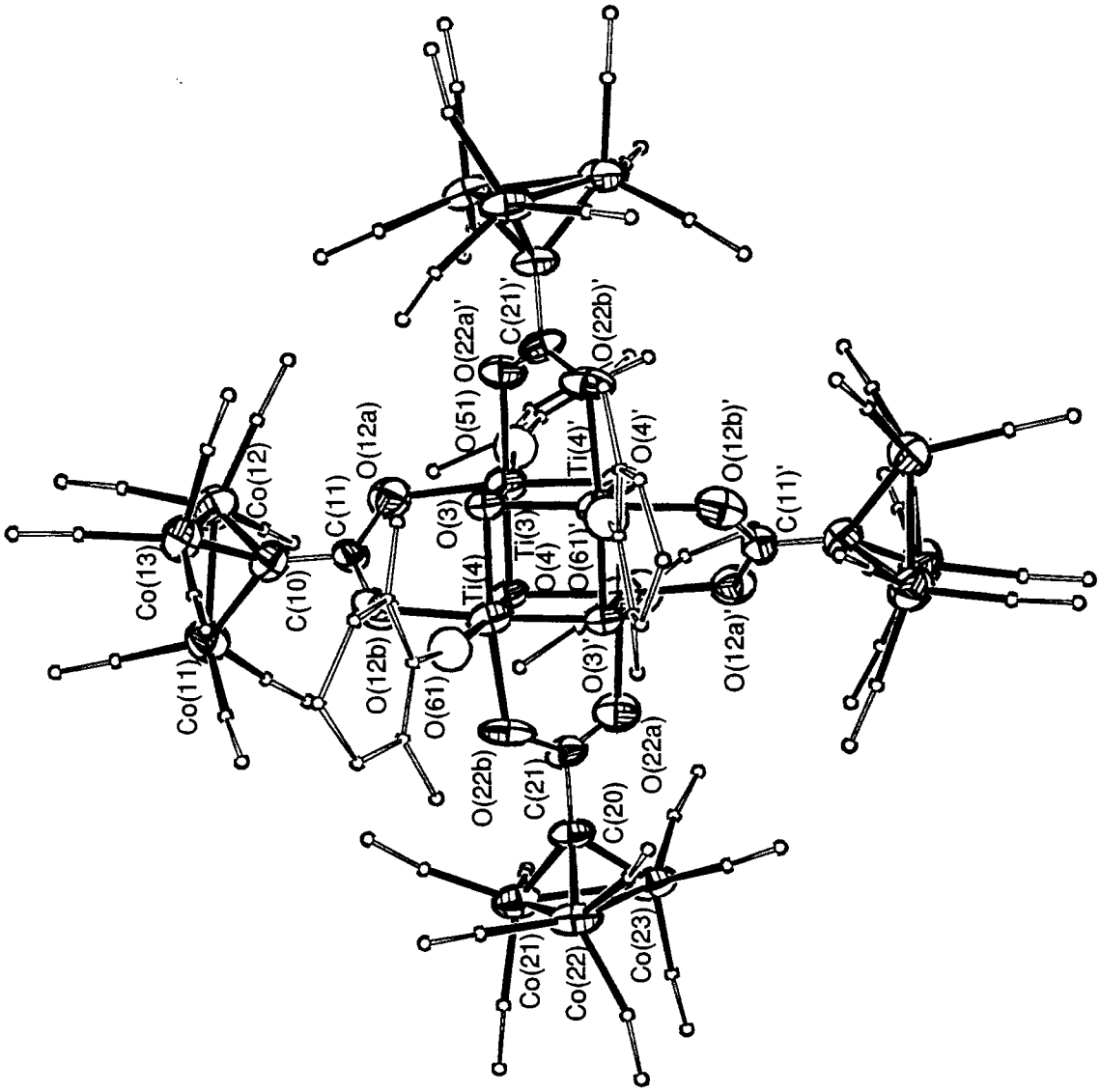


Table S1. Crystal data and structure refinement for $[Co_2Ti_2\{(OCH_2)_3CCH_3\}_2(OPr^i)_2\{(CO)_9Co_3CCO_2\}_4]$

Empirical formula	$C_{60}\ H_{32}\ Co_{14}\ O_{52}\ Ti_2$
Formula weight	2505.68
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 15.180(4) Å α = 90 deg.
	b = 21.579(5) Å β = 114.71(2)deg.
	c = 15.305(5) Å γ = 90 deg.
Volume, Z	4554(2) $Å^3$, 2
Density (calculated)	1.827 Mg/m^3
F(000)	2460
Wavelength	0.71073 Å
Absorption coefficient	2.734 mm^{-1}
Crystal size	0.45 x 0.28 x 0.15 mm
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9996 and 0.8249
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Monochromator	Graphite crystal, incident beam
Attenuator	Zr foil, factor 19.060
Take-off angle, deg	2.8
Detector aperture	1.95 to 2.39 mm horizontal
	4.0 mm vertical
Crystal-detector dist.	21 cm
Scan type	ω/2θ
Scan rate	1.27 - 8.23°/min
Scan width, deg	0.65 + 0.35tanθ
Theta range for data collection	2.39 to 23.01 deg.
Limiting indices	$-16 \le h \le 15,\ 0 \le k \le 23,\ 0 \le l \le 16$
Reflections collected	6613
Independent reflections	6335 [R(int) = 0.0556]
Unique observed data [$I>2\sigma(I)$]	4880
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6332 / 0 / 577
Goodness-of-fit on F^2	1.106
Final R indices [$I>2\sigma(I)$]	R_1 = 0.0515, wR_2 = 0.1265
R indices (all data)	R_1 = 0.0711, wR_2 = 0.1493
Largest diff. peak and hole	1.234 and -0.604 $e \cdot Å^{-3}$

