Synthesis and Characterization of tungsten(VI) alkylidene and alkylidyne complexes supported by an $[OCO]^{3-}$ trianionic pincer ligand: progress towards the $[^{t}BuOCO]W{\equiv}CC(CH_3)_3$ fragment.

Subramaniam Kuppuswamy, Andrew J. Peloquin, Ion Ghiviriga, Khalil A. Abboud, and

*Adam S. Veige**

Center for Catalysis, University of Florida, P.O. Box 177200, Gainesville, FL, 32611

Synthetic Procedures

General Considerations. Unless specified otherwise, all manipulations were performed under an inert atmosphere using standard Schlenk or glovebox techniques. Glassware was oven-dried before use. Pentane, toluene, diethyl ether (Et_2O), tetrahydrofuran (THF), 1,2-dimethoxyethane (DME) were dried using a GlassContours drying column. Benzene-d_6 (Cambridge Isotopes) was dried over sodium-benzophenone ketyl and distilled or vacuum transferred and stored over 4Å molecular sieves. $(^tBuO)_3W{\equiv}CC(CH_3)_3$ was purchased from Strem Chemicals Inc. and used as received. $(MeO)_3WCl_3$,[32] $(ArO)_3WCl_3$ (Ar = 2,6-diisopropylphenyl),[33] $(ArO)_2W{\equiv}CC(CH_3)_3Np$ (**8**),[21] $[^tBuOCO]H_3$ (**9**),[16b] $Np_3W{\equiv}CC(CH_3)_3$ (**11**),[26] $[^tBuOCHO]K_2(THF)_2$ (**15**),[15] $(DME)Cl_3W{\equiv}CC(CH_3)_3$ (**16**),[26b] were prepared according to the literature procedures. NMR spectra were obtained on Varian INOVA 500 MHz, Varian Mercury Broad Band 300 MHz, or Varian Mercury 300 MHz spectrometers. Chemical shifts are reported in δ (ppm). For ^1H and $^{13}C\{^1H\}$ NMR spectra the solvent resonance was referenced as an internal reference. Elemental analyses were performed at Complete Analysis Laboratory Inc., Parsippany, New Jersey. Accurate mass was determined by Atmospheric Pressure Chemical Ionization- Mass Spectrometric (APCI-MS) method in diluted dichloromethane solution, and the spectrum was recorded on Agilent 6210 TOF-MS at Mass spectrometry facility, University of Florida.

Synthesis of $[^tBuOCO]W{=}CHC(CH_3)_3(O\text{-}2,6\text{-}C_6H_3\text{-}^iPr_2)$ (10). A glass vial was charged with $[^tBuOCO]H_3$ (**9**) (41 mg, 0.11 mmol) and benzene (0.5 mL) and then frozen (-35 °C). $(^tBuO)_3W{\equiv}CC(CH_3)_3$ (52 mg, 0.11 mmol) was dissolved in benzene (0.5 mL) and then added to the frozen solution of **9**. All volatiles were removed in vacuo and triturated with pentane (3 x 1 mL) to provide a light red crystalline solid. The solid was redissolved in toluene (2 mL) and then the solution was cooled to -35 °C. 2,6-$^iPr_2$-C_6H_3OH (18.4 μL, 0.11 mmol) was dissolved in

toluene (5 mL) and cooled to -35 °C. The solutions were combined at -35 °C and the resulting mixture was shaken for 1 min and then all volatiles were removed, but the solution was kept cold. The crude mixture was checked by ^{1}H NMR spectroscopy to determine if additional 2,6-^{i}Pr$_2$-C$_6$H$_3$OH was needed to complete the reaction. The product was dried under vacuum and washed with cold pentane (3 x 1 mL) to provide **10** as a red crystalline solid (60 mg, 68%). ^{1}H NMR (300 MHz, C_6D_6) δ (ppm): 7.99 (d, *J*=7.9 Hz, 2H, Ar-*H*), 7.80 (dd, *J*=7.9 Hz, *J* = 1.5 Hz, 2H, Ar-*H*), 7.38 (t, *J*=7.9 Hz, 1H, Ar-*H*), 7.33 (dd, *J*=7.8 Hz, *J* = 1.5 Hz, 2H, Ar-*H*), 7.13-7.15 (m, 1H, Ar-*H*), 6.98 (overlapping doublets, *J*=7.9 Hz, *J* = 7.6 Hz, 2H, Ar-*H*), 6.87-6.89 (m, 2H, Ar-*H*), 5.55 (t, J_{HW}=8.7 Hz, 1H, W=C*H*C(CH$_3$)$_3$), 4.09 (sept, *J*=6.7 Hz, 1H, -C*H*(CH$_3$)$_2$), 2.40 (sept, *J*=6.7 Hz, 1H, -C*H*(CH$_3$)$_2$), 1.44 (s, 18H, -C(C*H$_3$*)$_3$), 1.42 (d, *J*=6.7Hz, 6H, -CH(C*H$_3$*)$_2$), 0.85 (s, 9H, W=CHC(C*H$_3$*)$_3$), 0.70 (d, *J*=6.7 Hz, 6H, -CH(C*H$_3$*)$_2$). ^{13}C{1H} NMR (75.36 Hz, C_6D_6) δ (ppm): 272.2 (s, W=*C*HC(CH$_3$)$_3$), 182.7 (s, W-*C$_{pincer}$*), 160.3, 158.5, 140.9, 138.2, 137.2, 137.1, 133.0, 130.0, 126.7, 126.4, 124.4, 123.9, 123.6, 122.3 (aryl), 47.8 (s, W=CH*C*(CH$_3$)$_3$), 35.6 (s, -*C*(CH$_3$)$_3$), 33.3 (s, W=CHC(*C*H$_3$)$_3$), 31.8 (s, -*C*H(CH$_3$)$_2$), 30.8 (s, -C(*C*H$_3$)$_3$), 27.5 (s, -*C*H(CH$_3$)$_2$), 23.9 (s, -CH(*C*H$_3$)$_2$), 23.6 (s, -*C*H(CH$_3$)$_2$). Anal. Calcd. for $C_{43}H_{54}O_3W$: C, 64.34; H, 6.78. Found: C, 64.42; H, 6.94.

Synthesis of [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$(^{t}BuOCO)] (12$_{therm}$). In a J. Young NMR tube, Np$_3$W≡CC(CH$_3$)$_3$ (**11**) (76 mg, 0.163 mmol), **9** (60 mg, 0.163 mmol), and PMe$_2$Ph (46 μL, 0.326 mmol) were combined in benzene-*d$_6$* (0.5 mL). The solution was degassed. The tube was heated at 100 °C and the progress of the reaction monitored periodically by ^{1}H NMR spectroscopy. In addition to the starting materials, the isomer **12$_{kin}$** was observed with appreciable intensity after 8 hours. ^{1}H NMR (300 MHz, C_6D_6), δ (ppm): 8.74 (s, 2H, W=C*H*C(CH$_3$)$_3$), 4.64 (s, 1H, Ar-H), 1.83 (s, 18H, -C(C*H$_3$*)$_3$), 1.65 (s, 18H, -C(C*H$_3$*)$_3$), 1.40 (s,

18H, -C(C*H*$_3$)$_3$), 0.61 (s, 18H, W=CHC(C*H*$_3$)$_3$). Further heating of the reaction mixture for a total of 48 hours completed the reaction. The solvent was removed in vacuo to yield a dark brown material. Extraction into hexanes followed by removal of all volatile material produced red oil. X-ray quality and analytically pure crystalline material was obtained by slow evaporation of an Et_2O solution of **12*$_{therm}$*** (45 mg, 51 %, based on [^{t}BuOCO]H$_3$ (**9**^{1}H NMR (300 MHz, C_6D_6), δ (ppm): 8.66 (t, J_{WH}=12.9 Hz, 2H, W=C*H*C(CH$_3$)$_3$), 7.75 (m, 2H, Ar-*H*), 7.66 (d, *J*=8.2 Hz, 2H, Ar-*H*), 7.38 (m, 4H, Ar-*H*), 7.28-7,32 (m, 4H, Ar-*H*), 7.00-7.07 (m, 3H, Ar-*H*), 6.91(m, 4H, Ar-*H*), 6.60 (m, 2H, Ar-*H*), 6.03-6.08 (m, 4H, Ar-*H*), 5.14 (t, *J*=7.6 Hz, 1H, Ar-*H*), 1.79 (s, 18H, -C(C*H*$_3$)$_3$), 1.68 (s, 18H, -C(C*H*$_3$)$_3$), 1.32 (s, 18H, -C(C*H*$_3$)$_3$), 0.56 (s, 18H, W=CHC(C*H*$_3$)$_3$). ^{13}C{1H} NMR (75.36 Hz, C_6D_6), δ (ppm): 280.7 (s, W=*C*HC(CH$_3$)$_3$), 184.3 (s, W-*C$_{pincer}$*), 161.4, 158.2, 155.7, 143.1, 140.6, 140.2, 140.0, 137.6, 136.5, 135.7, 135.4, 133.5, 132.8, 130.9, 129.0, 128.9, 127.8, 127.0, 126.9, 126.7, 126.4, 125.9, 124.5, 123.1, 121.8 (aryl), 49.2 (s, W=CH*C*(CH$_3$)$_3$), 36.3 (s, -*C*(CH$_3$)$_3$), 35.9 (s, -*C*(CH$_3$)$_3$), 35.4 (s, -*C*(CH$_3$)$_3$), 33.4 (s, W=CHC(*C*H$_3$)$_3$), 32.0 (s, -C(*C*H$_3$)$_3$), 31.7 (s, -C(*C*H$_3$)$_3$), 31.3 (s, -C(*C*H$_3$)$_3$). Anal. Calcd. for $C_{88}H_{102}O_6W_2$: C, 65.11; H, 6.33. Found: C, 64.98; H, 6.21.

Attempted synthesis of [^{t}BuOCHO]W≡CC(CH$_3$)$_3$Cl (17). In a 100 mL round bottom flask, (DME)Cl$_3$W≡CC(CH$_3$)$_3$ (**16**) (50 mg, 0.11 mmol) in 20 mL of Et_2O was added dropwise to [^{t}BuOCHO]K$_2$(THF)$_2$ (**15**) (66 mg, 0.11 mmol) in 60 mL of Et_2O at – 80 °C. The solution turned light to dark yellow within 10 min. The solvent was removed in vacuo to produce a red solid. The solid was extracted into cold hexanes and dried under vacuum to yield **17** (65 mg, 59 % of **17**, 17 % of [^{t}BuOCO]H$_3$ (**9**), and 6 % of **12*$_{kin}$***, along with other impurities. ^{1}H NMR (300 MHz, C_6D_6), δ (ppm): 9.75 (bs, 1H, Ar-*H*), 8.04 (bm, 2H, Ar-*H*), 7.31-7.36 (m, 4H, Ar-*H*), 6.39 (m,

3H, Ar-*H*), 3.27 (bm, 4H, -OC*H*$_2$CH$_3$), 1.69 (s, 18H, -C(C*H*$_3$)$_3$), 0.94 (bm, 6H, -OCH$_2$C*H*$_3$), 0.74 (s, 9H, W≡CC(C*H*$_3$)$_3$). APCI-MS, $[M+H]^+$=661.2085; ($C_{31}H_{38}O_2ClW$, theoretical = 661.2058).

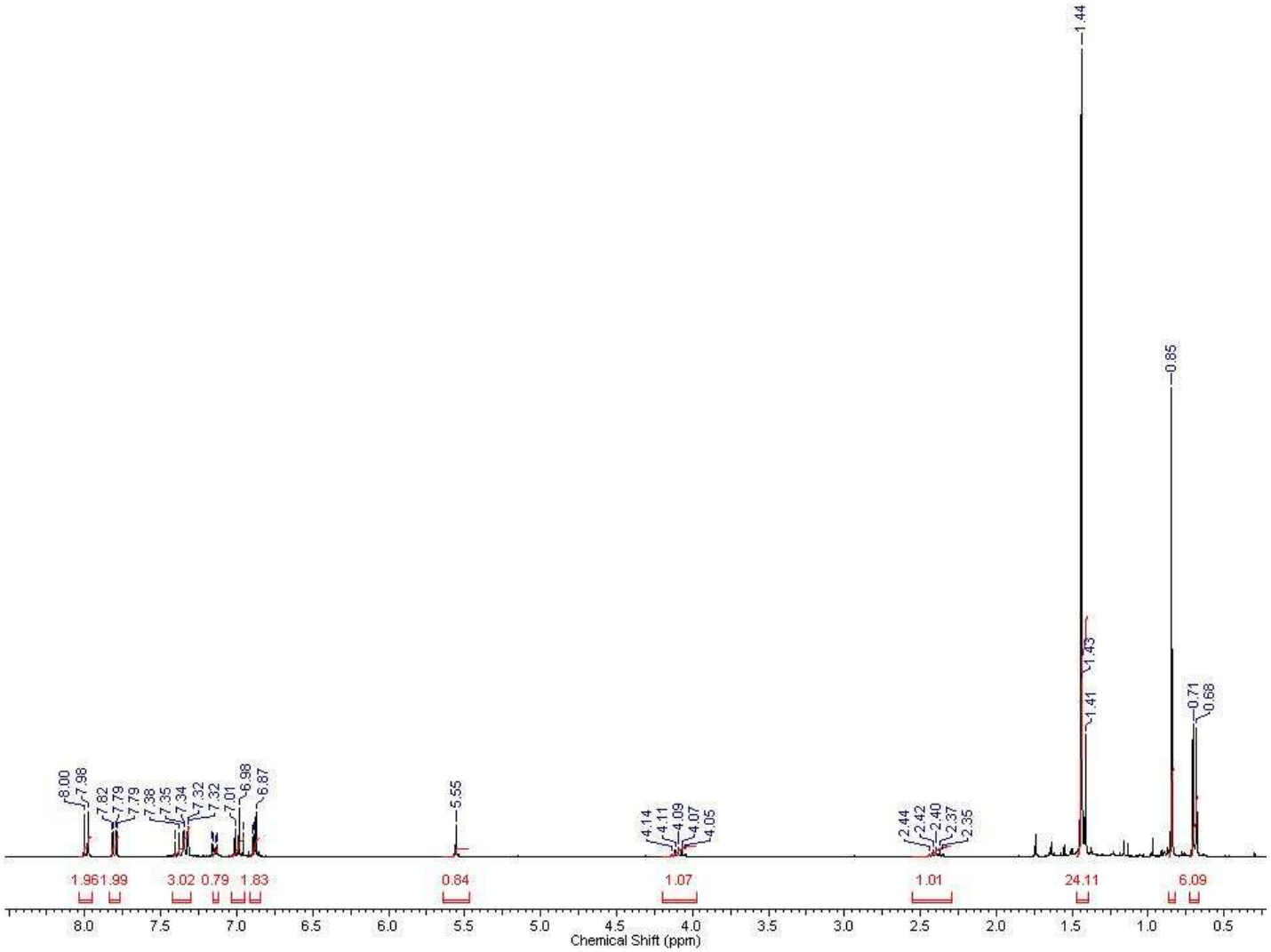

Figure S1. ^{1}H NMR spectrum of [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-C$_6$H$_3$-^{i}Pr$_2$) (**10**) in C$_6$D$_6$.

