

Electronic Supplementary Information for

Syntheses and Evaluation of κ^2 - β -Diketonate and β -Ketoesterate Tungsten (VI) Oxo- Alkoxide Complexes for Chemical Vapor Deposition of WO_x Thin Films

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Experimental Section

Synthesis of $\text{WO}_2(\text{dpm})_2$ (11a**):** Complex **11a** was obtained as a side product when reacting $[\text{WO}(\text{OCH}_2\text{C}(\text{CH}_3)_3)_4]_2$ (**19**, 0.910 mmol, 1.00 g) and more than 8 equiv Hdpm (8.00 mmol, 1.82 mL, 1.61 g) in THF. The mixture was refluxed for a total of 48 h. The pale yellow waxy residue obtained after removal of volatiles was characterized by NMR to consist of a mixture of **11** and **11a** (Figure S26). ^1H NMR of **11a** (C_6D_6 , 25 °C): δ 5.93 (s, 2H, COCHCO), 1.07 (s, 18H, $\text{C}(\text{CH}_3)_3$), 0.95 (s, 18H, $\text{C}(\text{CH}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR of **11a** (C_6D_6 , 25 °C): δ 205.43 (OC), 194.52 (OC), 95.43 (COCHCO), 41.50 ($\text{C}(\text{CH}_3)_3$), 40.31 ($\text{C}(\text{CH}_3)_3$), 27.52 ($(\text{CH}_3)_3\text{C}$), 27.07 ($(\text{CH}_3)_3\text{C}$). A single crystal selected for X-ray crystallographic study from a sample crystallized in toluene was representative of **11a** (Figure S28). Crystal data and structure refinement for **11a** are shown in Table S3.

Crystallographic Structure Determination of 11a. X-ray intensity data for **11a** were collected at 100 K on a Bruker **DUO** diffractometer using MoK α radiation ($\lambda = 0.71073 \text{ \AA}$) and an APEXII CCD area detector. Raw data frames were read by the program SAINT¹ and integrated using 3D profiling algorithms. The resulting data were reduced to produce hkl reflections and their intensities and estimated standard deviations. The data were corrected for Lorentz and polarization effects and numerical absorption corrections were applied based on indexed and measured faces. The structure was solved and refined in SHELXTL2013,¹ using full-matrix least-squares refinement. The non-H atoms were refined with anisotropic thermal parameters and all of the H atoms were calculated in idealized positions and refined riding on their parent atoms. The asymmetric unit consists of two chemically equivalent but crystallographically independent molecules, and a half pentane solvent molecule (located on an inversion symmetry element). Each molecule has the C19 t-butyl groups disordered and refined in two parts. Check for higher symmetry or a smaller unit cell did not provide any viable options, thus the use of the current space group and unit cell. In the final cycle of refinement, 11486 reflections (of which 8128 are observed with $I > 2\sigma(I)$) were used to refine 569 parameters and the resulting R_1 , wR_2 and S (goodness of fit) were 3.27%, 7.05% and 0.946, respectively. The refinement was carried out by minimizing the wR_2 function using F^2 rather than F values. R_1 is calculated to provide a reference to the conventional R value but its function is not minimized.