Table S2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Co_2Ti_2\{(OCH_2)_3CCH_3\}_2(OCH(CH_3)_2)_2\{(CO)_9Co_3CCO_2\}_4]$

	x	y	z	U(eq)
Co(1)	1087(1)	5202(1)	764(1)	35(1)
Ti(1)	-201(1)	6044(1)	-844(1)	35(1)
Co(11)	2906(1)	5160(1)	4604(1)	51(1)
Co(12)	2955(1)	4018(1)	4535(1)	52(1)
Co(13)	1572(1)	4541(1)	4658(1)	53(1)
Co(21)	3524(1)	6107(1)	-970(1)	69(1)
Co(22)	4114(1)	6391(1)	737(1)	69(1)
Co(23)	3111(1)	7127(1)	-517(1)	64(1)
O(11)	1695(3)	5082(2)	2238(3)	45(1)
O(12)	955(3)	4179(2)	2255(3)	42(1)
O(21)	2134(3)	5619(2)	451(3)	47(1)
O(22)	-1147(3)	3796(2)	790(3)	44(1)
O(31)	232(3)	5137(2)	-763(3)	34(1)
O(32)	439(3)	6047(2)	543(3)	39(1)
O(33)	1316(3)	4280(2)	690(3)	39(1)
O(41)	556(3)	3175(2)	1037(3)	49(1)
C(31)	649(5)	4821(3)	-1318(4)	40(2)
C(32)	-7(5)	6231(3)	1161(5)	51(2)
C(33)	1657(5)	4086(3)	-1(5)	47(2)
C(34)	897(5)	4136(3)	-1034(5)	45(2)
C(35)	1320(7)	3872(4)	-1702(6)	73(2)
C(41)	821(12)	2585(5)	1402(11)	134(5)
C(42)	140(27)	2156(8)	739(21)	347(21)
C(43)	1841(17)	2479(10)	1542(17)	269(15)
C(10)	2056(4)	4597(3)	3716(4)	38(1)
C(11)	1537(4)	4629(3)	2646(4)	38(2)
C(20)	2837(5)	6324(3)	-218(5)	50(2)
C(21)	1982(5)	6027(3)	-171(5)	41(2)
C(111)	3781(7)	5275(5)	4121(7)	81(3)
O(111)	4307(6)	5357(4)	3779(6)	130(3)
C(112)	2259(7)	5855(4)	4086(6)	77(3)
O(112)	1832(7)	6279(3)	3730(6)	125(3)
C(113)	3557(6)	5341(4)	5882(6)	68(2)
O(113)	3923(5)	5438(4)	6679(4)	108(3)
C(121)	3711(7)	3863(4)	5789(6)	78(3)
O(121)	4161(6)	3782(4)	6580(5)	126(3)
C(122)	2356(8)	3281(5)	4182(7)	90(3)
O(122)	2010(9)	2822(4)	3983(8)	161(4)
C(123)	3746(8)	3926(5)	3978(8)	94(3)
O(123)	4251(8)	3856(5)	3600(9)	165(4)
C(131)	1970(7)	4444(5)	5955(6)	79(3)
O(131)	2243(6)	4402(4)	6751(5)	124(3)
C(132)	769(8)	5171(6)	4409(8)	99(4)
O(132)	235(8)	5563(5)	4223(8)	156(4)
C(133)	671(7)	3959(6)	4106(7)	92(3)
O(133)	104(7)	3602(5)	3741(6)	146(4)
C(211)	2590(9)	6071(6)	-2176(8)	110(4)
O(211)	2017(9)	6011(6)	-2899(7)	192(6)
C(212)	4568(11)	6330(7)	-1188(11)	135(5)
O(212)	5247(10)	6456(7)	-1285(11)	233(8)
C(213)	3679(7)	5298(6)	-792(7)	83(3)