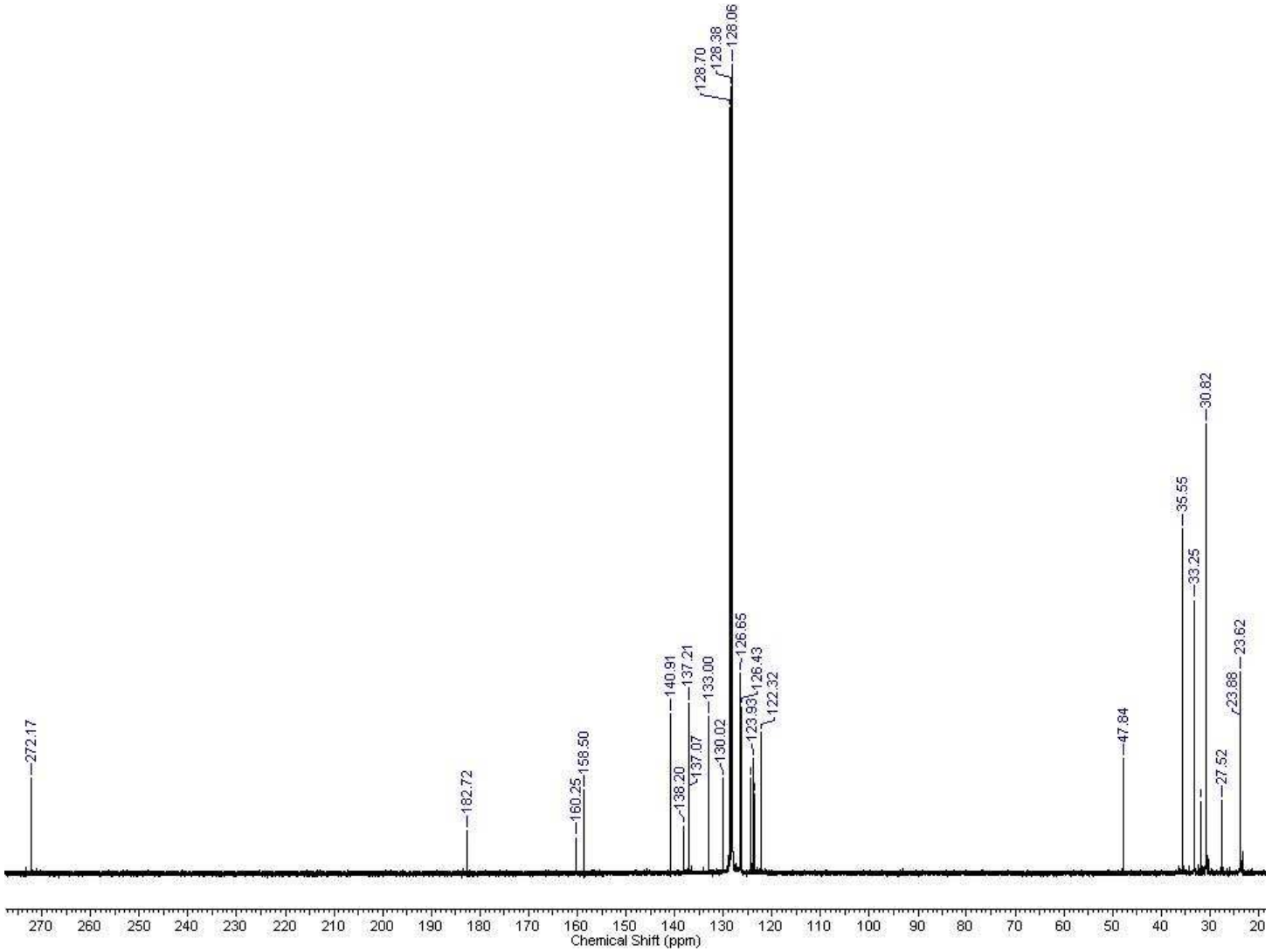

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-C$_6$H$_3$-^{i}Pr$_2$) (**10**) in C$_6$D$_6$.

Table S1. The assignment of the proton and carbon chemical shifts, given in Table S1, are based on the proton-proton and proton-carbon (both one-bond and long-range) couplings seen in the gDQCOSY, gHMQC and gHMBC spectra, correspondingly. The stereochemical discrimination between the two isopropyl groups was made on the nOe's seen in nOe difference experiment in which irradiation of H41 at 0.82 ppm produced an nOe at 4.06 ppm, assigned to H36. The NMR spectra of **10** were run in tolene-d_8 at 25 °C on a Varian Inova spectrometer, operating at 500 MHz for ^{1}H and at 125 MHz for ^{13}C. The probe was a 3-channel indirect detection, with z-axis gradients. Note: due to the higher resolution some of the resonances peak positions differ 300 MHz NMR spectrum in Figure S1 and S2.

Position	δ ^{1}H (ppm)	δ ^{13}C (ppm)	Carbons coupling to the protons in this position
1	-	159.7	
2	-	136.7	
3	7.30	126.0	1, 5, 25
4	6.96	121.7	2, 6
5	7.75	125.8	1, 3, 7
6	-	132.5	
7	-	140.4	
8	7.93	127.6	6, 8, 12
9	7.36	129.4	7
25	-	35.1	
26,27,28	1.41	30.3	2, 25, 26
19	-	157.9	
20	-	136.5	
21	6.83	123.2	19, 23, 33
22	6.86	123.8	20, 24
23	7.10	123.0	19, 21, 36
24	-	137.6	
33	2.36	31.1	
34,35	0.66	23.1	20, 33, 34
36	4.06	26.9	
37,38	1.40	23.3	24, 36, 37
39	5.50	271.5	40, 41
40	-	47.3	
41,42,43	0.82	32.7	39, 40, 41

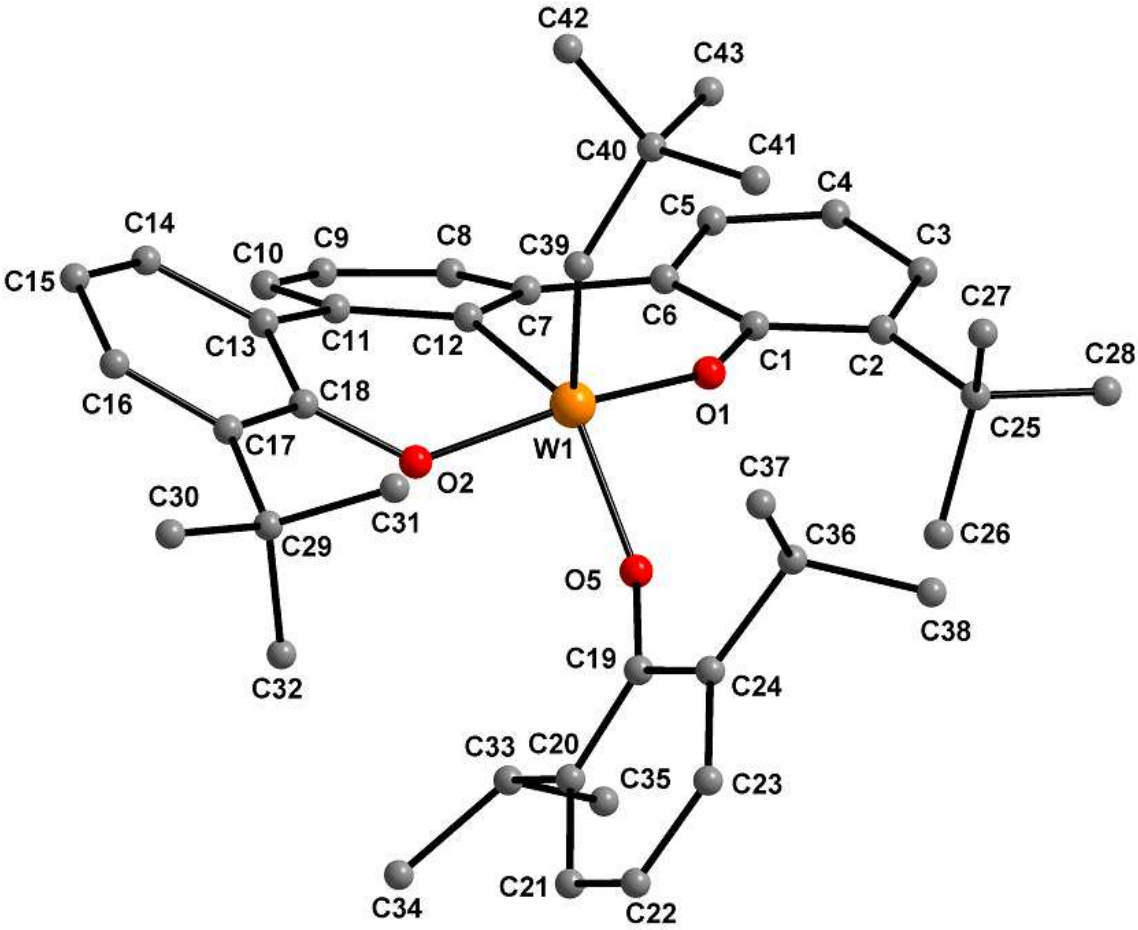

Figure S3. Molecular structure of **12**$_{therm}$ with complete labeling scheme to assign ^{1}H and ^{13}C NMR chemical shifts (refer Table S1).

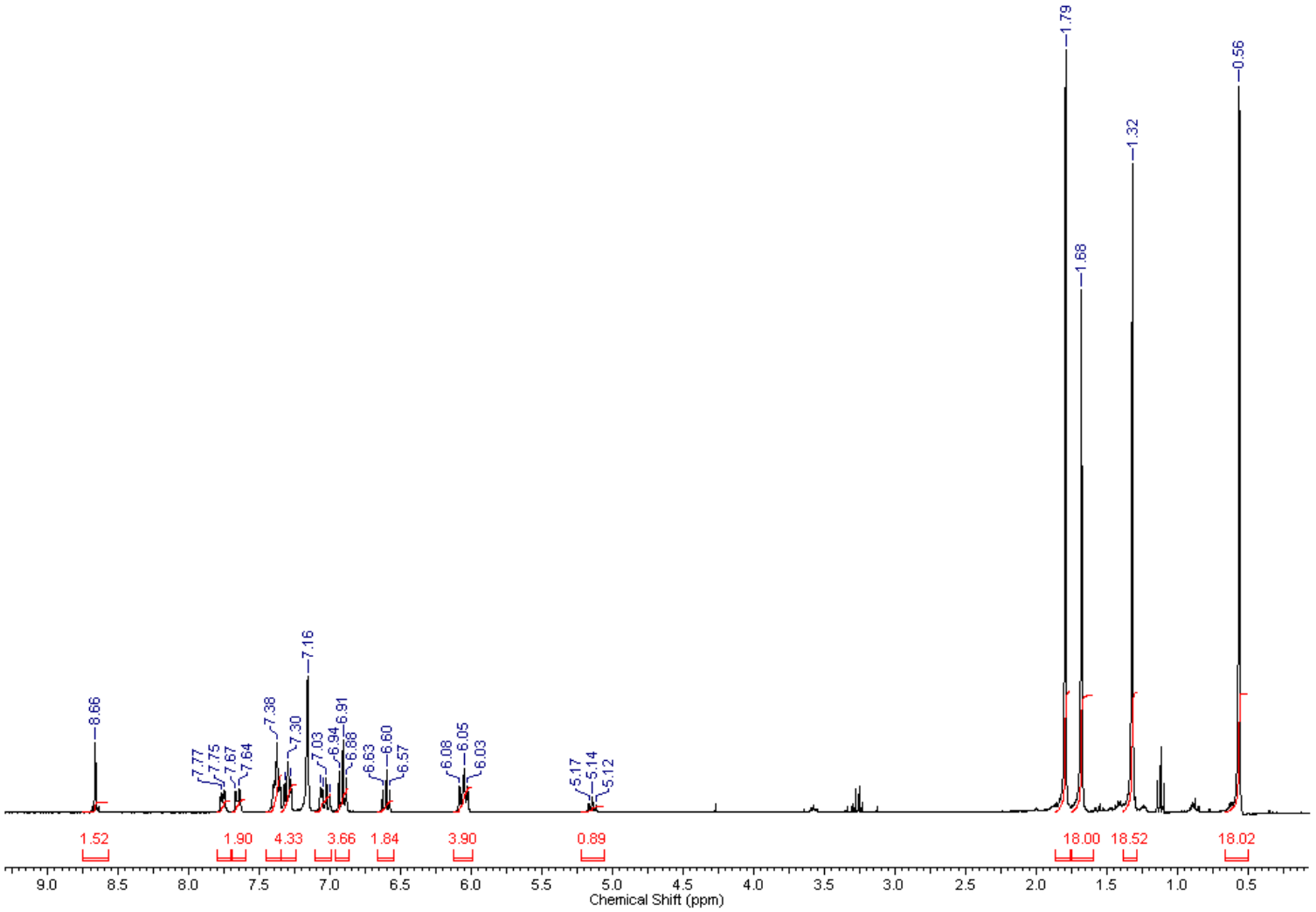

Figure S4. ^{1}H NMR spectrum of [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$(^{t}BuOCO)] (**12**$_{\boldsymbol{therm}}$) in C_6D_6.

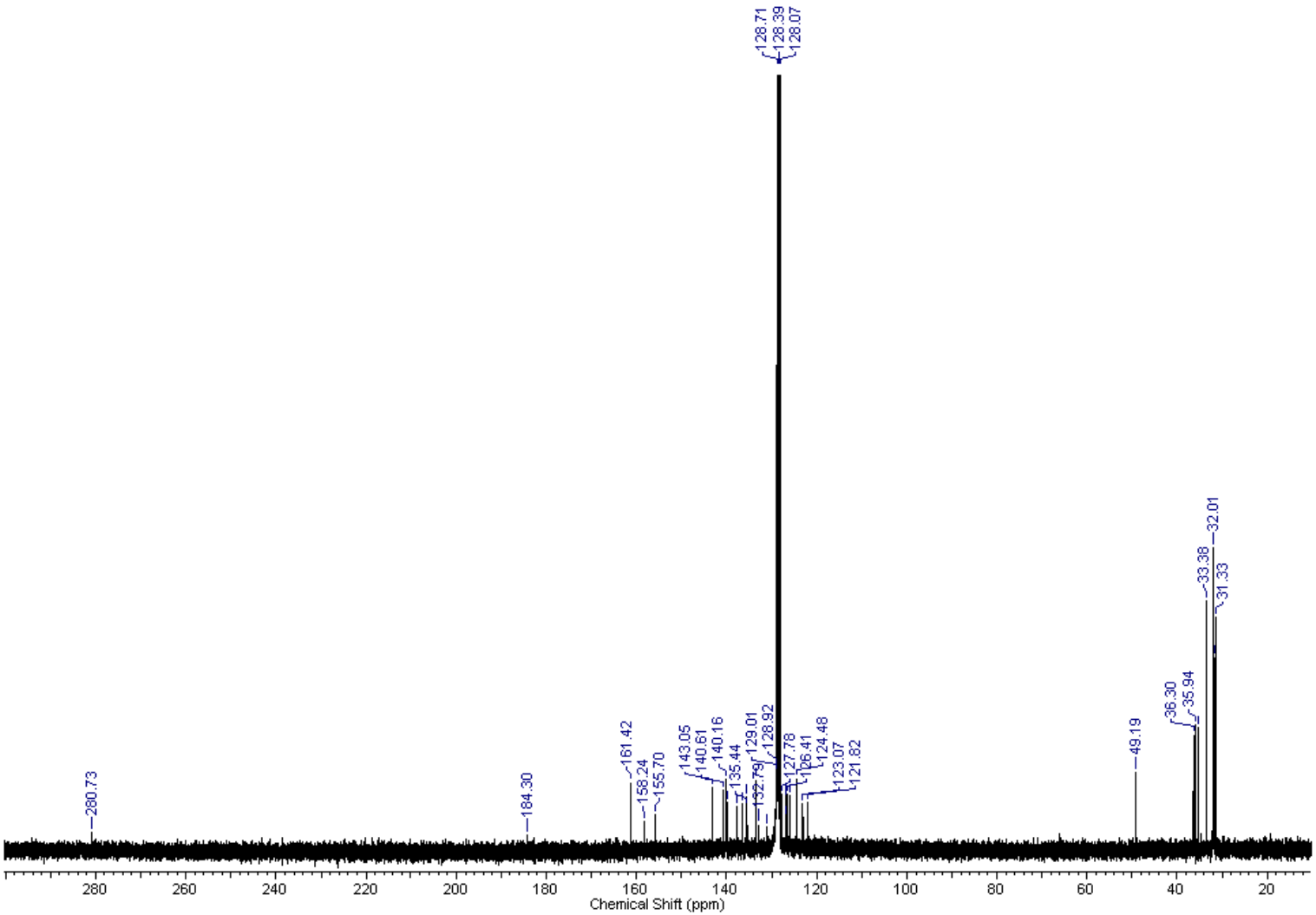

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$(^{t}BuOCO)] (**12**$_{\boldsymbol{therm}}$) in C_6D_6.

Table S2. The complete assignments of the ^{1}H and ^{13}C chemical shifts were made based on the ^{1}H-^{1}H and ^{1}H-^{13}C (one-bond and long-range) couplings seen in the DQCOSY, gHMQC and gHMBC spectra, correspondingly. The chemical shifts on the 'outer' ligands, the ones connected to just one of the W atoms, were assigned based on the nOes between H30 and H70-72 on one hand and between H26/H28 and H66-68 on the other. The NMR spectra of $\mathbf{12}_{\boldsymbol{therm}}$ were run in benzene-d_6 at 25 °C on a Varian Inova spectrometer, operating at 500 MHz for ^{1}H and at 125 MHz for ^{13}C. The probe was a 3-channel indirect detection, with z-axis gradients. Note: due to the higher resolution some of the resonances peak positions differ 300 MHz NMR spectrum in Figure S4 and S5.