Table S2 continued

O(213)	3740(6)	4778(4)	-714(7)	123(3)
C(221)	3837(9)	6695(6)	1680(8)	118(4)
O(221)	3590(10)	6832(7)	2257(7)	220(7)
C(222)	4333(7)	5629(6)	1231(7)	86(3)
O(222)	4425(7)	5156(4)	1545(6)	136(3)
C(223)	5331(9)	6655(6)	1004(10)	129(5)
O(223)	6082(7)	6832(6)	1175(9)	207(6)
C(231)	2081(8)	7287(4)	-1614(8)	91(3)
O(231)	1434(7)	7386(4)	-2303(6)	152(4)
C(232)	4051(9)	7621(5)	-562(8)	114(4)
O(232)	4674(8)	7899(5)	-568(8)	193(6)
C(233)	2749(12)	7580(6)	236(9)	123(5)
O(233)	2488(13)	7879(6)	690(8)	218(7)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Table S3. Full List of Bond lengths (Å) for $[Co_2Ti_2\{(OCH_2)_3CCH_3\}_2(OCH(CH_3)_2)_2\{(CO)_9Co_3CCO_2\}_4]$

Co(1)-O(33)	2.030(4)	O(33)-C(33)	1.422(8)
Co(1)-O(32)	2.033(4)	O(33)-Ti(1)#1	1.934(4)
Co(1)-O(21)	2.051(4)	O(41)-C(41)	1.381(10)
Co(1)-O(11)	2.065(4)	O(41)-Ti(1)#1	1.756(4)
Co(1)-O(31)#1	2.130(4)	C(31)-C(34)	1.542(9)
Co(1)-O(31)	2.152(4)	C(31)-H(31A)	0.97
Co(1)-Ti(1)	3.0276(14)	C(31)-H(31B)	0.97
Co(1)-Ti(1)#1	3.0311(14)	C(32)-C(34)#1	1.508(10)
Ti(1)-O(41)#1	1.756(4)	C(32)-H(32A)	0.97
Ti(1)-O(32)	1.931(4)	C(32)-H(32B)	0.97
Ti(1)-O(33)#1	1.934(4)	C(33)-C(34)	1.522(9)
Ti(1)-O(12)#1	2.034(4)	C(33)-H(33A)	0.97
Ti(1)-O(22)#1	2.043(4)	C(33)-H(33B)	0.97
Ti(1)-O(31)	2.053(4)	C(34)-C(32)#1	1.508(10)
Ti(1)-Co(1)#1	3.0311(14)	C(34)-C(35)	1.526(9)
Co(11)-C(111)	1.786(11)	C(35)-H(35A)	0.96
Co(11)-C(112)	1.785(9)	C(35)-H(35B)	0.96
Co(11)-C(113)	1.828(8)	C(35)-H(35C)	0.96
Co(11)-C(10)	1.877(6)	C(41)-C(42)	1.44(3)
Co(11)-Co(13)	2.457(2)	C(41)-C(43)	1.49(2)
Co(11)-Co(12)	2.470(2)	C(41)-H(41)	0.98
Co(12)-C(123)	1.750(12)	C(42)-H(42A)	0.96
Co(12)-C(122)	1.798(12)	C(42)-H(42B)	0.96
Co(12)-C(121)	1.810(8)	C(42)-H(42C)	0.96
Co(12)-C(10)	1.888(6)	C(43)-H(43A)	0.96
Co(12)-Co(13)	2.459(2)	C(43)-H(43B)	0.96
Co(13)-C(132)	1.759(12)	C(43)-H(43C)	0.96
Co(13)-C(133)	1.788(11)	C(10)-C(11)	1.493(8)
Co(13)-C(131)	1.829(9)	C(20)-C(21)	1.477(10)
Co(13)-C(10)	1.876(6)	C(21)-O(22)#1	1.284(8)
Co(21)-C(213)	1.768(12)	C(111)-O(111)	1.138(11)
Co(21)-C(211)	1.799(12)	C(112)-O(112)	1.122(10)
Co(21)-C(212)	1.816(13)	C(113)-O(113)	1.128(9)
Co(21)-C(20)	1.906(8)	C(121)-O(121)	1.127(10)
Co(21)-Co(22)	2.459(2)	C(122)-O(122)	1.104(12)
Co(21)-Co(23)	2.466(2)	C(123)-O(123)	1.148(12)
Co(22)-C(222)	1.782(12)	C(131)-O(131)	1.114(10)
Co(22)-C(221)	1.788(14)	C(132)-O(132)	1.123(12)
Co(22)-C(223)	1.809(12)	C(133)-O(133)	1.115(11)
Co(22)-C(20)	1.883(6)	C(211)-O(211)	1.091(13)
Co(22)-Co(23)	2.466(2)	C(212)-O(212)	1.134(14)
Co(23)-C(233)	1.764(14)	C(213)-O(213)	1.129(11)
Co(23)-C(231)	1.785(11)	C(221)-O(221)	1.133(14)
Co(23)-C(232)	1.804(11)	C(222)-O(222)	1.112(12)
Co(23)-C(20)	1.883(7)	C(223)-O(223)	1.124(12)
O(11)-C(11)	1.236(7)	C(231)-O(231)	1.121(11)
O(12)-C(11)	1.280(7)	C(232)-O(232)	1.125(12)
O(12)-Ti(1)#1	2.034(4)	C(233)-O(233)	1.134(14)
O(21)-C(21)	1.243(7)	Co(1)-O(33)	2.030(4)
O(22)-C(21)#1	1.284(8)	Co(1)-O(32)	2.033(4)
O(22)-Ti(1)#1	2.043(4)	Co(1)-O(21)	2.051(4)
O(31)-C(31)	1.427(7)	Co(1)-O(11)	2.065(4)
O(31)-Co(1)#1	2.130(4)	Co(1)-O(31)#1	2.130(4)
O(32)-C(32)	1.430(8)	Co(1)-O(31)	2.152(4)