Position	Alternate Position	δC	δH	Position	Alternate Position	δC	δH
1		155.2	-	20		139.7	-
2		137.1	-	21		126.3	7.33
3		125.4	7.27	22		121.3	6.57
4		124.0	6.88	23		128.5	6.00
5		126.4	7.62	24		132.9	-
6		135.2	-	25		142.6	-
7		139.5	-	26		124.0	6.04
8		126.5	7.73	27		130.4	5.11
9		127.6	6.99	30		132.3	7.03
10		127.7	7.35	55	60	280.2	8.63
11		140.1	-	56	61	48.7	-
12		183.8	-	57-59	62-64	32.9	0.53
13		134.9	-	65	77	35.4	-
14		127.3	7.36	66-68	78-80	31.2	1.64
15		122.6	6.88	69	73	34.9	-
16		125.9	7.26	70-72	74-76	30.8	1.28
17		136.0	-	81	85	35.8	-
18		157.7	-	82-84	86-88	31.5	1.76
19		160.9	-				

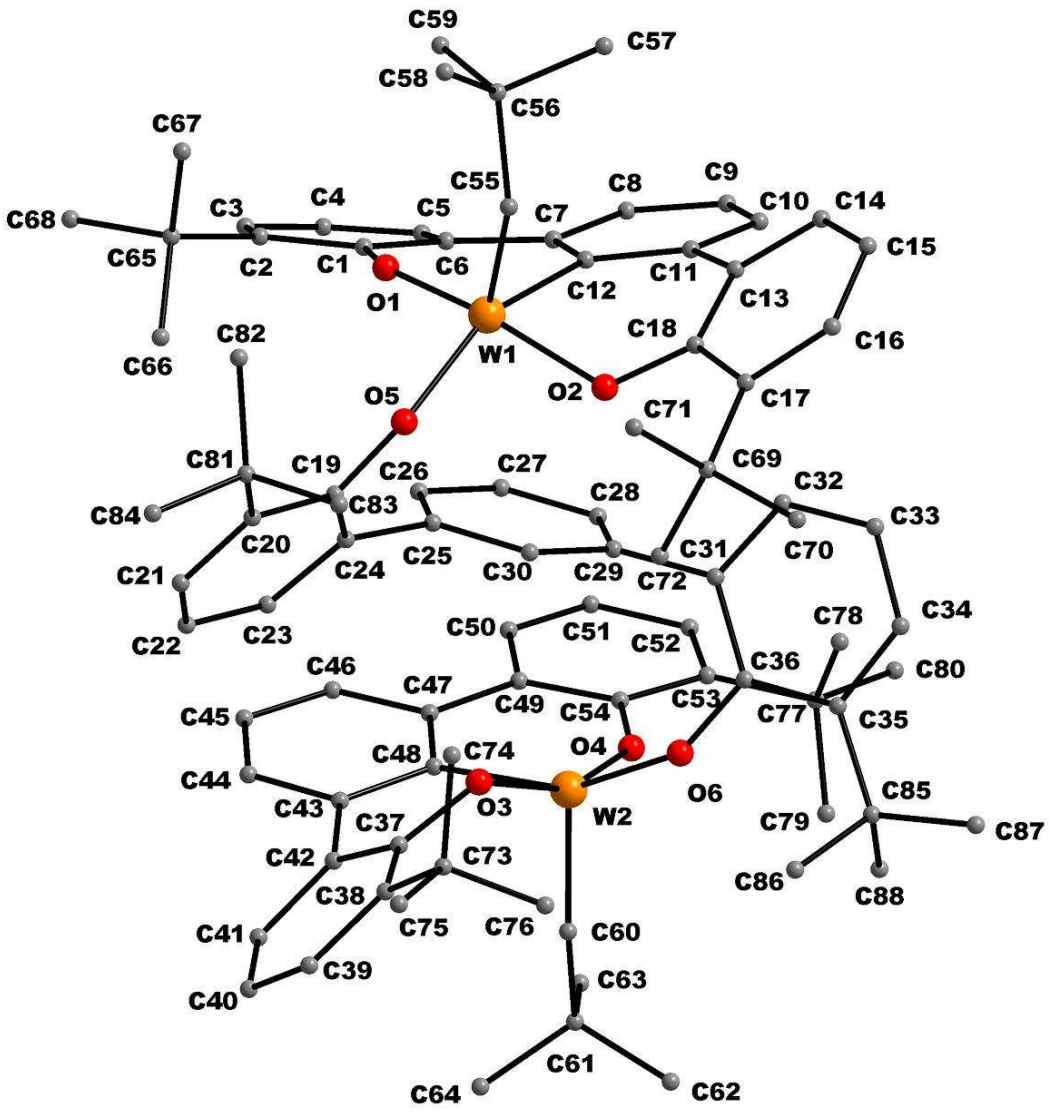

Figure S6. Molecular structure of **12**$_{therm}$ with complete labeling scheme to assign ^{1}H and ^{13}C NMR chemical shifts (refer Table S2).

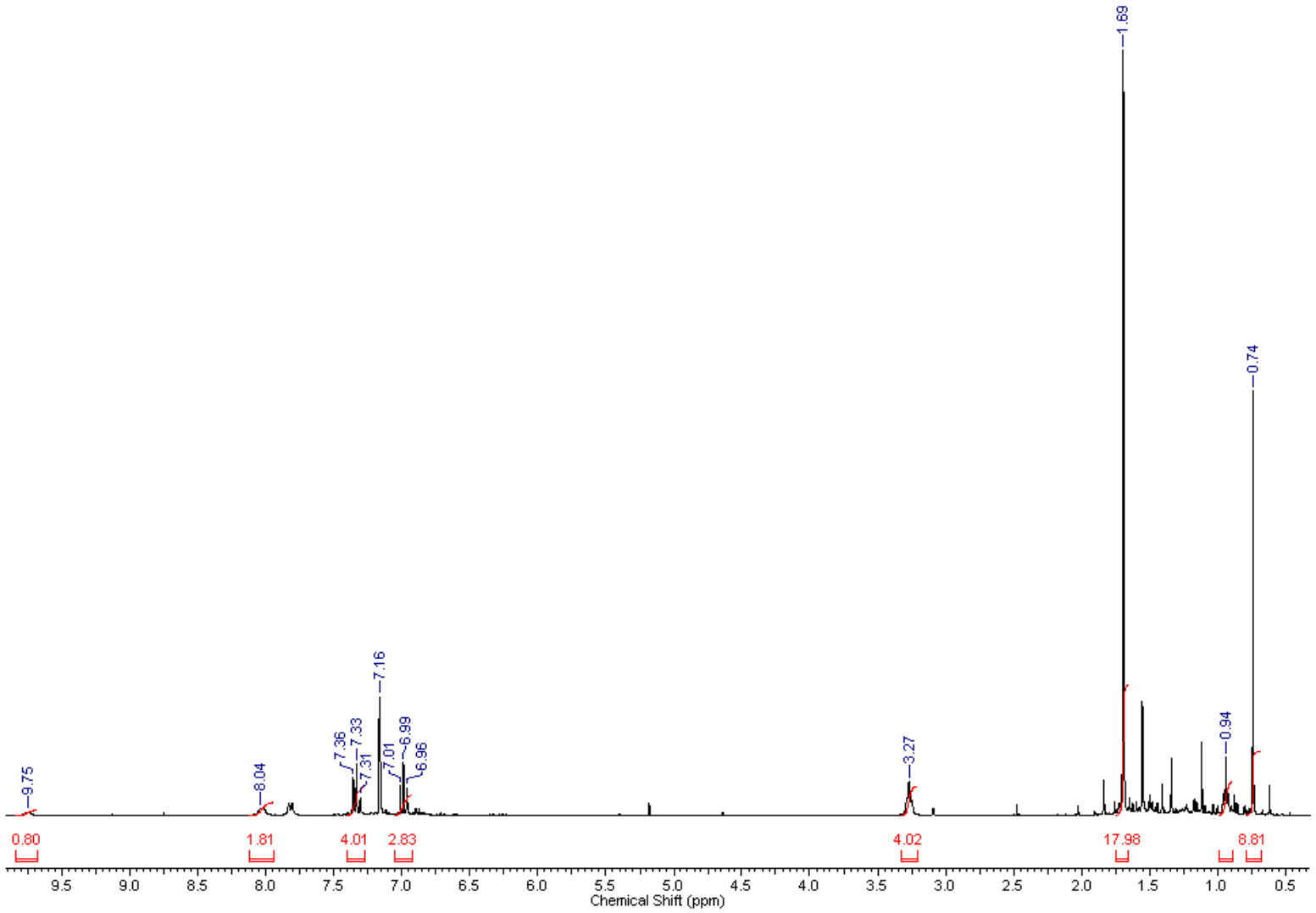

Figure S7. ^{1}H NMR spectrum of [^{t}BuOCHO]W≡CC(CH$_3$)$_3$Cl (**17**) as a mixture of **9** and **12**$_{kin}$ in C_6D_6.

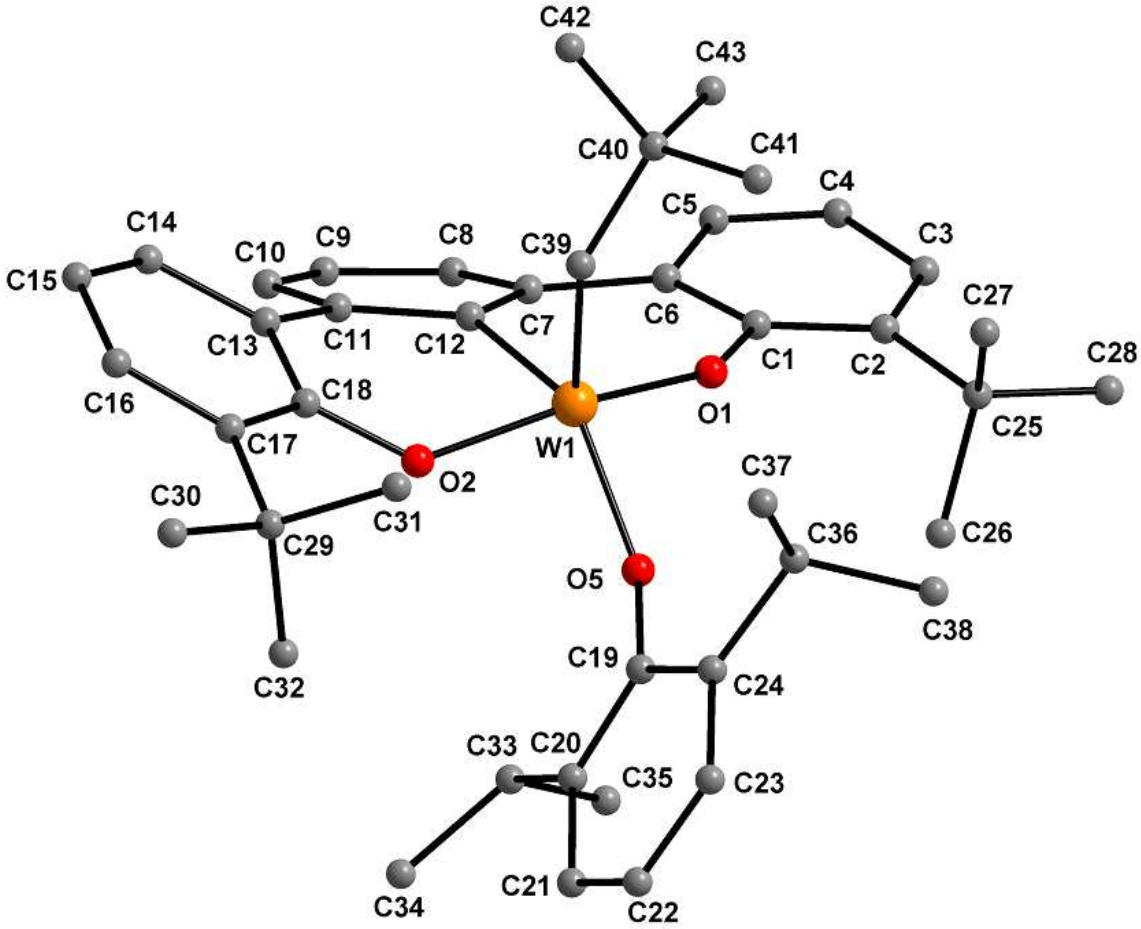

Figure S8. Molecular structure of [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-C$_6$H$_3$-^{i}Pr$_2$) (**10**).

X-ray Experimental for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(O-2,6-^{i}Pr$_2$C$_6$H$_3$) (10)

Data were collected at 173 K on a Siemens SMART PLATFORM equipped with A CCD area detector and a graphite monochromator utilizing MoK$_\alpha$ radiation (λ = 0.71073 Å). Cell parameters were refined using up to 8192 reflections. A full sphere of data (1850 frames) was collected using the ω-scan method (0.3° frame width). The first 50 frames were re-measured at the end of data collection to monitor instrument and crystal stability (maximum correction on I was < 1 %). Absorption corrections by integration were applied based on measured indexed crystal faces.

The structure was solved by the Direct Methods in *SHELXTL6,* and refined using full-matrix least squares. The non-H atoms were treated anisotropically, whereas the hydrogen atoms were calculated in ideal positions and were riding on their respective carbon atoms. A total of 847 parameters were refined in the final cycle of refinement using xxx reflections with I > 2σ(I) to yield R_1 and wR_2 of 5.20% and 12.04%, respectively. Refinement was done using F^2. The toluene molecule were disordered and could not be modeled properly, thus program SQUEEZE, a part of the PLATON package of crystallographic software, was used to calculate the solvent disorder area and remove its contribution to the overall intensity data.

P. van der Sluis & A.L. Spek (1990). SQUEEZE, Acta Cryst. A46, 194-201

SHELXTL6 (2000). Bruker-AXS, Madison, Wisconsin, USA.

Spek, A.L. (1990). PLATON, Acta Cryst. A46, C-34

Table S3. Crystal data, structure solution and refinement for [^{t}BuOCO]W=CHC(CH$_3$)$_3$ (O-2,6-^{i}Pr$_2$C$_6$H$_3$) (**10**).

identification code	pelo5t
empirical formula	$C_{43}H_{53}O_3W$
formula weight	801.70
T (K)	173(2) K
λ (Å)	0.71073 Å
crystal system	Monoclinic
space group	C(2)/c
a (Å)	39.001(2)
b (Å)	12.5405(8)
c (Å)	31.4372(19)
α (deg)	90
β (deg)	90.2150(10)
γ (deg)	90
V (Å^3)	15375.5(16)
Z	16
ρ_{calcd} (Mg mm^{-3})	1.385
crystal size (mm^3)	0.12 x 0.04 x 0.04
abs coeff (mm^{-1})	3.041
F(000)	6544
θ range for data collection	1.66 to 27.50
limiting indices	$-33 \le h \le 50$, $-16 \le k \le 16$, $-41 \le l \le 39$
no. of reflns collcd	51521
no. of ind reflns (R_{int})	17605 [R(int) = 0.0990]
completeness to θ = 27.50°	99.7 %
absorption corr	None
refinement method	Full-matrix least-squares on F^2
data / restraints / parameters	17605 / 0 / 847
$R1$,[a] $wR2$[b] [I > 2σ]	R1 = 0.0520, wR2 = 0.1204
$R1$,[a] $wR2$[b] (all data)	R1 = 0.1104, wR2 = 0.1351
GOF[c] on F^2	0.965
largest diff. peak and hole	1.308 and -1.282

$R1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$ $\quad wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w = 1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [^{t}BuOCO]W=CHC(CH_3)$_3$(O-2,6-^{i}Pr$_2$C$_6$H$_3$) (**10**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	X	Y	Z	U(eq)
W1	1336(1)	5376(1)	2116(1)	28(1)
W2	1408(1)	10030(1)	4354(1)	27(1)
O1	1147(1)	6692(4)	2212(2)	34(1)
O2	1503(1)	3986(4)	2200(2)	31(1)
O3	1261(1)	11398(4)	4261(2)	32(1)
O4	1536(1)	8566(4)	4251(2)	32(1)
O5	886(1)	4727(4)	2048(2)	36(1)
O6	946(1)	9499(4)	4432(2)	36(1)
C1	1148(2)	7618(6)	2445(3)	31(2)
C2	911(2)	8406(7)	2348(3)	43(2)
C3	944(2)	9353(7)	2580(3)	52(3)
C4	1207(3)	9460(8)	2879(3)	58(3)
C5	1414(3)	8647(7)	2978(3)	51(3)
C6	1393(2)	7663(7)	2764(3)	37(2)
C7	1618(2)	6735(6)	2880(2)	32(2)
C8	1773(2)	6819(7)	3285(3)	42(2)
C9	2003(2)	6065(8)	3427(3)	47(2)
C10	2094(2)	5230(7)	3164(3)	43(2)
C11	1935(2)	5086(7)	2770(2)	33(2)
C12	1681(2)	5813(6)	2626(2)	32(2)
C13	2048(2)	4151(7)	2523(3)	41(2)
C14	2389(2)	3733(8)	2566(3)	47(2)
C15	2492(2)	2839(8)	2364(3)	50(3)
C16	2257(2)	2271(7)	2109(3)	45(2)
C17	1919(2)	2620(7)	2050(3)	37(2)
C18	1823(2)	3590(6)	2252(3)	33(2)
C19	687(2)	3955(6)	1907(3)	33(2)
C20	581(2)	3176(7)	2205(3)	35(2)
C21	376(2)	2328(6)	2054(3)	40(2)
C22	275(2)	2273(7)	1637(3)	45(2)
C23	362(2)	3057(7)	1349(3)	45(2)
C24	575(2)	3917(6)	1479(3)	35(2)

C25	621(2)	8260(7)	2028(3)	48(2)
C26	403(2)	7313(9)	2164(3)	71(3)
C27	754(3)	8115(8)	1583(3)	60(3)
C28	392(3)	9247(9)	2030(4)	96(5)
C29	1664(2)	1974(7)	1781(3)	46(2)
C30	1834(3)	964(7)	1594(3)	64(3)
C31	1526(3)	2626(7)	1397(3)	54(3)
C32	1367(2)	1627(7)	2050(3)	57(3)
C33	670(2)	3313(6)	2668(3)	35(2)
C34	667(2)	2272(7)	2928(3)	52(3)
C35	443(2)	4157(7)	2879(3)	45(2)
C36	663(2)	4793(7)	1166(3)	40(2)
C37	850(3)	4389(8)	775(3)	69(3)
C38	347(3)	5453(9)	1048(4)	84(4)
C39	1626(2)	5649(7)	1639(2)	35(2)
C41	1505(3)	6602(8)	974(3)	65(3)
C42	2103(3)	6364(9)	1219(4)	81(4)
C43	1742(3)	7624(7)	1602(3)	52(3)
C44	1266(2)	12258(6)	3996(3)	29(2)
C45	1041(2)	13102(7)	4080(3)	35(2)
C46	1071(2)	13992(7)	3816(3)	42(2)
C47	1307(2)	14020(6)	3504(3)	39(2)
C49	1505(2)	12240(6)	3667(2)	34(2)
C50	1736(2)	11316(6)	3587(2)	32(2)
C52	2163(2)	10575(7)	3107(3)	44(2)
C53	2219(2)	9731(7)	3387(3)	40(2)
C54	2022(2)	9635(6)	3757(2)	30(2)
C55	1762(2)	10384(6)	3860(2)	31(2)
C56	2109(2)	8714(6)	4037(2)	30(2)
C57	2450(2)	8345(7)	4073(3)	38(2)
C58	2526(2)	7480(7)	4317(3)	40(2)
C59	2265(2)	6951(7)	4538(3)	40(2)
C60	1926(2)	7245(6)	4514(2)	31(2)
C61	1865(2)	8170(6)	4270(2)	31(2)
C62	731(2)	8742(6)	4575(3)	38(2)

C63	608(2)	7980(7)	4289(3)	39(2)
C64	392(2)	7185(8)	4441(3)	54(3)
C65	297(3)	7194(9)	4863(4)	66(3)
C66	403(2)	7982(8)	5140(3)	55(3)
C68	753(2)	13023(7)	4416(3)	44(2)
C69	520(2)	12072(7)	4313(3)	56(3)
C70	904(2)	12905(7)	4866(3)	50(2)
C71	520(2)	14025(8)	4404(4)	70(3)
C72	1652(2)	6617(7)	4740(3)	38(2)
C73	1383(2)	6228(7)	4410(3)	48(2)
C74	1467(2)	7290(7)	5080(3)	44(2)
C75	1785(2)	5628(7)	4956(3)	57(3)
C76	696(2)	8059(8)	3825(3)	54(3)
C77	468(3)	8952(10)	3629(3)	84(4)
C78	655(3)	7047(9)	3566(3)	77(4)
C79	721(2)	9686(8)	5296(3)	50(2)
C80	923(3)	9302(9)	5679(3)	81(4)
C81	412(3)	10319(9)	5448(4)	81(4)
C82	1730(2)	10171(6)	4804(2)	33(2)
C83	1959(2)	10981(6)	5021(3)	37(2)
C84	1850(2)	12128(7)	4901(3)	53(3)
C85	2322(2)	10779(8)	4861(4)	67(3)
C86	1942(3)	10823(8)	5496(3)	75(4)

Table S5. Bond lengths (in Å) for [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-^{i}Pr$_2$-C$_6$H$_3$) (**10**).

Bond	Length	Bond	Length
W1-O1	1.834(5)	W1-O2	1.880(5)
W1-O5	1.945(5)	W2-O3	1.833(5)
W2-O4	1.931(5)	W2-O6	1.937(5)
W1-C12	2.162(8)	W1-C39	1.913(8)
W2-C55	2.128(8)	W2-C82	1.895(8)
O1-C1	1.373(9)	O3-C44	1.363(9)
O4-C61	1.376(9)	O5-C19	1.315(9)
C1-C2	1.386(11)	C2-C3	1.398(12)
C2-C25	1.521(12)	C4-C3	1.397(12)
C5-C4	1.336(13)	C6-C1	1.385(10)
C6-C5	1.408(11)	C6-C7	1.500(11)
C8-C7	1.412(10)	C8-C9	1.376(12)
C10-C9	1.382(12)	C10-C11	1.396(10)
C12-C7	1.428(11)	C12-C11	1.418(11)
C13-C11	1.476(12)	C13-C14	1.433(11)
C14-C15	1.351(12)	C16-C15	1.410(12)
C17-C16	1.401(11)	C17-C18	1.424(11)
C17-C29	1.536(12)	C18-O2	1.352(9)
C18-C13	1.409(11)	C19-C24	1.415(11)
C20-C19	1.417(11)	C20-C21	1.411(11)
C20-C33	1.506(11)	C21-C22	1.370(11)
C23-C22	1.379(12)	C23-C24	1.419(11)
C25-C26	1.523(13)	C25-C27	1.504(13)
C25-C28	1.528(13)	C29-C32	1.502(12)
C29-C30	1.546(12)	C31-C29	1.553(12)
C33-C34	1.541(11)	C33-C35	1.531(11)
C36-C24	1.515(11)	C36-C37	1.520(12)
C36-C38	1.529(12)	C39-C40	1.505(11)
C40-C41	1.550(12)	C40-C42	1.493(12)
C43-C40	1.522(12)	C45-C44	1.401(11)
C45-C46	1.398(11)	C45-C68	1.546(12)
C46-C47	1.349(11)	C48-C47	1.388(11)

C49-C44	1.395(11)	C49-C48	1.401(11)
C49-C50	1.490(11)	C50-C51	1.415(11)
C51-C52	1.370(11)	C53-C52	1.392(11)
C54-C53	1.404(11)	C55-C50	1.454(10)
C55-C54	1.419(11)	C56-C54	1.492(11)
C56-C57	1.411(11)	C56-C61	1.385(11)
C57-C58	1.361(11)	C59-C58	1.399(11)
C59-C60	1.376(11)	C61-C60	1.409(11)
C62-O6	1.345(9)	C62-C63	1.398(11)
C62-C67	1.395(12)	C63-C76	1.504(12)
C64-C63	1.391(12)	C64-C65	1.376(14)
C65-C66	1.380(14)	C67-C66	1.400(12)
C67-C79	1.515(12)	C68-C69	1.533(12)
C68-C70	1.536(12)	C68-C71	1.552(12)
C72-C60	1.508(11)	C72-C73	1.553(10)
C74-C72	1.543(12)	C75-C72	1.504(11)
C77-C76	1.556(13)	C78-C76	1.515(13)
C79-C80	1.515(12)	C79-C81	1.520(13)
C82-C83	1.512(10)	C83-C86	1.509(12)
C84-C83	1.545(11)	C85-H83	1.527(12)

Table S6. Bond angles (in deg) for [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-^{i}Pr$_2$-C$_6$H$_3$) (**10**).

Bond	Angle	Bond	Angle
O1-W1-O2	162.0(2)	O1-W1-O5	91.8(2)
O1-W1-C39	102.0(3)	O1-W1-C12	84.2(3)
O2-W1-C39	94.0(3)	O2-W1-O5	86.6(2)
O2-W1-C12	85.1(3)	O3-W2-O6	92.9(2)
O3-W2-C82	103.8(3)	O5-W1-C12	138.3(3)
C39-W1-O5	121.7(3)	C39-W1-C12	99.5(3)
O3-W2-O4	160.8(2)	O3-W2-C55	83.8(3)
O4-W2-C55	84.7(3)	O6-W2-O4	86.3(2)
O6-W2-C55	140.3(2)	C82-W2-O4	92.4(3)
C82-W2-O6	123.5(3)	C82-W2-C55	95.4(3)
C1-C6-C5	114.9(8)	C1-C6-C7	123.1(7)
C1-O1-W1	148.1(5)	C7-C12-W1	120.8(5)
C11-C12-W1	120.4(6)	C19-O5-W1	151.0(5)
C44-O3-W2	146.4(5)	C50-C55-W2	123.8(6)
C54-C55-W2	119.6(5)	C61-O4-W2	125.3(4)
O1-C1-C2	119.1(7)	O1-C1-C6	114.9(7)
O2-C18-C13	117.6(7)	O2-C18-C17	120.2(7)
O3-C44-C45	118.1(7)	O3-C44-C49	116.9(7)
O4-C61-C56	116.2(7)	O4-C61-C60	118.5(7)
O5-C19-C20	117.4(7)	O5-C19-C24	121.6(7)
O6-C62-C63	118.7(8)	O6-C62-C67	118.7(8)
C1-C2-C3	115.6(8)	C1-C2-C25	123.5(8)
C2-C1-C6	126.0(8)	C2-C3-C4	119.9(9)
C2-C25-C26	108.8(8)	C2-C25-C28	109.5(8)
C3-C2-C25	120.9(8)	C4-C5-C6	121.6(9)
C5-C6-C7	122.0(8)	C5-C4-C3	121.7(9)
C8-C9-C10	119.8(8)	C8-C7-C6	114.2(7)
C8-C7-C12	119.4(7)	C9-C8-C7	121.1(8)
C9-C10-C11	120.9(8)	C10-C11-C12	120.6(8)
C10-C11-C13	115.8(8)	C11-C12-C7	117.6(7)
C12-C7-C6	126.4(7)	C12-C11-C13	123.6(7)

C13-C18-C17	122.2(8)	C14-C15-C16	119.4(8)
C14-C13-C11	121.4(8)	C15-C14-C13	122.6(9)
C16-C17-C18	117.2(8)	C16-C17-C29	121.0(8)
C17-C29-C30	111.3(8)	C17-C29-C31	111.9(7)
C17-C16-C15	121.8(8)	C18-C17-C29	121.8(7)
C18-C13-C11	121.8(8)	C18-C13-C14	116.7(9)
C18-O2-W1	132.6(5)	C19-C20-C33	119.5(7)
C19-C24-C23	118.5(8)	C19-C24-C36	121.6(7)
C20-C33-C34	114.5(7)	C20-C33-C35	111.4(6)
C21-C20-C19	117.7(8)	C21-C20-C33	122.6(8)
C21-C22-C23	121.4(8)	C22-C23-C24	119.9(8)
C22-C21-C20	121.3(9)	C23-C24-C36	119.9(7)
C24-C36-C37	113.2(8)	C24-C36-C38	111.4(8)
C24-C19-C20	121.0(7)	C26-C25-C28	107.6(9)
C27-C25-C2	111.9(8)	C27-C25-C26	111.2(8)
C27-C25-C28	107.7(9)	C31-C29-C30	106.5(8)
C32-C29-C17	110.0(8)	C32-C29-C30	108.1(8)
C32-C29-C31	109.0(8)	C35-C33-C34	110.6(7)
C37-C36-C38	111.9(8)	C39-C40-C41	106.8(7)
C39-C40-C43	112.8(8)	C51-C52-C53	119.8(8)
C39-C40-C41	106.8(7)	C39-C40-C43	112.8(8)
C42-C40-C39	109.9(7)	C42-C40-C41	108.7(9)
C42-C40-C43	107.9(8)	C43-C40-C41	110.7(7)
C42-C40-C39	109.9(7)	C42-C40-C41	108.7(9)
C42-C40-C43	107.9(8)	C43-C40-C41	110.7(7)
C44-C49-C48	115.6(8)	C44-C49-C50	123.0(7)
C44-C45-C46	115.9(8)	C44-C45-C68	122.5(7)
C45-C68-C71	111.0(7)	C45-C68-C69	109.7(8)
C46-C47-C48	122.3(8)	C46-C45-C68	121.4(8)
C47-C48-C49	120.2(8)	C47-C46-C45	120.9(9)
C48-C49-C50	121.3(8)	C49-C44-C45	125.0(7)
C51-C50-C49	116.3(7)	C51-C50-C55	119.2(7)
C52-C51-C50	122.0(8)	C52-C53-C54	120.2(8)
C53-C54-C55	121.9(7)	C53-C54-C56	115.4(7)
C54-C55-C50	116.3(7)	C55-C54-C56	122.7(7)

C55-C50-C49	124.4(7)	C56-C61-C60	125.3(8)
C57-C58-C59	120.1(8)	C57-C56-C54	121.0(7)
C58-C57-C56	120.6(8)	C59-C60-C61	114.3(7)
C59-C60-C72	121.1(7)	C60-C59-C58	123.0(8)
C60-C72-C73	109.0(7)	C60-C72-C74	112.0(7)
C60-C72-C75	113.6(7)	C61-C56-C57	116.4(7)
C61-C60-C72	124.6(7)	C61-C56-C54	122.5(7)
C62-C63-C64	118.4(9)	C62-C63-C76	120.0(8)
C62-C67-C66	117.7(8)	C62-C67-C79	122.9(8)
C63-C76-C77	107.3(8)	C63-C76-C78	116.2(9)
C64-C63-C76	121.6(8)	C64-C65-C66	122.3(10)
C65-C64-C63	119.4(9)	C66-C67-C79	119.4(9)
C67-C66-C65	119.7(9)	C67-C79-C80	112.7(8)
C67-C79-C81	112.7(8)	C67-C62-C63	122.4(8)
C70-C68-C45	111.1(7)	C70-C68-C71	108.8(8)
C70-C68-C69	110.1(8)	C71-C68-C69	106.1(7)
C74-C72-C73	108.6(7)	C75-C72-C73	105.9(7)
C75-C72-C74	107.4(7)	C78-C76-C77	109.4(8)
C80-C79-C81	108.9(8)	C82-C83-C84	110.8(6)
C82-C83-C85	106.6(7)	C85-C83-C84	109.2(8)
C86-C83-C82	109.4(7)	C86-C83-C84	110.5(8)
C86-C83-C85	110.3(8)		

Table S7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [^{t}BuOCO]W(=CHC(CH$_3$)$_3$)(O-2,6-^{i}Pr$_2$-C$_6$H$_3$) (**10**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W1	28(1)	32(1)	24(1)	0(1)	-2(1)	-3(1)
W2	24(1)	33(1)	24(1)	3(1)	1(1)	-3(1)
C39	26(5)	50(5)	30(5)	5(4)	-13(4)	-24(4)
O3	29(3)	37(3)	32(3)	4(3)	0(2)	8(2)
O5	28(3)	36(3)	44(3)	1(3)	-5(3)	-4(3)
O1	30(3)	35(3)	36(3)	-5(3)	-3(3)	-5(2)
C82	47(5)	22(5)	30(4)	-1(3)	5(4)	-5(4)
O4	30(3)	33(3)	35(3)	-4(2)	6(2)	1(2)
C55	42(5)	30(4)	22(4)	3(4)	-5(3)	-7(4)
C56	27(5)	36(5)	26(4)	-5(4)	-6(4)	0(4)
C17	35(5)	49(6)	27(5)	2(4)	6(4)	-8(4)
C45	32(5)	42(5)	32(5)	-1(4)	5(4)	-16(4)
C16	34(6)	55(6)	48(6)	15(5)	16(4)	32(5)
C20	11(4)	52(6)	42(5)	-12(4)	-1(4)	-4(4)
C49	38(5)	42(5)	24(4)	4(4)	2(4)	-12(4)
C50	23(5)	44(5)	29(5)	8(4)	-2(4)	7(4)
C18	31(5)	39(5)	30(5)	7(4)	1(4)	-10(4)
C54	26(4)	41(5)	23(4)	-5(4)	2(3)	-3(4)
C19	21(4)	33(5)	44(5)	-3(4)	9(4)	6(4)
C12	29(5)	39(5)	28(4)	6(4)	9(4)	-6(4)
C6	29(5)	48(5)	34(5)	-7(4)	5(4)	-18(4)
C46	37(6)	53(6)	37(5)	4(4)	2(4)	-1(4)
C21	41(6)	34(5)	45(6)	-2(4)	3(4)	7(4)
C62	29(5)	28(5)	56(6)	13(4)	1(4)	-8(4)
C44	16(4)	33(5)	38(5)	4(4)	-15(4)	-7(3)
C43	67(7)	42(6)	47(6)	9(5)	7(5)	-16(5)
C1	21(4)	37(5)	36(5)	-6(4)	9(4)	-3(4)
C36	20(4)	61(6)	41(5)	-1(4)	-15(4)	-3(4)
C74	33(5)	60(6)	38(5)	5(5)	-1(4)	0(4)
C61	30(5)	30(5)	32(5)	-5(4)	2(4)	-1(4)
C53	39(5)	53(6)	29(5)	-5(4)	-1(4)	-3(4)