Table S3 continued

Co(1)-Ti(1)	3.0276(14)	O(33)-C(33)	1.422(8)
Co(1)-Ti(1)#1	3.0311(14)	O(33)-Ti(1)#1	1.934(4)
Ti(1)-O(41)#1	1.756(4)	O(41)-C(41)	1.381(10)
Ti(1)-O(32)	1.931(4)	O(41)-Ti(1)#1	1.756(4)
Ti(1)-O(33)#1	1.934(4)	C(31)-C(34)	1.542(9)
Ti(1)-O(12)#1	2.034(4)	C(31)-H(31A)	0.97
Ti(1)-O(22)#1	2.043(4)	C(31)-H(31B)	0.97
Ti(1)-O(31)	2.053(4)	C(32)-C(34)#1	1.508(10)
Ti(1)-Co(1)#1	3.0311(14)	C(32)-H(32A)	0.97
Co(11)-C(111)	1.786(11)	C(32)-H(32B)	0.97
Co(11)-C(112)	1.785(9)	C(33)-C(34)	1.522(9)
Co(11)-C(113)	1.828(8)	C(33)-H(33A)	0.97
Co(11)-C(10)	1.877(6)	C(33)-H(33B)	0.97
Co(11)-Co(13)	2.457(2)	C(34)-C(32)#1	1.508(10)
Co(11)-Co(12)	2.470(2)	C(34)-C(35)	1.526(9)
Co(12)-C(123)	1.750(12)	C(35)-H(35A)	0.96
Co(12)-C(122)	1.798(12)	C(35)-H(35B)	0.96
Co(12)-C(121)	1.810(8)	C(35)-H(35C)	0.96
Co(12)-C(10)	1.888(6)	C(41)-C(42)	1.44(3)
Co(12)-Co(13)	2.459(2)	C(41)-C(43)	1.49(2)
Co(13)-C(132)	1.759(12)	C(41)-H(41)	0.98
Co(13)-C(133)	1.788(11)	C(42)-H(42A)	0.96
Co(13)-C(131)	1.829(9)	C(42)-H(42B)	0.96
Co(13)-C(10)	1.876(6)	C(42)-H(42C)	0.96
Co(21)-C(213)	1.768(12)	C(43)-H(43A)	0.96
Co(21)-C(211)	1.799(12)	C(43)-H(43B)	0.96
Co(21)-C(212)	1.816(13)	C(43)-H(43C)	0.96
Co(21)-C(20)	1.906(8)	C(10)-C(11)	1.493(8)
Co(21)-Co(22)	2.459(2)	C(20)-C(21)	1.477(10)
Co(21)-Co(23)	2.466(2)	C(21)-O(22)#1	1.284(8)
Co(22)-C(222)	1.782(12)	C(111)-O(111)	1.138(11)
Co(22)-C(221)	1.788(14)	C(112)-O(112)	1.122(10)
Co(22)-C(223)	1.809(12)	C(113)-O(113)	1.128(9)
Co(22)-C(20)	1.883(6)	C(121)-O(121)	1.127(10)
Co(22)-Co(23)	2.466(2)	C(122)-O(122)	1.104(12)
Co(23)-C(233)	1.764(14)	C(123)-O(123)	1.148(12)
Co(23)-C(231)	1.785(11)	C(131)-O(131)	1.114(10)
Co(23)-C(232)	1.804(11)	C(132)-O(132)	1.123(12)
Co(23)-C(20)	1.883(7)	C(133)-O(133)	1.115(11)
O(11)-C(11)	1.236(7)	C(211)-O(211)	1.091(13)
O(12)-C(11)	1.280(7)	C(212)-O(212)	1.134(14)
O(12)-Ti(1)#1	2.034(4)	C(213)-O(213)	1.129(11)
O(21)-C(21)	1.243(7)	C(221)-O(221)	1.133(14)
O(22)-C(21)#1	1.284(8)	C(222)-O(222)	1.112(12)
O(22)-Ti(1)#1	2.043(4)	C(223)-O(223)	1.124(12)
O(31)-C(31)	1.427(7)	C(231)-O(231)	1.121(11)
O(31)-Co(1)#1	2.130(4)	C(232)-O(232)	1.125(12)
O(32)-C(32)	1.430(8)	C(233)-O(233)	1.134(14)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

Table S4. Full List of Bond Angles (deg) for $[Co_2Ti_2\{(OCH_2)_3CCH_3\}_2(OCH(CH_3)_2)_2\{(CO)_9Co_3CCO_2\}_4]$