C23	27(5)	62(6)	45(6)	-14(5)	-6(4)	-17(4)
C40	40(6)	40(5)	43(6)	10(4)	1(4)	-4(4)
C67	31(5)	56(6)	36(5)	10(4)	-1(4)	6(4)
C48	36(5)	43(5)	38(5)	5(4)	6(4)	-14(4)
C51	44(6)	40(5)	39(5)	15(4)	6(4)	10(4)
C8	43(6)	50(6)	33(5)	4(4)	-5(4)	-5(4)
C47	44(6)	27(5)	46(6)	1(4)	-8(4)	-10(4)
C57	40(6)	41(5)	34(5)	-2(4)	8(4)	-6(4)
C59	43(6)	39(5)	38(5)	-4(4)	1(4)	1(4)
C58	18(5)	57(6)	44(6)	-10(5)	-10(4)	-7(4)
C10	36(5)	63(7)	31(5)	9(4)	-7(4)	-18(4)
C13	46(6)	43(5)	34(5)	19(4)	10(4)	-3(4)
C5	59(7)	44(6)	49(6)	-6(5)	0(5)	-4(5)
C2	46(6)	44(6)	39(5)	-3(4)	6(4)	1(4)
C7	21(4)	44(5)	31(5)	5(4)	-5(4)	-1(4)
C4	68(8)	42(6)	65(7)	-21(5)	6(6)	-19(5)
C33	22(5)	37(5)	46(5)	0(4)	-11(4)	-9(4)
C11	28(5)	44(5)	28(4)	4(4)	4(3)	-18(4)
C85	21(5)	64(7)	116(10)	-17(7)	-11(6)	0(5)
C68	30(5)	43(5)	59(6)	12(5)	8(4)	11(4)
C31	67(7)	40(6)	54(7)	-6(5)	-10(5)	-10(5)
C9	47(6)	67(7)	28(5)	-4(5)	-9(4)	-24(5)
C84	53(7)	41(5)	66(7)	-17(5)	-26(5)	-11(5)
C69	30(6)	62(7)	76(8)	11(6)	4(5)	7(5)
C52	34(5)	71(7)	26(5)	0(4)	3(4)	-7(5)
C29	47(6)	34(5)	56(6)	1(4)	15(5)	7(4)
C75	41(6)	53(6)	75(7)	21(5)	-2(5)	-8(5)
C41	97(9)	60(7)	39(6)	19(5)	5(6)	0(6)
C64	31(6)	64(7)	65(7)	0(6)	3(5)	-14(5)
C71	47(7)	64(7)	99(9)	20(6)	30(6)	10(5)
C79	47(6)	65(7)	39(5)	1(5)	6(4)	-1(5)
C72	27(5)	44(5)	43(5)	8(4)	-13(4)	-8(4)
C35	48(6)	44(5)	44(6)	0(4)	0(4)	12(5)
C63	34(5)	46(5)	37(5)	8(4)	-1(4)	-4(4)
C22	48(6)	34(5)	54(6)	-15(5)	10(5)	-11(4)

C83	31(5)	43(5)	36(5)	-10(4)	-11(4)	0(4)
C60	30(5)	33(5)	30(5)	-2(4)	-1(4)	-7(4)
C37	85(9)	70(8)	51(7)	8(6)	21(6)	6(6)
C25	38(6)	43(6)	63(7)	-7(5)	-12(5)	-7(4)
C24	16(4)	45(5)	44(5)	3(4)	-10(4)	8(4)
C65	57(8)	65(8)	77(9)	24(6)	10(6)	-14(6)
C78	59(8)	120(10)	53(7)	-24(7)	-6(6)	-38(7)
C73	38(6)	43(5)	64(7)	1(5)	-1(5)	-17(4)
C26	29(6)	108(10)	75(8)	-17(7)	-10(6)	1(6)
C27	66(8)	61(7)	54(7)	6(5)	-29(6)	4(5)
C3	50(6)	47(6)	58(7)	-8(5)	5(5)	2(5)
C32	59(7)	34(5)	79(8)	0(5)	18(6)	-6(5)
C30	76(8)	42(6)	73(8)	-6(5)	2(6)	11(5)
C77	80(9)	125(11)	46(7)	22(7)	-13(6)	12(8)
C76	32(6)	78(7)	52(6)	8(5)	-12(5)	6(5)
C14	18(5)	75(7)	49(6)	23(5)	2(4)	10(4)
C15	29(5)	70(7)	51(6)	18(5)	3(5)	9(5)
C42	60(8)	72(8)	111(10)	42(7)	43(7)	13(6)
C66	48(7)	68(7)	48(6)	15(5)	13(5)	-10(5)
C38	98(10)	64(8)	91(9)	12(7)	-13(8)	14(7)
C70	44(6)	58(6)	47(6)	2(5)	17(5)	-1(5)
C34	54(7)	50(6)	53(6)	5(5)	7(5)	-5(5)
C80	87(9)	87(9)	69(8)	-14(7)	-15(7)	31(7)
C28	67(8)	82(9)	139(12)	-49(8)	-37(8)	28(7)
C86	130(11)	53(6)	42(6)	-7(5)	-27(6)	-26(7)
C81	87(9)	85(9)	72(8)	-17(7)	-8(7)	31(7)
O2	17(3)	42(3)	34(3)	-6(3)	-6(2)	2(2)
O6	27(3)	45(3)	35(3)	6(3)	-4(2)	-11(3)

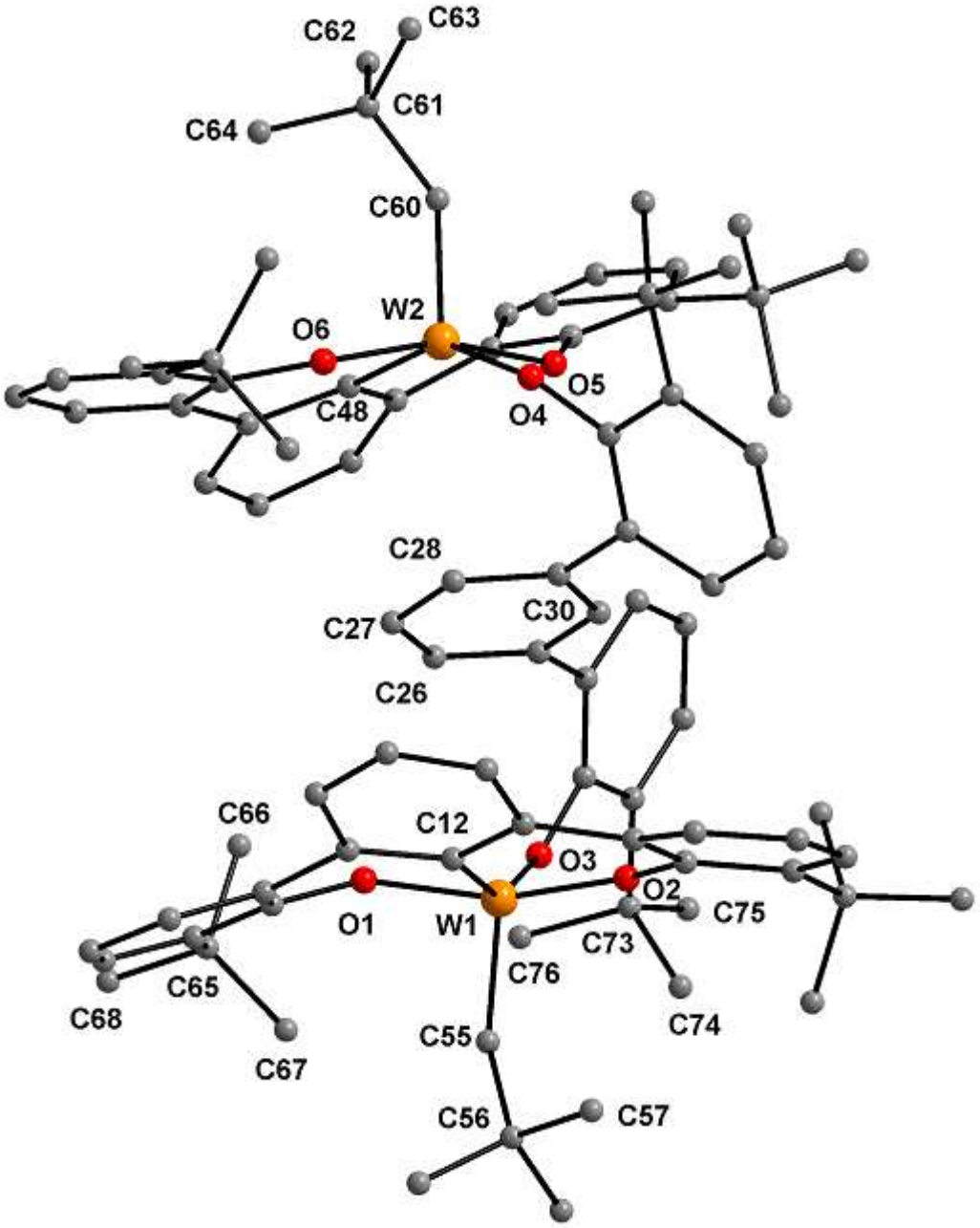

Figure S9. Molecular structure of [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$(^{t}BuOCO)] (**12**$_{kin}$).

X-ray Experimental for [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$ [^{t}BuOCO]} (12$_{kin}$)

Data were collected at 173 K on a Siemens SMART PLATFORM equipped with A CCD area detector and a graphite monochromator utilizing MoKα radiation (λ = 0.71073 Å). Cell parameters were refined using up to 8192 reflections. A full sphere of data (1850 frames) was collected using the ω-scan method (0.3° frame width). The first 50 frames were re-measured at the end of data collection to monitor instrument and crystal stability (maximum correction on I was < 1 %). Absorption corrections by integration were applied based on measured indexed crystal faces.

The structure was solved by the Direct Methods in *SHELXTL6,* and refined using full-matrix least squares. The non-H atoms were treated anisotropically, whereas the hydrogen atoms were calculated in ideal positions and were riding on their respective carbon atoms. A total of 865 parameters were refined in the final cycle of refinement using 9568 reflections with I > 2σ(I) to yield R_1 and wR_2 of 4.38% and 6.83%, respectively. Refinement was done using F^2.

SHELXTL6 (2000). Bruker-AXS, Madison, Wisconsin, USA.

Table S8. Crystal data, structure solution and refinement for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{kin}$)·

identification code	pelo6
empirical formula	$C_{88}H_{102}O_6W_2$
formula weight	1623.40
T (K)	173(2) K
λ (Å)	0.71073 Å
crystal system	Monoclinic
space group	P2(1)/n
a (Å)	13.5918(11)
b (Å)	35.213(3)
c (Å)	17.2146(15)
α (deg)	90
β (deg)	111.897(2)
γ (deg)	90
V (Å^3)	7644.7(11)
Z	4
ρ_{calcd} (Mg mm^{-3})	1.411
crystal size (mm^3)	0.15 x 0.15 x 0.02
abs coeff (mm^{-1})	3.059
F(000)	3304
θ range for data collection	1.64 to 27.50
limiting indices	$-17 \le h \le 17$, $-31 \le k \le 45$, $-19 \le l \le 22$
no. of reflns collcd	51986
no. of ind reflns (R_{int})	17559 [R(int) = 0.0879]
completeness to θ = 27.50°	99.9 %
absorption corr	Integration
refinement method	Full-matrix least-squares on F^2
data / restraints / parameters	17559 / 0 / 865
$R1$,[a] $wR2$[b] [I > 2σ]	R1 = 0.0438, wR2 = 0.0683
$R1$,[a] $wR2$[b] (all data)	R1 = 0.1061, wR2 = 0.0809
GOF[c] on F^2	0.855
largest diff. peak and hole (e.Å^{-3})	1.380 and -1.310

$R1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$ $\quad wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w = 1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [^{t}BuOCO]W=CHC(CH_3)$_3$(μ-^{t}BuOCHO)W{=CHC(CH_3)$_3$[^{t}BuOCO] (**12**$_{kin}$) U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	Y	Z	U(eq)
W1	1720(1)	1072(1)	4750(1)	41(1)
W2	2864(1)	1311(1)	883(1)	32(1)
O1	3049(3)	841(1)	5080(2)	57(1)
O2	454(3)	1290(1)	4124(2)	49(1)
O3	2431(3)	1563(1)	5061(2)	42(1)
O4	1341(3)	1216(1)	385(2)	38(1)
O5	2535(2)	1790(1)	1228(2)	32(1)
O6	3231(3)	807(1)	887(2)	38(1)
C1	3411(5)	475(2)	5207(4)	53(2)
C2	4365(5)	406(2)	5886(4)	59(2)
C3	4668(6)	26(2)	5967(5)	75(2)
C4	4103(7)	-254(2)	5435(6)	86(3)
C5	3174(6)	-170(2)	4785(5)	71(2)
C6	2792(5)	204(2)	4630(5)	56(2)
C7	1832(5)	305(2)	3891(4)	53(2)
C8	1615(6)	68(2)	3172(5)	63(2)
C9	745(6)	132(2)	2463(5)	67(2)
C10	52(5)	407(2)	2451(4)	58(2)
C11	198(5)	649(2)	3128(4)	46(2)
C12	1154(5)	617(2)	3851(4)	46(2)
C13	-660(5)	920(2)	3029(4)	48(2)
C14	-1699(5)	860(2)	2433(4)	62(2)
C15	-2464(5)	1128(2)	2306(4)	70(2)
C16	-2267(5)	1457(2)	2761(4)	62(2)
C17	-1305(5)	1533(2)	3386(4)	52(2)
C18	-509(5)	1248(2)	3503(4)	44(2)
C19	2621(4)	1895(2)	4731(3)	34(1)
C20	2826(4)	2228(2)	5230(4)	44(2)
C21	2948(4)	2564(2)	4855(4)	48(2)

C22	2897(5)	2579(2)	4064(4)	56(2)
C23	2715(4)	2255(2)	3572(4)	45(2)
C24	2565(4)	1906(2)	3904(3)	35(1)
C25	2330(4)	1568(2)	3347(3)	36(1)
C26	3008(4)	1257(2)	3506(3)	33(1)
C27	2808(4)	963(1)	2931(3)	35(1)
C28	1945(4)	979(1)	2191(3)	35(1)
C29	1248(4)	1288(2)	2009(3)	31(1)
C30	1448(4)	1572(2)	2607(3)	33(1)
C31	305(4)	1315(1)	1216(3)	32(1)
C32	-687(4)	1394(1)	1241(4)	43(2)
C33	-1568(5)	1413(2)	529(4)	51(2)
C34	-1494(5)	1351(2)	-246(4)	53(2)
C35	-522(4)	1277(2)	-320(4)	44(2)
C36	379(4)	1265(1)	428(3)	35(1)
C37	3130(4)	2113(1)	1503(3)	32(1)
C38	2670(4)	2472(1)	1224(3)	35(1)
C39	3352(5)	2781(2)	1502(3)	43(2)
C40	4400(5)	2741(2)	2020(4)	47(2)
C41	4793(4)	2392(2)	2305(4)	44(2)
C42	4161(4)	2070(2)	2065(3)	33(1)
C43	4572(4)	1691(2)	2432(3)	32(1)
C44	5253(4)	1693(2)	3261(4)	40(1)
C45	5762(4)	1367(2)	3645(4)	45(2)
C46	5622(4)	1041(2)	3176(4)	44(2)
C47	4923(4)	1017(2)	2344(3)	35(1)
C48	4312(4)	1344(2)	1965(3)	33(1)
C49	4874(4)	646(2)	1922(4)	39(1)
C50	5716(5)	389(2)	2205(4)	49(2)
C51	5643(5)	47(2)	1819(4)	57(2)
C52	4742(5)	-64(2)	1175(4)	56(2)
C53	3857(5)	173(2)	855(4)	47(2)
C54	3997(5)	538(2)	1231(4)	39(1)
C55	1378(6)	849(2)	5613(4)	85(3)
C56	618(7)	674(2)	5918(5)	82(2)

C57	-517(6)	685(2)	5163(5)	109(3)
C58	558(8)	902(3)	6643(6)	159(4)
C59	917(9)	272(2)	6170(6)	165(5)
C60	3398(4)	1523(2)	112(3)	47(2)
C61	4177(5)	1458(2)	-323(5)	63(2)
C62	4994(7)	1776(2)	-78(7)	153(5)
C63	3543(8)	1466(3)	-1256(5)	164(5)
C64	4751(5)	1082(2)	-88(4)	68(2)
C65	5006(5)	713(2)	6481(4)	68(2)
C66	5317(5)	1027(2)	6003(4)	81(2)
C67	4381(5)	887(2)	6975(4)	70(2)
C68	6024(5)	553(2)	7133(5)	101(3)
C69	-1082(5)	1888(2)	3936(4)	54(2)
C70	-2061(4)	2153(2)	3672(5)	77(2)
C71	-835(5)	1781(2)	4854(4)	71(2)
C72	-171(4)	2118(2)	3847(4)	66(2)
C73	2913(5)	2219(2)	6154(4)	62(2)
C74	1867(5)	2085(2)	6221(4)	90(3)
C75	3141(6)	2619(2)	6547(4)	86(2)
C76	3814(5)	1959(2)	6658(4)	69(2)
C77	-476(5)	1193(2)	-1175(4)	56(2)
C78	-1557(5)	1229(2)	-1891(4)	99(3)
C79	280(5)	1465(2)	-1391(4)	62(2)
C80	-78(5)	785(2)	-1177(4)	74(2)
C81	1506(4)	2523(2)	670(4)	42(2)
C82	813(4)	2356(2)	1126(4)	53(2)
C83	1195(5)	2947(2)	512(4)	59(2)
C84	1220(4)	2333(2)	-174(3)	51(2)
C85	2814(5)	49(2)	180(4)	53(2)
C86	1902(5)	98(2)	498(4)	64(2)
C87	2840(5)	-378(2)	-41(4)	81(2)
C88	2567(5)	278(2)	-625(4)	59(2)

Table S10. Bond lengths (in Å) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{kin}$)

Bond	Length	Bond	Length
W1-O2	1.824(4)	W1-O1	1.866(4)
W1-C55	1.885(6)	W1-O3	1.954(3)
W1-C12	2.162(6)	W2-O6	1.844(3)
W2-C60	1.887(5)	W2-O5	1.894(3)
W2-O4	1.951(3)	W2-C48	2.150(5)
O1-C1	1.369(7)	O2-C18	1.355(6)
O3-C19	1.367(6)	O4-C36	1.348(5)
O5-C37	1.375(5)	O6-C54	1.369(6)
C1-C2	1.406(8)	C1-C6	1.407(8)
C2-C3	1.390(9)	C2-C65	1.521(9)
C3-C4	1.371(10)	C4-C5	1.372(10)
C5-C6	1.404(8)	C6-C7	1.486(9)
C7-C12	1.418(8)	C7-C8	1.430(8)
C8-C9	1.365(9)	C9-C10	1.345(8)
C10-C11	1.395(8)	C11-C12	1.430(8)
C11-C13	1.467(8)	C13-C18	1.386(7)
C13-C14	1.418(8)	C14-C15	1.359(8)
C15-C16	1.368(9)	C16-C17	1.375(8)
C17-C18	1.432(8)	C17-C69	1.531(8)
C19-C24	1.396(7)	C19-C20	1.420(7)
C20-C21	1.386(8)	C20-C73	1.551(8)
C21-C22	1.337(8)	C22-C23	1.388(7)
C23-C24	1.403(7)	C24-C25	1.487(7)
C25-C30	1.386(7)	C25-C26	1.391(7)
C26-C27	1.386(7)	C27-C28	1.375(7)
C28-C29	1.399(6)	C29-C30	1.385(7)
C29-C31	1.487(7)	C31-C32	1.393(6)
C31-C36	1.408(7)	C32-C33	1.359(7)
C33-C34	1.392(8)	C34-C35	1.398(7)
C35-C36	1.408(7)	C35-C77	1.525(8)
C37-C42	1.383(7)	C37-C38	1.410(6)

C38-C39	1.394(7)	C38-C81	1.524(7)
C39-C40	1.377(7)	C40-C41	1.354(7)
C41-C42	1.390(7)	C42-C43	1.492(7)
C43-C44	1.381(7)	C43-C48	1.433(7)
C44-C45	1.375(7)	C45-C46	1.377(7)
C46-C47	1.394(7)	C47-C48	1.429(7)
C47-C49	1.485(7)	C49-C54	1.387(7)
C49-C50	1.396(7)	C50-C51	1.362(8)
C51-C52	1.367(8)	C52-C53	1.398(7)
C53-C54	1.418(7)	C53-C85	1.523(8)
C55-C56	1.459(8)	C56-C59	1.490(10)
C56-C58	1.513(10)	C56-C57	1.605(10)
C60-C61	1.524(7)	C61-C64	1.512(7)
C61-C63	1.514(10)	C61-C62	1.521(10)
C65-C66	1.527(8)	C65-C68	1.528(8)
C65-C67	1.535(8)	C69-C71	1.534(8)
C69-C72	1.535(7)	C69-C70	1.547(8)
C73-C76	1.516(8)	C73-C75	1.542(8)
C73-C74	1.543(8)	C77-C78	1.531(8)
C77-C80	1.534(8)	C77-C79	1.548(8)
C81-C84	1.512(7)	C81-C83	1.547(7)
C81-C82	1.548(7)	C85-C88	1.527(8)
C85-C86	1.539(7)	C85-C87	1.558(7)

Table S111. Bond angles (in deg) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{kin}$)

Bond	Angle	Bond	Angle
O2-W1-O1	162.91(16)	C59-C56-C58	110.9(8)
O2-W1-C55	100.6(3)	C55-C56-C57	107.1(6)
O1-W1-C55	94.2(3)	C59-C56-C57	109.5(7)
O2-W1-O3	92.97(15)	C58-C56-C57	108.9(7)
O1-W1-O3	88.80(16)	C55-W1-O3	113.3(2)
O1-W1-C12	86.5(2)	O2-W1-C12	83.3(2)
C55-W1-C12	97.4(2)	O6-W2-C60	102.0(2)
O3-W1-C12	149.29(17)	O6-W2-O5	161.88(14)
C60-W2-O5	93.85(19)	O5-W2-O4	87.37(13)
O6-W2-O4	94.49(14)	O6-W2-C48	83.69(17)
C60-W2-O4	112.46(19)	C60-W2-C48	96.9(2)
C1-O1-W1	135.2(4)	O5-W2-C48	85.80(17)
C18-O2-W1	147.4(4)	O4-W2-C48	150.25(15)
C19-O3-W1	142.5(3)	C61-C60-W2	143.7(4)
C36-O4-W2	147.8(3)	C64-C61-C63	109.4(6)
C37-O5-W2	131.9(3)	C64-C61-C62	108.6(6)
C54-O6-W2	146.1(4)	C63-C61-C62	110.4(7)
O1-C1-C2	117.4(6)	C64-C61-C60	112.6(5)
O1-C1-C6	116.1(6)	C63-C61-C60	107.1(6)
C2-C1-C6	126.4(7)	C62-C61-C60	108.8(6)
C3-C2-C1	113.4(7)	C3-C4-C5	120.3(8)
C3-C2-C65	122.9(7)	C4-C5-C6	121.5(8)
C1-C2-C65	123.8(6)	C5-C6-C7	122.1(7)
C4-C3-C2	123.7(8)	C1-C6-C7	123.0(6)
C5-C6-C1	114.8(7)	C12-C7-C8	119.3(6)
C9-C8-C7	120.6(7)	C12-C7-C6	125.0(6)
C10-C9-C8	120.0(6)	C8-C7-C6	115.6(6)
C9-C10-C11	123.0(7)	C2-C65-C66	110.8(6)
C10-C11-C12	118.7(6)	C2-C65-C68	111.5(6)
C10-C11-C13	116.1(6)	C66-C65-C68	107.8(6)
C12-C11-C13	125.2(5)	C2-C65-C67	111.1(5)

C7-C12-C11	117.8(5)	C66-C65-C67	109.3(6)
C7-C12-W1	119.2(5)	C68-C65-C67	106.1(6)
C11-C12-W1	122.1(4)	C17-C69-C71	110.7(5)
C18-C13-C14	116.0(6)	C17-C69-C72	110.5(5)
C18-C13-C11	122.5(5)	C71-C69-C72	110.9(5)
C14-C13-C11	121.5(6)	C17-C69-C70	111.1(5)
C15-C14-C13	120.6(6)	C71-C69-C70	106.5(5)
C14-C15-C16	121.4(7)	C72-C69-C70	106.8(5)
C15-C16-C17	122.5(7)	O2-C18-C17	119.5(5)
C16-C17-C18	115.0(6)	C13-C18-C17	124.2(6)
C16-C17-C69	123.6(6)	O3-C19-C24	120.0(5)
C18-C17-C69	121.3(5)	O3-C19-C20	118.7(5)
O2-C18-C13	116.3(5)	C24-C19-C20	121.3(5)
C21-C22-C23	121.2(6)	C21-C20-C19	116.9(6)
C22-C23-C24	119.5(6)	C21-C20-C73	121.3(5)
C19-C24-C23	118.5(5)	C19-C20-C73	121.8(5)
C19-C24-C25	123.6(5)	C22-C21-C20	122.6(6)
C23-C24-C25	117.9(5)	C76-C73-C75	108.3(6)
C30-C25-C26	118.1(5)	C76-C73-C74	110.0(6)
C30-C25-C24	119.3(5)	C75-C73-C74	106.6(5)
C26-C25-C24	122.4(5)	C76-C73-C20	109.6(5)
C27-C26-C25	120.5(5)	C75-C73-C20	110.9(6)
C28-C27-C26	120.2(5)	C74-C73-C20	111.3(5)
C27-C28-C29	120.8(5)	C30-C29-C28	117.6(5)
C30-C29-C31	120.1(5)	C32-C31-C36	118.2(5)
C28-C29-C31	122.3(5)	C32-C31-C29	119.9(5)
C29-C30-C25	122.6(5)	C36-C31-C29	122.0(4)
C33-C32-C31	121.3(5)	C35-C77-C78	112.9(5)
C32-C33-C34	120.1(6)	C35-C77-C80	109.0(5)
C33-C34-C35	121.7(6)	C78-C77-C80	108.0(5)
C34-C35-C36	116.8(5)	C35-C77-C79	112.4(5)
C34-C35-C77	120.3(5)	C78-C77-C79	106.2(6)
C36-C35-C77	122.8(5)	C80-C77-C79	108.2(5)
O4-C36-C35	118.9(5)	O5-C37-C38	119.7(5)
O4-C36-C31	119.2(5)	C42-C37-C38	122.8(5)

C35-C36-C31	121.8(5)	C39-C38-C37	115.4(5)
O5-C37-C42	117.5(5)	C39-C38-C81	121.6(5)
C40-C39-C38	122.5(5)	C37-C38-C81	122.9(5)
C41-C40-C39	120.0(5)	C84-C81-C38	112.6(4)
C40-C41-C42	121.0(6)	C84-C81-C83	107.5(5)
C37-C42-C41	118.1(5)	C38-C81-C83	112.1(5)
C37-C42-C43	121.1(5)	C84-C81-C82	109.4(5)
C41-C42-C43	120.8(5)	C38-C81-C82	108.9(4)
C44-C43-C48	120.9(5)	C83-C81-C82	106.1(4)
C44-C43-C42	115.8(5)	C44-C45-C46	118.6(6)
C48-C43-C42	123.3(5)	C45-C46-C47	123.1(5)
C45-C44-C43	121.1(5)	C53-C85-C88	111.6(5)
C46-C47-C48	118.5(5)	C53-C85-C86	110.0(5)
C46-C47-C49	116.5(5)	C88-C85-C86	109.3(5)
C48-C47-C49	125.0(5)	C53-C85-C87	111.3(5)
C47-C48-C43	116.9(5)	C88-C85-C87	107.8(5)
C47-C48-W2	122.7(4)	C86-C85-C87	106.7(5)
C43-C48-W2	119.2(4)	C50-C51-C52	121.9(6)
C54-C49-C50	116.9(5)	C51-C52-C53	121.9(6)
C54-C49-C47	121.9(5)	C52-C53-C54	114.3(6)
C50-C49-C47	121.2(6)	C52-C53-C85	123.3(6)
C51-C50-C49	120.1(6)	C54-C53-C85	122.3(5)
C55-C56-C59	110.8(7)	O6-C54-C49	116.9(5)
C55-C56-C58	109.6(7)	O6-C54-C53	118.6(5)
C56-C55-W1	151.2(6)	C49-C54-C53	124.5(5)

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{kin}$). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W1	48(1)	41(1)	41(1)	-5(1)	25(1)	-14(1)
W2	41(1)	25(1)	37(1)	-1(1)	22(1)	0(1)
O1	67(3)	45(3)	59(3)	-5(2)	23(2)	-6(2)
O2	48(2)	54(3)	46(3)	-19(2)	20(2)	-13(2)
O3	49(2)	41(2)	38(2)	-9(2)	21(2)	-15(2)
O4	51(2)	31(2)	38(2)	-7(2)	23(2)	-2(2)
O5	34(2)	23(2)	43(2)	-4(2)	19(2)	-3(2)
O6	50(2)	29(2)	40(2)	0(2)	23(2)	2(2)
C1	61(5)	47(4)	67(5)	9(4)	44(4)	1(4)
C2	64(5)	63(5)	65(5)	21(4)	41(4)	10(4)
C3	90(6)	80(6)	78(6)	35(5)	58(5)	27(5)
C4	130(8)	54(6)	111(8)	36(5)	87(7)	26(5)
C5	95(6)	45(5)	99(6)	11(4)	65(5)	-3(4)
C6	71(5)	31(4)	88(6)	8(4)	56(4)	0(4)
C7	61(5)	46(4)	67(5)	1(3)	40(4)	-22(3)
C8	95(6)	31(4)	87(6)	-14(4)	60(5)	-22(4)
C9	99(6)	61(5)	59(5)	-32(4)	50(5)	-42(4)
C10	66(5)	53(5)	68(5)	-20(4)	41(4)	-30(4)
C11	63(4)	35(4)	49(4)	-11(3)	33(4)	-29(3)
C12	69(4)	34(4)	53(4)	-3(3)	45(4)	-12(3)
C13	49(4)	55(4)	50(4)	-15(3)	31(3)	-22(3)
C14	63(5)	76(5)	56(5)	-21(4)	32(4)	-41(4)
C15	45(4)	118(7)	55(5)	-13(5)	29(4)	-26(5)
C16	43(4)	100(6)	51(4)	-11(4)	27(4)	-9(4)
C17	44(4)	69(5)	51(4)	-13(4)	27(3)	-12(3)
C18	46(4)	57(4)	38(4)	-11(3)	27(3)	-18(3)
C19	32(3)	32(3)	42(4)	-4(3)	19(3)	-6(2)
C20	34(3)	54(4)	49(4)	-17(3)	21(3)	-14(3)
C21	59(4)	31(4)	52(4)	-19(3)	19(3)	-8(3)

C22	66(5)	33(4)	62(5)	1(3)	17(4)	-9(3)
C23	51(4)	42(4)	44(4)	-4(3)	21(3)	-13(3)
C24	30(3)	40(4)	34(3)	-11(3)	11(3)	-8(3)
C25	37(3)	39(4)	36(3)	-3(3)	20(3)	-9(3)
C26	35(3)	40(4)	30(3)	1(3)	18(3)	-12(3)
C27	39(3)	27(3)	44(4)	8(3)	23(3)	0(2)
C28	49(4)	28(3)	42(4)	-2(2)	34(3)	-8(3)
C29	35(3)	32(3)	35(3)	1(3)	24(3)	-4(3)
C30	29(3)	35(3)	42(4)	-4(3)	21(3)	-7(2)
C31	37(3)	25(3)	39(3)	-11(3)	20(3)	-3(3)
C32	53(4)	35(4)	44(4)	-4(3)	23(3)	-8(3)
C33	40(4)	42(4)	72(5)	-10(3)	21(4)	-7(3)
C34	43(4)	50(4)	54(4)	-6(3)	5(3)	-6(3)
C35	46(4)	35(4)	51(4)	-15(3)	20(3)	-6(3)
C36	39(3)	25(3)	47(4)	-7(3)	21(3)	-1(3)
C37	44(3)	27(3)	35(3)	-3(2)	26(3)	-2(3)
C38	50(4)	23(3)	37(3)	3(2)	22(3)	4(3)
C39	71(4)	22(3)	41(4)	2(3)	25(3)	2(3)
C40	58(4)	34(4)	46(4)	-7(3)	16(3)	-15(3)
C41	45(4)	37(4)	51(4)	-2(3)	19(3)	-8(3)
C42	37(3)	34(3)	33(3)	-2(3)	18(3)	1(3)
C43	31(3)	33(3)	37(3)	-2(3)	18(3)	-2(2)
C44	42(4)	30(3)	52(4)	2(3)	21(3)	0(3)
C45	42(3)	55(4)	37(4)	1(3)	14(3)	-4(3)
C46	48(4)	42(4)	55(4)	16(3)	32(3)	5(3)
C47	39(3)	33(3)	38(3)	1(3)	21(3)	-4(3)
C48	38(3)	31(3)	42(3)	6(3)	29(3)	2(3)
C49	51(4)	30(3)	46(4)	13(3)	31(3)	6(3)
C50	61(4)	39(4)	57(4)	8(3)	33(3)	11(3)
C51	62(5)	45(4)	75(5)	12(4)	38(4)	16(3)
C52	79(5)	31(4)	70(5)	9(3)	42(4)	21(4)
C53	70(4)	33(4)	48(4)	2(3)	34(4)	5(3)
C54	55(4)	29(3)	44(4)	7(3)	32(3)	8(3)
C55	113(6)	112(6)	49(5)	-10(4)	52(4)	-63(5)
C56	117(7)	79(6)	74(6)	-7(4)	65(5)	-26(5)