O(33)-Co(1)-O(32)	162.2(2)	Co(1)-Ti(1)-Co(1)#1	65.23(4)
O(33)-Co(1)-O(21)	104.5(2)	C(111)-Co(11)-C(112)	93.8(5)
O(32)-Co(1)-O(21)	86.3(2)	C(111)-Co(11)-C(113)	104.5(4)
O(33)-Co(1)-O(11)	86.0(2)	C(112)-Co(11)-C(113)	104.3(4)
O(32)-Co(1)-O(11)	105.0(2)	C(111)-Co(11)-C(10)	101.3(4)
O(21)-Co(1)-O(11)	105.9(2)	C(112)-Co(11)-C(10)	98.0(3)
O(33)-Co(1)-O(31)#1	81.2(2)	C(113)-Co(11)-C(10)	144.4(3)
O(32)-Co(1)-O(31)#1	85.3(2)	C(111)-Co(11)-Co(13)	148.8(3)
O(21)-Co(1)-O(31)#1	166.0(2)	C(112)-Co(11)-Co(13)	99.4(3)
O(11)-Co(1)-O(31)#1	87.1(2)	C(113)-Co(11)-Co(13)	99.4(3)
O(33)-Co(1)-O(31)	85.1(2)	C(10)-Co(11)-Co(13)	49.1(2)
O(32)-Co(1)-O(31)	81.2(2)	C(111)-Co(11)-Co(12)	94.6(3)
O(21)-Co(1)-O(31)	87.1(2)	C(112)-Co(11)-Co(12)	147.1(3)
O(11)-Co(1)-O(31)	165.8(2)	C(113)-Co(11)-Co(12)	104.3(3)
O(31)#1-Co(1)-O(31)	80.6(2)	C(10)-Co(11)-Co(12)	49.2(2)
O(33)-Co(1)-Ti(1)	127.62(12)	Co(13)-Co(11)-Co(12)	59.88(4)
O(32)-Co(1)-Ti(1)	38.97(11)	C(123)-Co(12)-C(122)	96.8(5)
O(21)-Co(1)-Ti(1)	81.14(12)	C(123)-Co(12)-C(121)	103.6(5)
O(11)-Co(1)-Ti(1)	143.60(13)	C(122)-Co(12)-C(121)	99.9(4)
O(31)#1-Co(1)-Ti(1)	85.29(11)	C(123)-Co(12)-C(10)	101.8(4)
O(31)-Co(1)-Ti(1)	42.65(11)	C(122)-Co(12)-C(10)	104.6(4)
O(33)-Co(1)-Ti(1)#1	38.96(12)	C(121)-Co(12)-C(10)	142.1(4)
O(32)-Co(1)-Ti(1)#1	127.66(13)	C(123)-Co(12)-Co(13)	150.5(3)
O(21)-Co(1)-Ti(1)#1	143.07(14)	C(122)-Co(12)-Co(13)	95.0(4)
O(11)-Co(1)-Ti(1)#1	81.28(12)	C(121)-Co(12)-Co(13)	100.8(3)
O(31)#1-Co(1)-Ti(1)#1	42.56(11)	C(10)-Co(12)-Co(13)	49.0(2)
O(31)-Co(1)-Ti(1)#1	84.84(11)	C(123)-Co(12)-Co(11)	99.9(4)
Ti(1)-Co(1)-Ti(1)#1	114.77(4)	C(122)-Co(12)-Co(11)	151.0(3)
O(41)#1-Ti(1)-O(32)	99.2(2)	C(121)-Co(12)-Co(11)	99.0(3)
O(41)#1-Ti(1)-O(33)#1	98.4(2)	C(10)-Co(12)-Co(11)	48.8(2)
O(32)-Ti(1)-O(33)#1	86.1(2)	Co(13)-Co(12)-Co(11)	59.78(4)
O(41)#1-Ti(1)-O(12)#1	93.0(2)	C(132)-Co(13)-C(133)	96.7(6)
O(32)-Ti(1)-O(12)#1	165.8(2)	C(132)-Co(13)-C(131)	102.0(5)
O(33)#1-Ti(1)-O(12)#1	84.9(2)	C(133)-Co(13)-C(131)	105.8(4)
O(41)#1-Ti(1)-O(22)#1	94.4(2)	C(132)-Co(13)-C(10)	104.0(4)
O(32)-Ti(1)-O(22)#1	85.4(2)	C(133)-Co(13)-C(10)	98.6(4)
O(33)#1-Ti(1)-O(22)#1	165.6(2)	C(131)-Co(13)-C(10)	141.6(3)
O(12)#1-Ti(1)-O(22)#1	101.1(2)	C(132)-Co(13)-Co(11)	94.5(4)
O(41)#1-Ti(1)-O(31)	173.5(2)	C(133)-Co(13)-Co(11)	147.6(3)
O(32)-Ti(1)-O(31)	86.3(2)	C(131)-Co(13)-Co(11)	101.3(3)
O(33)#1-Ti(1)-O(31)	85.5(2)	C(10)-Co(13)-Co(11)	49.1(2)
O(12)#1-Ti(1)-O(31)	82.1(2)	C(132)-Co(13)-Co(12)	151.0(3)
O(22)#1-Ti(1)-O(31)	82.4(2)	C(133)-Co(13)-Co(12)	98.6(4)
O(41)#1-Ti(1)-Co(1)	139.6(2)	C(131)-Co(13)-Co(12)	97.2(3)
O(32)-Ti(1)-Co(1)	41.45(12)	C(10)-Co(13)-Co(12)	49.4(2)
O(33)#1-Ti(1)-Co(1)	89.09(12)	Co(11)-Co(13)-Co(12)	60.33(4)
O(12)#1-Ti(1)-Co(1)	127.33(13)	C(213)-Co(21)-C(211)	96.4(5)
O(22)#1-Ti(1)-Co(1)	76.86(12)	C(213)-Co(21)-C(212)	102.7(6)
O(31)-Ti(1)-Co(1)	45.27(11)	C(211)-Co(21)-C(212)	101.3(7)
O(41)#1-Ti(1)-Co(1)#1	138.4(2)	C(213)-Co(21)-C(20)	102.7(4)
O(32)-Ti(1)-Co(1)#1	89.21(12)	C(211)-Co(21)-C(20)	103.7(4)
O(33)#1-Ti(1)-Co(1)#1	41.30(12)	C(212)-Co(21)-C(20)	141.8(5)
O(12)#1-Ti(1)-Co(1)#1	76.73(12)	C(213)-Co(21)-Co(22)	96.7(3)
O(22)#1-Ti(1)-Co(1)#1	126.99(13)	C(211)-Co(21)-Co(22)	151.9(4)
O(31)-Ti(1)-Co(1)#1	44.59(11)	C(212)-Co(21)-Co(22)	99.8(5)

Table S4 continued

C(20)-Co(21)-Co(22)	49.1(2)	O(31)-C(31)-H(31B)	108.7(3)
C(213)-Co(21)-Co(23)	150.6(3)	C(34)-C(31)-H(31B)	108.7(3)
C(211)-Co(21)-Co(23)	98.3(4)	H(31A)-C(31)-H(31B)	107.6
C(212)-Co(21)-Co(23)	99.2(5)	O(32)-C(32)-C(34)#1	114.5(5)
C(20)-Co(21)-Co(23)	49.0(2)	O(32)-C(32)-H(32A)	108.6(3)
Co(22)-Co(21)-Co(23)	60.09(5)	C(34)#1-C(32)-H(32A)	108.6(4)
C(222)-Co(22)-C(221)	93.5(6)	O(32)-C(32)-H(32B)	108.6(3)
C(222)-Co(22)-C(223)	101.7(5)	C(34)#1-C(32)-H(32B)	108.6(4)
C(221)-Co(22)-C(223)	105.3(7)	H(32A)-C(32)-H(32B)	107.6
C(222)-Co(22)-C(20)	101.9(4)	O(33)-C(33)-C(34)	113.5(5)
C(221)-Co(22)-C(20)	98.1(4)	O(33)-C(33)-H(33A)	108.9(3)
C(223)-Co(22)-C(20)	145.3(5)	C(34)-C(33)-H(33A)	108.9(3)
C(222)-Co(22)-Co(21)	98.1(3)	O(33)-C(33)-H(33B)	108.9(3)
C(221)-Co(22)-Co(21)	147.6(4)	C(34)-C(33)-H(33B)	108.9(4)
C(223)-Co(22)-Co(21)	101.7(5)	H(33A)-C(33)-H(33B)	107.7
C(20)-Co(22)-Co(21)	49.9(2)	C(32)#1-C(34)-C(33)	110.2(5)
C(222)-Co(22)-Co(23)	150.4(3)	C(32)#1-C(34)-C(35)	108.8(6)
C(221)-Co(22)-Co(23)	96.6(4)	C(33)-C(34)-C(35)	108.7(6)
C(223)-Co(22)-Co(23)	102.3(4)	C(32)#1-C(34)-C(31)	111.5(6)
C(20)-Co(22)-Co(23)	49.1(2)	C(33)-C(34)-C(31)	110.6(5)
Co(21)-Co(22)-Co(23)	60.09(5)	C(35)-C(34)-C(31)	106.9(5)
C(233)-Co(23)-C(231)	96.8(6)	C(34)-C(35)-H(35A)	109.5(5)
C(233)-Co(23)-C(232)	99.5(7)	C(34)-C(35)-H(35B)	109.5(4)
C(231)-Co(23)-C(232)	104.2(5)	H(35A)-C(35)-H(35B)	109.5
C(233)-Co(23)-C(20)	100.9(5)	C(34)-C(35)-H(35C)	109.5(4)
C(231)-Co(23)-C(20)	102.2(3)	H(35A)-C(35)-H(35C)	109.5
C(232)-Co(23)-C(20)	144.2(5)	H(35B)-C(35)-H(35C)	109.5
C(233)-Co(23)-Co(21)	149.6(4)	O(41)-C(41)-C(42)	108(2)
C(231)-Co(23)-Co(21)	97.7(3)	O(41)-C(41)-C(43)	108.0(12)
C(232)-Co(23)-Co(21)	102.6(5)	C(42)-C(41)-C(43)	114(2)
C(20)-Co(23)-Co(21)	49.8(2)	O(41)-C(41)-H(41)	109.1(6)
C(233)-Co(23)-Co(22)	96.2(4)	C(42)-C(41)-H(41)	109.1(12)
C(231)-Co(23)-Co(22)	150.4(3)	C(43)-C(41)-H(41)	109.1(10)
C(232)-Co(23)-Co(22)	99.7(4)	C(41)-C(42)-H(42A)	109.5(14)
C(20)-Co(23)-Co(22)	49.1(2)	C(41)-C(42)-H(42B)	109.5(13)