C57	101(7)	111(8)	137(9)	-22(6)	69(7)	-43(5)
C58	221(12)	190(11)	129(9)	-34(8)	139(9)	-30(9)
C59	310(15)	68(7)	120(9)	32(6)	85(9)	-27(8)
C60	55(4)	38(4)	54(4)	10(3)	26(3)	12(3)
C61	76(5)	59(5)	79(5)	29(4)	56(4)	29(4)
C62	120(7)	69(6)	335(16)	40(8)	161(10)	1(6)
C63	210(11)	248(13)	85(7)	85(7)	111(8)	165(10)
C64	84(5)	56(5)	91(6)	16(4)	65(4)	21(4)
C65	54(5)	92(6)	61(5)	15(4)	24(4)	6(4)
C66	83(5)	94(6)	72(5)	10(4)	35(4)	-24(4)
C67	65(5)	97(6)	46(4)	10(4)	20(4)	-2(4)
C68	73(6)	136(8)	90(7)	16(5)	27(5)	15(5)
C69	47(4)	67(5)	62(5)	-1(4)	35(3)	-1(3)
C70	49(4)	91(6)	106(6)	4(5)	47(4)	10(4)
C71	78(5)	83(5)	70(5)	-19(4)	48(4)	0(4)
C72	47(4)	71(5)	84(5)	-5(4)	29(4)	2(3)
C73	71(5)	74(5)	52(5)	-29(4)	35(4)	-29(4)
C74	88(5)	123(7)	87(6)	-47(5)	64(5)	-51(5)
C75	109(6)	90(6)	70(5)	-48(4)	44(5)	-36(5)
C76	89(5)	69(5)	50(5)	-9(4)	26(4)	-23(4)
C77	64(4)	50(5)	50(4)	-15(3)	16(4)	-3(3)
C78	76(5)	156(9)	45(5)	-34(5)	0(4)	-11(5)
C79	96(5)	52(4)	34(4)	-5(3)	21(4)	-13(4)
C80	117(6)	49(5)	70(5)	-29(4)	53(5)	-26(4)
C81	52(4)	26(3)	50(4)	4(3)	23(3)	10(3)
C82	48(4)	49(4)	69(5)	12(3)	31(3)	15(3)
C83	74(4)	34(4)	64(5)	6(3)	20(4)	13(3)
C84	62(4)	38(4)	48(4)	2(3)	16(3)	3(3)
C85	85(5)	26(4)	60(5)	-4(3)	39(4)	6(3)
C86	78(5)	44(4)	71(5)	-4(3)	28(4)	-15(3)
C87	117(6)	29(4)	91(6)	-23(4)	30(5)	-2(4)
C88	77(5)	50(4)	55(5)	-5(3)	31(4)	7(3)

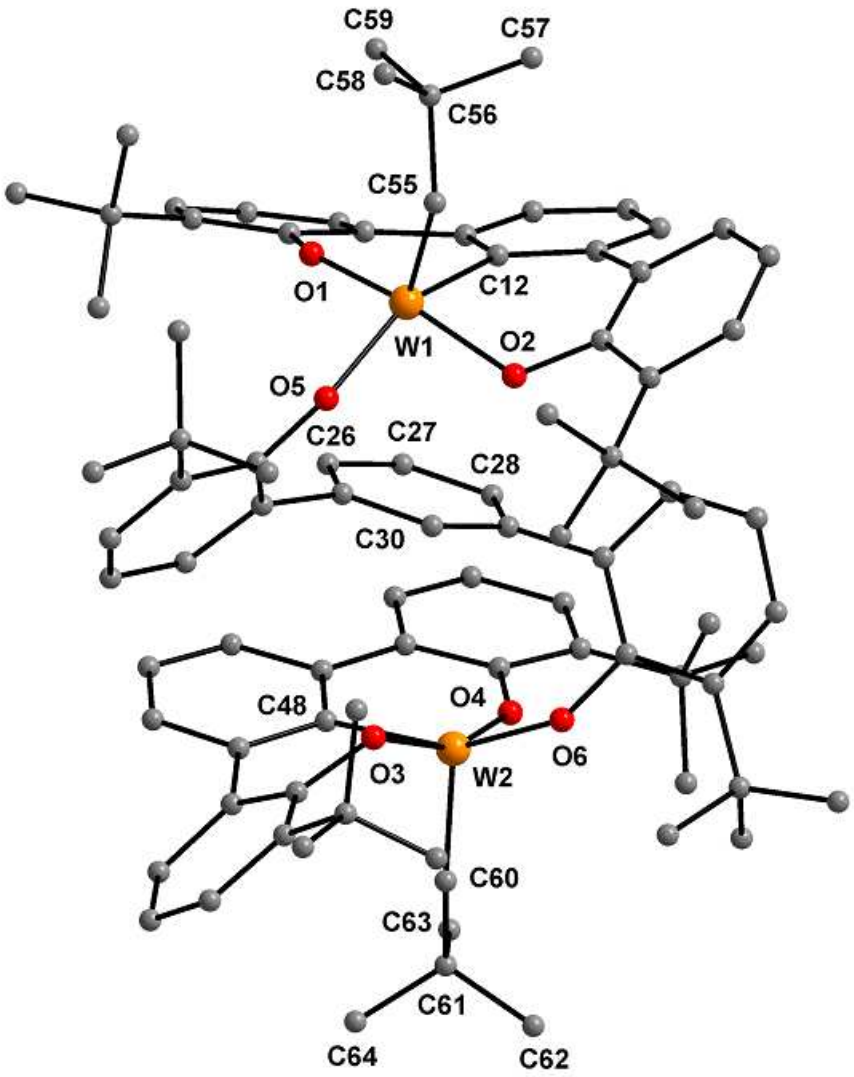

Figure S10. Molecular structure of [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{therm}$).

X-ray Experimental for [(^{t}BuOCO)W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W=CHC(CH$_3$)$_3$ [^{t}BuOCO]} (12$_{therm}$).

Data were collected at 173 K on a Siemens SMART PLATFORM equipped with A CCD area detector and a graphite monochromator utilizing MoK$_\alpha$ radiation (λ = 0.71073 Å). Cell parameters were refined using up to 8192 reflections. A full sphere of data (1850 frames) was collected using the ω-scan method (0.3° frame width). The first 50 frames were re-measured at the end of data collection to monitor instrument and crystal stability (maximum correction on I was < 1 %). Absorption corrections by integration were applied based on measured indexed crystal faces.

The structure was solved by the Direct Methods in *SHELXTL6,* and refined using full-matrix least squares. The non-H atoms were treated anisotropically, whereas the hydrogen atoms were calculated in ideal positions and were riding on their respective carbon atoms. A total of 865 parameters were refined in the final cycle of refinement using 8982 reflections with I > 2σ(I) to yield R$_1$ and wR$_2$ of 4.70% and 7.47%, respectively. Refinement was done using F^2. The toluene molecule were disordered and could not be modeled properly, thus program SQUEEZE, a part of the PLATON package of crystallographic software, was used to calculate the solvent disorder area and remove its contribution to the overall intensity data.

P. van der Sluis & A.L. Spek (1990). SQUEEZE, Acta Cryst. A46, 194-201

SHELXTL6 (2000). Bruker-AXS, Madison, Wisconsin, USA.

Spek, A.L. (1990). PLATON, Acta Cryst. A46, C-34.

Table S13. Crystal data, structure solution and refinement for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{therm}$).

identification code	pelo7t
empirical formula	$C_{88}H_{102}O_6W_2$
formula weight	1623.40
T (K)	173(2) K
λ (Å)	0.71073 Å
crystal system	Monoclinic
space group	P2(1)/c
a (Å)	12.8904(8)
b (Å)	20.2444(13)
c (Å)	29.2372(18)
α (deg)	90
β (deg)	100.7990(10)
γ (deg)	90
V (Å^3)	7494.6(8)
Z	4
ρ_{calcd} (Mg mm^{-3})	1.439
crystal size (mm^3)	0.16 x 0.04 x 0.04
abs coeff (mm^{-1})	3.121
F(000)	3304
θ range for data collection	1.23 to 27.50
limiting indices	$-16 \le h \le 15$, $-26 \le k \le 26$, $-37 \le l \le 27$
no. of reflns collcd	50772
no. of ind reflns (R_{int})	17182 (0.1164)
completeness to θ = 27.50°	99.8 %
absorption corr	Integration
refinement method	Full-matrix least-squares on F^2
data / restraints / parameters	17182 / 0 / 865
$R1$,[a] $wR2$[b] [I > 2σ]	R1 = 0.0470, wR2 = 0.0747
$R1$,[a] $wR2$[b] (all data)	R1 = 0.1207, wR2 = 0.1004
GOF[c] on F^2	0.817
largest diff. peak and hole (e.Å^{-3})	1.313 and -0.690

$R1 = \Sigma(||F_o| - |F_c||) / \Sigma|F_o|$ $\quad wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2}$

$S = [\Sigma[w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$

$w = 1/[\sigma^2(F_o^2)+(m*p)^2+n*p]$, $p = [\max(F_o^2,0)+ 2* F_c^2]/3$, m & n are constants.

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [^{t}BuOCO]W=CHC$(CH_3)_3$(μ-^{t}BuOCHO)W{=CHC$(CH_3)_3$[^{t}BuOCO] (**12**$_{therm}$). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	X	Y	Z	U(eq)
W1	2846(1)	5902(1)	3082(1)	23(1)
W2	1520(1)	7759(1)	4941(1)	25(1)
O5	1353(3)	6133(2)	2975(1)	26(1)
O4	2683(4)	7592(2)	5399(2)	30(1)
O3	460(4)	7588(2)	4408(1)	26(1)
O1	2667(3)	5063(2)	3319(1)	24(1)
O6	2269(4)	8291(2)	4553(2)	28(1)
C12	4361(5)	5840(3)	3524(2)	22(2)
C48	944(6)	6880(3)	5211(2)	26(2)
C25	1682(5)	6263(3)	3977(2)	24(2)
C29	3046(5)	7085(3)	4259(2)	24(2)
C9	6334(5)	5883(4)	4127(2)	32(2)
C30	2139(5)	6879(3)	3944(2)	28(2)
C47	1570(6)	6422(3)	5511(2)	32(2)
C20	-519(5)	5959(3)	2907(2)	29(2)
C36	3092(5)	8332(3)	4325(2)	24(2)
C51	4235(7)	6199(5)	6284(3)	50(2)
C2	2358(5)	4094(3)	3750(2)	25(2)
C49	2677(6)	6542(3)	5754(2)	28(2)
C26	2130(5)	5840(3)	4342(2)	26(2)
C60	708(5)	8341(3)	5233(2)	28(2)
C31	3519(5)	7738(3)	4190(2)	25(2)
C19	493(5)	6074(3)	3186(2)	23(2)
C1	2984(5)	4654(3)	3693(2)	23(2)
C23	-219(6)	5967(3)	3882(3)	33(2)
C6	3896(5)	4841(3)	4002(2)	24(2)
C37	-593(6)	7546(3)	4408(2)	23(2)
C7	4605(5)	5383(3)	3903(2)	25(2)
C24	661(5)	6097(3)	3678(2)	25(2)
C56	3871(6)	5225(3)	2265(2)	32(2)

C13	5002(5)	6811(3)	3088(2)	25(2)
C77	4804(6)	7944(4)	5880(3)	38(2)
C65	1400(6)	3865(3)	3394(2)	30(2)
C42	-894(6)	7144(3)	4755(2)	29(2)
C54	3220(6)	7138(3)	5705(2)	30(2)
C3	2677(6)	3752(3)	4160(3)	32(2)
C18	4013(6)	7102(3)	2936(2)	29(2)
C53	4243(6)	7288(4)	5938(3)	38(2)
C17	3854(6)	7676(3)	2653(2)	31(2)
C15	5716(6)	7561(4)	2591(3)	40(2)
C10	6112(5)	6319(3)	3761(2)	27(2)
C5	4136(5)	4473(3)	4416(2)	28(2)
C61	490(6)	8597(3)	5693(2)	32(2)
C11	5151(5)	6305(3)	3459(2)	24(2)
C35	3490(6)	8949(3)	4233(2)	30(2)
C52	4734(7)	6799(4)	6232(3)	44(2)
C50	3239(7)	6074(4)	6053(3)	45(2)
C16	4754(6)	7875(3)	2484(2)	36(2)
C8	5606(6)	5421(4)	4191(2)	33(2)
C27	3022(6)	6042(4)	4647(2)	34(2)
C44	-528(7)	6097(4)	5147(2)	39(2)
C41	-1971(7)	7174(4)	4798(3)	47(2)
C28	3481(6)	6657(3)	4610(2)	32(2)
C81	-707(6)	5989(4)	2372(3)	40(2)
C21	-1327(6)	5844(4)	3145(3)	40(2)
C69	2804(6)	8026(4)	2511(3)	36(2)
C79	4143(7)	8517(4)	6007(3)	55(2)
C14	5841(6)	7051(3)	2896(2)	34(2)
C33	4791(6)	8385(4)	3882(3)	49(2)
C32	4383(6)	7778(4)	3980(3)	40(2)
C39	-2367(6)	7895(4)	4147(3)	46(2)
C87	3602(8)	10199(4)	4231(4)	79(3)
C78	4982(7)	8019(4)	5389(3)	48(2)
C34	4347(6)	8946(4)	4012(3)	43(2)
C38	-1321(6)	7894(3)	4080(2)	30(2)

C4	3526(6)	3945(3)	4488(2)	35(2)
C43	-134(6)	6710(3)	5045(2)	30(2)
C62	782(7)	9328(4)	5741(3)	55(3)
C40	-2674(6)	7553(4)	4507(3)	46(2)
C22	-1183(6)	5832(4)	3627(3)	39(2)
C64	-676(6)	8500(4)	5704(3)	52(2)
C66	521(6)	4375(4)	3331(3)	54(2)
C63	1168(7)	8208(4)	6101(2)	48(2)
C46	1122(7)	5808(4)	5602(3)	50(2)
C71	2208(7)	7689(5)	2079(3)	87(4)
C88	3161(10)	9631(4)	4906(4)	101(4)
C45	107(8)	5644(4)	5419(3)	52(2)
C68	933(6)	3227(4)	3550(3)	48(2)
C83	-394(7)	6661(4)	2212(3)	55(2)
C70	2983(7)	8763(4)	2391(3)	67(3)
C72	2140(7)	8055(4)	2887(3)	62(3)
C85	3041(7)	9594(4)	4377(3)	47(2)
O2	3159(3)	6825(2)	3077(2)	27(1)
C55	3329(5)	5739(3)	2521(2)	29(2)
C73	-1035(6)	8259(4)	3671(2)	36(2)
C59	4022(7)	4582(4)	2520(3)	50(2)
C58	3213(7)	5134(4)	1777(3)	53(2)
C57	4955(6)	5505(4)	2219(3)	50(2)
C82	-67(6)	5457(4)	2175(3)	54(2)
C80	5881(7)	7985(4)	6208(3)	63(3)
C67	1705(7)	3726(5)	2925(3)	69(3)
C75	-1965(7)	8443(6)	3314(3)	92(4)
C76	-502(13)	8875(6)	3831(4)	193(9)
C84	-1868(6)	5874(5)	2157(3)	71(3)
C74	-362(11)	7858(7)	3426(4)	183(9)
C86	1879(7)	9642(4)	4146(4)	96(4)

Table S15. Bond lengths (in Å) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{therm}$).

Bond	Length	Bond	Length
W1-O1	1.865(4)	W1-C55	1.888(6)
W1-O2	1.914(4)	W1-O5	1.948(4)
W1-C12	2.134(7)	W2-O4	1.844(5)
W2-C60	1.883(6)	W2-O3	1.903(5)
W2-O6	1.947(4)	W2-C48	2.136(7)
O5-C19	1.371(7)	O4-C54	1.375(8)
O3-C37	1.361(7)	O1-C1	1.371(7)
O6-C36	1.357(7)	C33-C34	1.357(10)
C12-C11	1.426(8)	C33-C32	1.386(10)
C12-C7	1.433(9)	C69-C70	1.560(10)
C48-C47	1.419(9)	C25-C26	1.405(9)
C48-C43	1.426(10)	C39-C40	1.379(10)
C25-C30	1.388(9)	C39-C38	1.398(9)
C25-C24	1.476(9)	C87-C85	1.522(10)
C29-C28	1.378(9)	C29-C31	1.486(9)
C29-C30	1.409(9)	C9-C8	1.363(9)
C47-C46	1.416(10)	C9-C10	1.376(9)
C47-C49	1.491(10)	C38-C73	1.509(9)
C20-C21	1.377(9)	C36-C35	1.395(9)
C20-C19	1.423(9)	C36-C31	1.411(9)
C20-C81	1.538(9)	C51-C50	1.357(11)
C2-C3	1.377(9)	C51-C52	1.397(11)
C2-C1	1.421(9)	C46-C45	1.358(11)
C2-C65	1.530(9)	C60-C61	1.516(9)
C49-C50	1.396(10)	C31-C32	1.372(9)
C49-C54	1.415(9)	C19-C24	1.415(9)
C26-C27	1.380(9)	C88-C85	1.525(12)
C1-C6	1.394(9)	C6-C5	1.405(9)
C23-C22	1.352(10)	C6-C7	1.490(9)
C23-C24	1.402(9)	C37-C38	1.399(9)
C56-C55	1.525(9)	C37-C42	1.412(9)

C56-C58	1.529(10)	C7-C8	1.405(9)
C56-C57	1.535(9)	C56-C59	1.496(9)
C13-C18	1.400(9)	C85-C86	1.526(12)
C13-C14	1.394(9)	C73-C76	1.458(11)
C13-C11	1.477(9)	C73-C74	1.468(11)
C77-C53	1.537(10)	C73-C75	1.481(11)
C77-C79	1.527(10)	C65-C66	1.519(10)
C77-C78	1.504(10)	C65-C68	1.530(9)
C77-C80	1.534(11)	C42-C41	1.418(10)
C65-C67	1.523(9)	C42-C43	1.463(10)
C18-O2	1.366(7)	C54-C53	1.401(10)
C18-C17	1.418(9)	C3-C4	1.369(10)
C53-C52	1.384(10)	C81-C84	1.529(10)
C17-C16	1.402(9)	C21-C22	1.386(9)
C17-C69	1.515(10)	C69-C72	1.517(10)
C15-C14	1.356(9)	C61-C64	1.522(10)
C15-C16	1.377(10)	C61-C62	1.525(10)
C10-C11	1.381(9)	C61-C63	1.555(10)
C5-C4	1.366(9)	C35-C34	1.381(9)
C81-C82	1.534(10)	C35-C85	1.521(10)
C69-C71	1.511(11)	C81-C83	1.516(10)
C27-C28	1.391(9)	C41-C40	1.357(10)
C44-C43	1.394(9)	C44-C45	1.379(10)

Table S16. Bond angles (in deg) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{therm}$).