Co(21)-Co(23)-Co(22)	59.82(5)	H(42A)-C(42)-H(42B)	109.5
C(11)-O(11)-Co(1)	123.9(4)	C(41)-C(42)-H(42C)	109.5(12)
C(11)-O(12)-Ti(1)#1	130.4(4)	H(42A)-C(42)-H(42C)	109.5
C(21)-O(21)-Co(1)	125.2(4)	H(42B)-C(42)-H(42C)	109.5
C(21)#1-O(22)-Ti(1)#1	130.0(4)	C(41)-C(43)-H(43A)	109.5(12)
C(31)-O(31)-Ti(1)	129.1(3)	C(41)-C(43)-H(43B)	109.5(10)
C(31)-O(31)-Co(1)#1	119.1(3)	H(43A)-C(43)-H(43B)	109.5
Ti(1)-O(31)-Co(1)#1	92.9(2)	C(41)-C(43)-H(43C)	109.5(9)
C(31)-O(31)-Co(1)	117.5(3)	H(43A)-C(43)-H(43C)	109.5
Ti(1)-O(31)-Co(1)	92.1(2)	H(43B)-C(43)-H(43C)	109.5
Co(1)#1-O(31)-Co(1)	99.4(2)	C(11)-C(10)-Co(11)	130.7(5)
C(32)-O(32)-Ti(1)	124.6(4)	C(11)-C(10)-Co(13)	130.5(5)
C(32)-O(32)-Co(1)	118.0(4)	Co(11)-C(10)-Co(13)	81.8(3)
Ti(1)-O(32)-Co(1)	99.6(2)	C(11)-C(10)-Co(12)	131.5(5)
C(33)-O(33)-Ti(1)#1	126.4(4)	Co(11)-C(10)-Co(12)	82.0(2)
C(33)-O(33)-Co(1)	117.1(4)	Co(13)-C(10)-Co(12)	81.6(2)
Ti(1)#1-O(33)-Co(1)	99.7(2)	O(11)-C(11)-O(12)	127.2(5)
C(41)-O(41)-Ti(1)#1	165.8(6)	O(11)-C(11)-C(10)	117.8(6)
O(31)-C(31)-C(34)	114.0(5)	O(12)-C(11)-C(10)	115.0(5)
O(31)-C(31)-H(31A)	108.7(3)	C(21)-C(20)-Co(22)	129.5(5)
C(34)-C(31)-H(31A)	108.7(4)	C(21)-C(20)-Co(23)	134.4(5)

Table S4 continued

Co(22)-C(20)-Co(23)	81.8(3)	O(131)-C(131)-Co(13)	177.1(9)
C(21)-C(20)-Co(21)	129.5(5)	O(132)-C(132)-Co(13)	177.6(13)
Co(22)-C(20)-Co(21)	80.9(3)	O(133)-C(133)-Co(13)	178.3(10)
Co(23)-C(20)-Co(21)	81.2(3)	O(211)-C(211)-Co(21)	175.6(14)
O(21)-C(21)-O(22)#1	125.8(6)	O(212)-C(212)-Co(21)	177(2)
O(21)-C(21)-C(20)	117.3(6)	O(213)-C(213)-Co(21)	176.9(10)
O(22)#1-C(21)-C(20)	116.8(5)	O(221)-C(221)-Co(22)	172(2)
O(111)-C(111)-Co(11)	177.1(9)	O(222)-C(222)-Co(22)	176.3(10)
O(112)-C(112)-Co(11)	177.4(8)	O(223)-C(223)-Co(22)	179(2)
O(113)-C(113)-Co(11)	176.5(8)	O(231)-C(231)-Co(23)	179.8(12)
O(121)-C(121)-Co(12)	177.3(9)	O(232)-C(232)-Co(23)	175.9(13)
O(122)-C(122)-Co(12)	178.2(10)	O(233)-C(233)-Co(23)	177.4(14)
O(123)-C(123)-Co(12)	178.4(12)		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Co_2Ti_2\{(OCH_2)_3CCH_3\}_2(OCH(CH_3)_2)_2\{(CO)_9Co_3CCO_2\}_4]$