Bond	Angle	Bond	Angle
O1-W1-C55	104.4(2)	C55-W1-O2	93.5(2)
O1-W1-O2	158.91(18)	O1-W1-O5	95.22(18)
C55-W1-O5	112.3(2)	C15-C14-C13	121.7(7)
O2-W1-O5	88.12(18)	C34-C33-C32	119.2(7)
O1-W1-C12	83.3(2)	C31-C32-C33	121.1(7)
C55-W1-C12	95.9(3)	C40-C39-C38	121.9(7)
O2-W1-C12	83.7(2)	O4-W2-C60	103.4(3)
O5-W1-C12	151.1(2)	O4-W2-O3	157.35(18)
O3-W2-O6	88.89(18)	C60-W2-O3	96.4(3)
O4-W2-C48	82.6(2)	O4-W2-O6	95.7(2)
C60-W2-C48	95.3(3)	C60-W2-O6	107.2(2)
O3-W2-C48	84.6(2)	O6-W2-C48	157.1(2)
C19-O5-W1	139.9(4)	C33-C34-C35	123.4(7)
C54-O4-W2	146.6(4)	C36-O6-W2	147.0(4)
C37-O3-W2	125.0(4)	C11-C12-C7	118.1(6)
C1-O1-W1	143.8(4)	C11-C12-W1	118.4(5)
C47-C48-W2	125.2(5)	C7-C12-W1	123.3(5)
C43-C48-W2	117.3(5)	C47-C48-C43	117.3(6)
C30-C25-C26	118.7(7)	C37-C38-C39	116.4(7)
C30-C25-C24	120.5(6)	C37-C38-C73	123.8(6)
C26-C25-C24	120.2(6)	C39-C38-C73	119.8(7)
C28-C29-C30	118.2(6)	C3-C4-C5	121.5(6)
C28-C29-C31	122.7(6)	C44-C43-C48	120.8(7)
C30-C29-C31	119.1(6)	C44-C43-C42	115.3(7)
C8-C9-C10	120.0(7)	C48-C43-C42	123.9(6)
C25-C30-C29	122.1(6)	C46-C47-C48	119.0(7)
C46-C47-C49	116.2(7)	C48-C47-C49	124.8(6)
C21-C20-C81	122.1(6)	C21-C20-C19	115.9(7)
C19-C20-C81	122.0(6)	C23-C22-C21	119.5(7)
O6-C36-C35	120.0(6)	C35-C36-C31	122.2(6)
O6-C36-C31	117.9(6)	C50-C51-C52	121.4(8)

C3-C2-C1	114.8(6)	C50-C49-C54	115.8(7)
C3-C2-C65	120.7(6)	C50-C49-C47	121.7(7)
C1-C2-C65	124.5(6)	C54-C49-C47	122.5(6)
C61-C60-W2	145.8(5)	C27-C26-C25	118.9(7)
C32-C31-C36	117.8(7)	C36-C31-C29	121.9(6)
C32-C31-C29	120.2(6)	O5-C19-C24	118.2(6)
O5-C19-C20	119.2(6)	C45-C46-C47	122.5(8)
C24-C19-C20	122.6(6)	C1-C6-C5	115.8(6)
O1-C1-C6	116.3(6)	C1-C6-C7	123.1(6)
O1-C1-C2	118.9(6)	C5-C6-C7	121.0(6)
C6-C1-C2	124.7(6)	O3-C37-C38	120.6(6)
C22-C23-C24	122.4(7)	C46-C45-C44	119.2(8)
O3-C37-C42	116.4(6)	C12-C7-C6	124.9(6)
C38-C37-C42	122.9(7)	C19-C24-C23	116.4(6)
C8-C7-C12	118.2(6)	C19-C24-C25	123.9(6)
C8-C7-C6	116.8(6)	C23-C24-C25	119.6(6)
C55-C56-C58	108.3(6)	C59-C56-C55	112.2(6)
C59-C56-C57	109.2(7)	C59-C56-C58	111.0(6)
C55-C56-C57	107.4(6)	C18-C13-C14	117.0(6)
C58-C56-C57	108.6(6)	C18-C13-C11	120.7(6)
C14-C13-C11	122.2(7)	C53-C77-C80	111.6(6)
C53-C77-C79	109.5(6)	C79-C77-C80	106.7(6)
C53-C77-C78	110.6(6)	C78-C77-C80	108.0(7)
C79-C77-C78	110.3(7)	C2-C65-C67	111.0(6)
C67-C65-C66	109.1(7)	C2-C65-C66	111.5(6)
C2-C65-C68	111.4(6)	C66-C65-C68	106.5(6)
C67-C65-C68	107.1(6)	C37-C42-C41	116.4(7)
C41-C42-C43	122.4(7)	C37-C42-C43	121.2(6)
C35-C85-C87	112.8(7)	C86-C85-C35	108.9(7)
C86-C85-C88	110.5(8)	C86-C85-C87	107.7(7)
O4-C54-C53	119.0(7)	C35-C85-C88	110.5(7)
O4-C54-C49	116.1(7)	C87-C85-C88	106.4(7)
C53-C54-C49	125.0(7)	C18-O2-W1	125.9(4)
C2-C3-C4	122.4(7)	C56-C55-W1	143.2(5)
O2-C18-C13	118.0(6)	C76-C73-C74	110.0(11)

O2-C18-C17	118.5(6)	C76-C73-C75	106.3(8)
C13-C18-C17	123.6(6)	C74-C73-C75	105.7(8)
C52-C53-C54	115.3(8)	C76-C73-C38	109.6(7)
C52-C53-C77	121.1(7)	C74-C73-C38	111.7(7)
C54-C53-C77	123.6(7)	C75-C73-C38	113.3(7)
C16-C17-C18	113.8(7)	C9-C10-C11	121.0(7)
C16-C17-C69	121.6(6)	C4-C5-C6	120.5(7)
C18-C17-C69	124.5(6)	C60-C61-C64	108.8(6)
C14-C15-C16	119.5(7)	C60-C61-C62	109.2(6)
C64-C61-C62	110.6(6)	C10-C11-C13	115.6(6)
C60-C61-C63	109.6(6)	C12-C11-C13	124.0(6)
C64-C61-C63	109.5(6)	C36-C35-C34	116.3(7)
C62-C61-C63	109.1(6)	C36-C35-C85	122.9(6)
C10-C11-C12	120.4(6)	C34-C35-C85	120.8(6)
C51-C50-C49	121.0(8)	C53-C52-C51	121.5(8)
C15-C16-C17	123.8(7)	C26-C27-C28	122.0(7)
C9-C8-C7	122.2(7)	C43-C44-C45	121.1(8)
C40-C41-C42	121.3(7)	C20-C81-C84	111.6(6)
C29-C28-C27	120.0(7)	C83-C81-C82	108.7(6)
C83-C81-C20	110.4(6)	C20-C81-C82	111.1(6)
C83-C81-C84	107.8(7)	C84-C81-C82	107.0(7)
C17-C69-C71	107.8(6)	C20-C21-C22	123.1(7)
C17-C69-C72	114.6(6)	C71-C69-C70	108.6(7)
C71-C69-C72	110.8(8)	C72-C69-C70	104.6(7)
C17-C69-C70	110.3(6)		

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [^{t}BuOCO]W=CHC(CH$_3$)$_3$(μ-^{t}BuOCHO)W{=CHC(CH$_3$)$_3$[^{t}BuOCO] (**12**$_{therm}$).). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W1	23(1)	23(1)	23(1)	2(1)	4(1)	-2(1)
W2	34(1)	18(1)	23(1)	0(1)	7(1)	1(1)
O5	26(3)	30(3)	22(3)	0(2)	4(2)	-6(2)
O4	38(3)	20(3)	32(3)	-2(2)	5(2)	1(2)
O3	35(3)	21(3)	23(3)	5(2)	12(2)	0(2)
O1	31(3)	21(3)	18(3)	3(2)	1(2)	-1(2)
O6	37(3)	21(3)	29(3)	1(2)	10(2)	-4(2)
C12	27(4)	19(4)	23(4)	-6(3)	9(3)	-2(3)
C48	43(5)	19(4)	17(4)	0(3)	9(3)	12(3)
C25	30(4)	23(4)	21(4)	-4(3)	11(3)	-1(3)
C29	27(4)	25(4)	17(4)	-8(3)	1(3)	5(3)
C9	23(4)	41(5)	28(4)	0(4)	-3(3)	-7(4)
C30	25(4)	28(4)	28(5)	-3(3)	-2(3)	12(3)
C47	53(5)	24(4)	26(4)	9(3)	21(4)	2(4)
C20	23(4)	28(4)	36(5)	3(4)	4(3)	2(3)
C36	18(4)	35(4)	16(4)	1(3)	-1(3)	3(3)
C51	56(6)	64(7)	29(5)	5(4)	5(5)	28(5)
C2	25(4)	23(4)	28(4)	-2(4)	4(3)	2(3)
C49	40(5)	25(4)	23(4)	-2(3)	12(4)	11(4)
C26	36(4)	23(4)	20(4)	2(3)	6(3)	9(4)
C60	37(5)	21(4)	25(4)	3(3)	6(3)	6(3)
C31	26(4)	29(4)	18(4)	-8(3)	-1(3)	1(4)
C19	31(4)	13(4)	25(4)	2(3)	8(3)	2(3)
C1	26(4)	24(4)	19(4)	0(3)	6(3)	5(3)
C23	38(5)	29(4)	35(5)	2(4)	13(4)	8(4)
C6	25(4)	19(4)	26(4)	-1(3)	2(3)	7(3)
C37	32(4)	22(4)	15(4)	-4(3)	3(3)	1(3)
C7	30(4)	21(4)	26(4)	-8(3)	8(3)	4(3)
C24	26(4)	13(4)	35(5)	4(3)	6(4)	3(3)
C56	40(5)	32(5)	26(5)	3(4)	9(4)	-3(4)

C13	28(4)	22(4)	29(4)	-2(3)	10(3)	-5(3)
C77	36(5)	42(5)	32(5)	-5(4)	-4(4)	-6(4)
C65	34(5)	27(4)	28(5)	-3(3)	3(4)	-8(3)
C42	36(5)	31(4)	18(4)	-2(3)	2(3)	-7(4)
C54	46(5)	22(4)	23(4)	-3(3)	11(4)	13(4)
C3	34(5)	26(4)	37(5)	13(4)	10(4)	-9(4)
C18	36(5)	19(4)	34(5)	-2(3)	13(4)	-10(3)
C53	44(5)	38(5)	30(5)	-4(4)	4(4)	10(4)
C17	32(5)	31(4)	28(4)	2(3)	0(3)	-6(4)
C15	33(5)	46(5)	42(5)	11(4)	13(4)	-10(4)
C10	26(4)	26(4)	31(5)	-1(3)	7(4)	2(3)
C5	29(4)	36(5)	17(4)	3(3)	-5(3)	-1(4)
C61	45(5)	24(4)	29(5)	-1(3)	11(4)	6(4)
C11	23(4)	24(4)	25(4)	-5(3)	6(3)	0(3)
C35	33(4)	27(4)	29(4)	1(3)	1(3)	-6(3)
C52	49(6)	55(6)	27(5)	-9(4)	0(4)	12(5)
C50	61(6)	30(5)	43(6)	3(4)	8(5)	9(4)
C16	42(5)	27(5)	35(5)	1(3)	1(4)	-7(4)
C8	38(5)	41(5)	21(4)	0(4)	3(4)	8(4)
C27	38(5)	35(5)	27(5)	3(4)	0(4)	11(4)
C44	57(6)	33(5)	28(5)	3(4)	11(4)	-16(4)
C41	54(6)	54(6)	35(5)	-3(4)	15(4)	-23(5)
C28	33(5)	30(4)	29(5)	-12(4)	-2(4)	4(4)
C81	31(5)	51(5)	37(5)	0(4)	0(4)	0(4)
C21	31(5)	46(5)	42(5)	13(4)	5(4)	2(4)
C69	34(5)	39(5)	34(5)	5(4)	3(4)	-1(4)
C79	57(6)	41(5)	69(7)	-30(5)	15(5)	-2(5)
C14	36(5)	32(5)	34(5)	0(4)	8(4)	-4(4)
C33	24(5)	65(6)	61(6)	4(5)	17(4)	-10(5)
C32	30(5)	46(5)	41(5)	-10(4)	1(4)	4(4)
C39	36(5)	66(6)	30(5)	-2(4)	-7(4)	4(4)
C87	90(8)	23(5)	123(9)	14(5)	16(7)	-14(5)
C78	58(6)	40(5)	48(6)	-7(4)	11(5)	-8(4)
C34	36(5)	37(5)	58(6)	7(4)	11(4)	-9(4)
C38	27(4)	31(5)	26(5)	-7(3)	-5(3)	-1(3)

C4	48(5)	32(5)	22(4)	13(3)	2(4)	-2(4)
C43	48(5)	28(4)	18(4)	-3(3)	13(4)	-6(4)
C62	81(7)	38(5)	49(6)	-15(4)	20(5)	-2(5)
C40	30(5)	66(6)	41(6)	-2(5)	1(4)	-2(4)
C22	33(5)	35(5)	55(6)	12(4)	24(4)	5(4)
C64	57(6)	61(6)	43(6)	1(4)	20(5)	11(5)
C66	43(6)	46(5)	64(7)	-2(5)	-9(5)	-12(4)
C63	65(6)	54(6)	27(5)	-6(4)	12(4)	16(5)
C46	63(6)	46(6)	39(5)	16(4)	3(5)	-2(5)
C71	63(7)	93(8)	86(8)	-18(7)	-34(6)	24(6)
C88	178(13)	34(6)	103(10)	-30(6)	60(9)	-19(7)
C45	75(7)	30(5)	52(6)	5(4)	12(5)	-13(5)
C68	52(6)	35(5)	53(6)	6(4)	0(4)	-15(4)
C83	63(6)	63(6)	37(5)	27(5)	0(4)	7(5)
C70	68(7)	36(5)	100(8)	38(5)	26(6)	14(5)
C72	58(6)	62(6)	72(7)	31(5)	24(5)	33(5)
C85	48(6)	14(4)	80(7)	7(4)	16(5)	-8(4)
O2	24(3)	21(3)	37(3)	3(2)	6(2)	-1(2)
C55	32(4)	21(4)	31(4)	4(3)	0(3)	-8(3)
C73	47(5)	34(5)	27(5)	8(4)	4(4)	10(4)
C59	66(6)	39(5)	50(6)	4(4)	22(5)	17(5)
C58	67(6)	51(6)	42(6)	-12(4)	12(5)	-7(5)
C57	40(5)	55(6)	58(6)	-7(5)	22(4)	-3(4)
C82	50(6)	69(6)	41(6)	-13(5)	1(4)	-3(5)
C80	58(7)	71(7)	51(6)	-11(5)	-13(5)	-11(5)
C67	86(8)	84(7)	40(6)	-32(5)	20(5)	-40(6)
C75	68(8)	151(11)	55(7)	49(7)	4(6)	12(7)
C76	360(20)	131(12)	52(8)	47(7)	-60(10)	-187(14)
C84	36(5)	124(9)	46(6)	11(6)	-10(4)	-2(6)
C74	248(17)	222(16)	123(11)	136(11)	149(12)	200(14)
C86	51(7)	36(6)	198(13)	22(7)	12(7)	19(5)

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