	U11	U22	U33	U23	U13	U12
Co(1)	40(1)	33(1)	24(1)	6(1)	7(1)	-2(1)
Ti(1)	40(1)	29(1)	26(1)	5(1)	6(1)	-1(1)
Co(11)	51(1)	57(1)	32(1)	-2(1)	5(1)	-7(1)
Co(12)	53(1)	58(1)	33(1)	7(1)	5(1)	14(1)
Co(13)	49(1)	76(1)	33(1)	9(1)	15(1)	0(1)
Co(21)	66(1)	82(1)	65(1)	2(1)	34(1)	-7(1)
Co(22)	47(1)	84(1)	59(1)	15(1)	5(1)	-10(1)
Co(23)	68(1)	55(1)	58(1)	12(1)	16(1)	-16(1)
O(11)	54(3)	45(3)	24(2)	6(2)	5(2)	-9(2)
O(12)	46(3)	42(3)	25(2)	9(2)	5(2)	-3(2)
O(21)	42(3)	49(3)	43(3)	16(2)	11(2)	-3(2)
O(22)	41(3)	46(3)	35(2)	12(2)	7(2)	-1(2)
O(31)	41(2)	33(2)	25(2)	4(2)	11(2)	1(2)
O(32)	49(3)	35(2)	26(2)	0(2)	9(2)	-2(2)
O(33)	43(2)	38(2)	34(2)	9(2)	12(2)	8(2)
O(41)	64(3)	27(2)	45(3)	9(2)	12(2)	7(2)
C(31)	48(4)	40(4)	33(3)	3(3)	19(3)	4(3)
C(32)	74(5)	37(4)	44(4)	-7(3)	25(4)	-1(4)
C(33)	52(4)	43(4)	49(4)	8(3)	24(4)	12(3)
C(34)	61(4)	42(4)	38(4)	3(3)	27(3)	10(3)
C(35)	107(7)	66(5)	61(5)	7(4)	50(5)	23(5)
C(41)	226(16)	61(7)	159(12)	46(8)	122(12)	66(9)
C(42)	643(64)	73(11)	422(41)	-103(18)	317(44)	-124(22)
C(43)	317(28)	251(24)	328(30)	180(23)	224(26)	231(24)
C(10)	35(3)	40(4)	29(3)	4(3)	5(3)	-3(3)
C(11)	38(4)	46(4)	24(3)	2(3)	7(3)	5(3)
C(20)	44(4)	52(4)	37(4)	11(3)	1(3)	-2(3)
C(21)	47(4)	37(4)	34(4)	1(3)	13(3)	-8(3)
C(111)	74(6)	91(7)	65(6)	0(5)	17(5)	-21(5)
O(111)	99(6)	188(9)	125(7)	6(6)	71(6)	-38(6)
C(112)	92(7)	50(5)	58(5)	-7(4)	1(5)	-4(5)
O(112)	161(7)	52(4)	106(6)	4(4)	0(5)	13(5)
C(113)	60(5)	77(6)	52(5)	-14(4)	9(4)	-15(4)
O(113)	98(5)	158(7)	43(4)	-31(4)	6(3)	-19(5)
C(121)	76(6)	89(7)	49(5)	10(5)	5(5)	24(5)
O(121)	124(6)	159(7)	48(4)	26(4)	-11(4)	42(5)
C(122)	115(8)	70(7)	72(6)	3(5)	28(6)	9(6)
O(122)	238(12)	58(5)	172(9)	-27(5)	72(9)	-33(6)
C(123)	90(7)	98(8)	93(8)	10(6)	35(6)	21(6)
O(123)	164(9)	184(10)	205(11)	6(8)	136(9)	36(8)
C(131)	79(6)	117(8)	52(6)	8(5)	37(5)	-10(5)
O(131)	138(7)	198(9)	36(4)	11(4)	36(4)	-22(6)
C(132)	95(8)	135(10)	88(7)	42(7)	59(7)	32(7)
O(132)	161(8)	173(9)	183(10)	85(8)	120(8)	103(8)
C(133)	72(6)	140(10)	60(6)	9(6)	22(5)	-36(6)
O(133)	121(7)	188(9)	110(6)	-15(6)	30(5)	-90(7)
C(211)	114(9)	133(10)	67(7)	-20(7)	23(7)	35(8)
O(211)	203(11)	242(13)	66(6)	-27(7)	-8(6)	94(10)
C(212)	133(11)	148(12)	157(13)	-18(10)	95(11)	-32(10)
O(212)	218(12)	260(15)	335(19)	-74(13)	227(14)	-106(11)
C(213)	64(6)	95(8)	86(7)	7(6)	27(5)	13(6)
O(213)	121(7)	92(6)	147(8)	-2(5)	46(6)	22(5)
C(221)	106(9)	146(11)	64(7)	-13(7)	-3(6)	37(8)