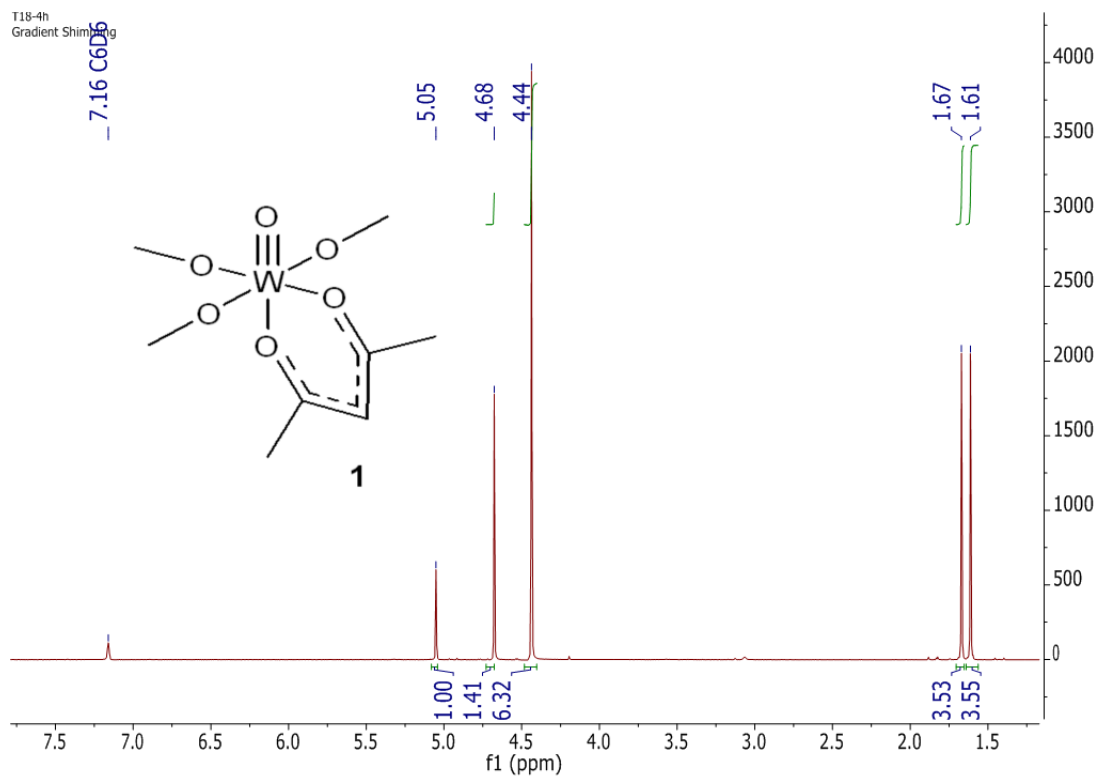


Figure S1: Room temperature ^1H NMR of **1** in C_6D_6 .

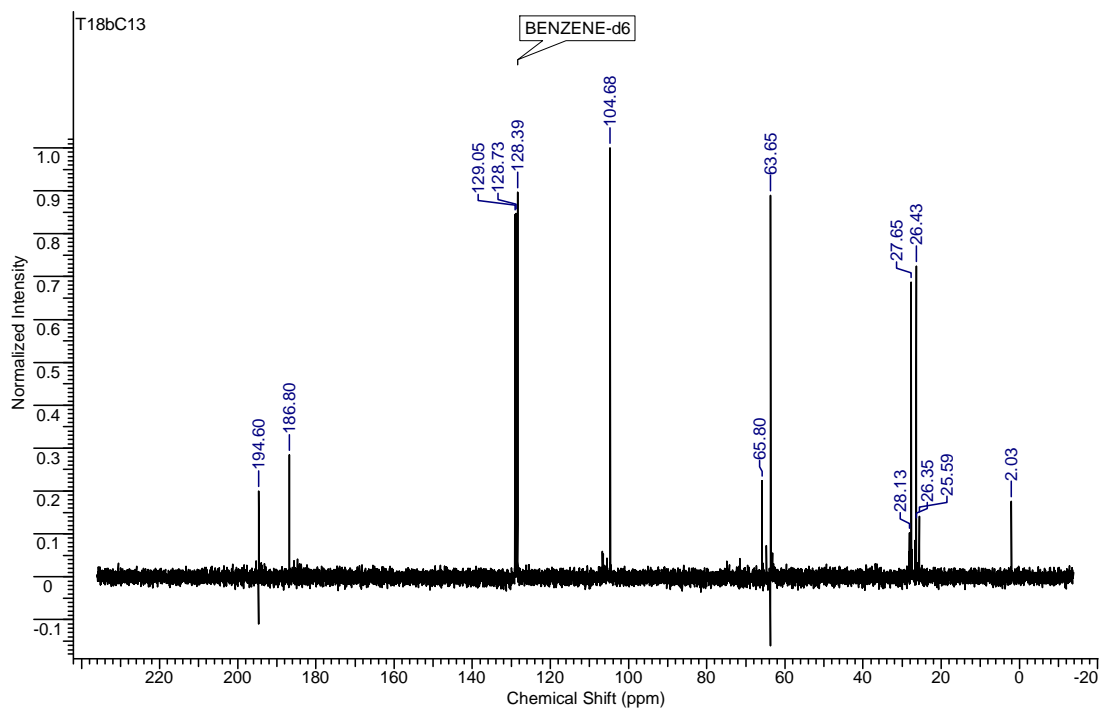


Figure S2: Room temperature ^{13}C NMR of **1** in C_6D_6 .

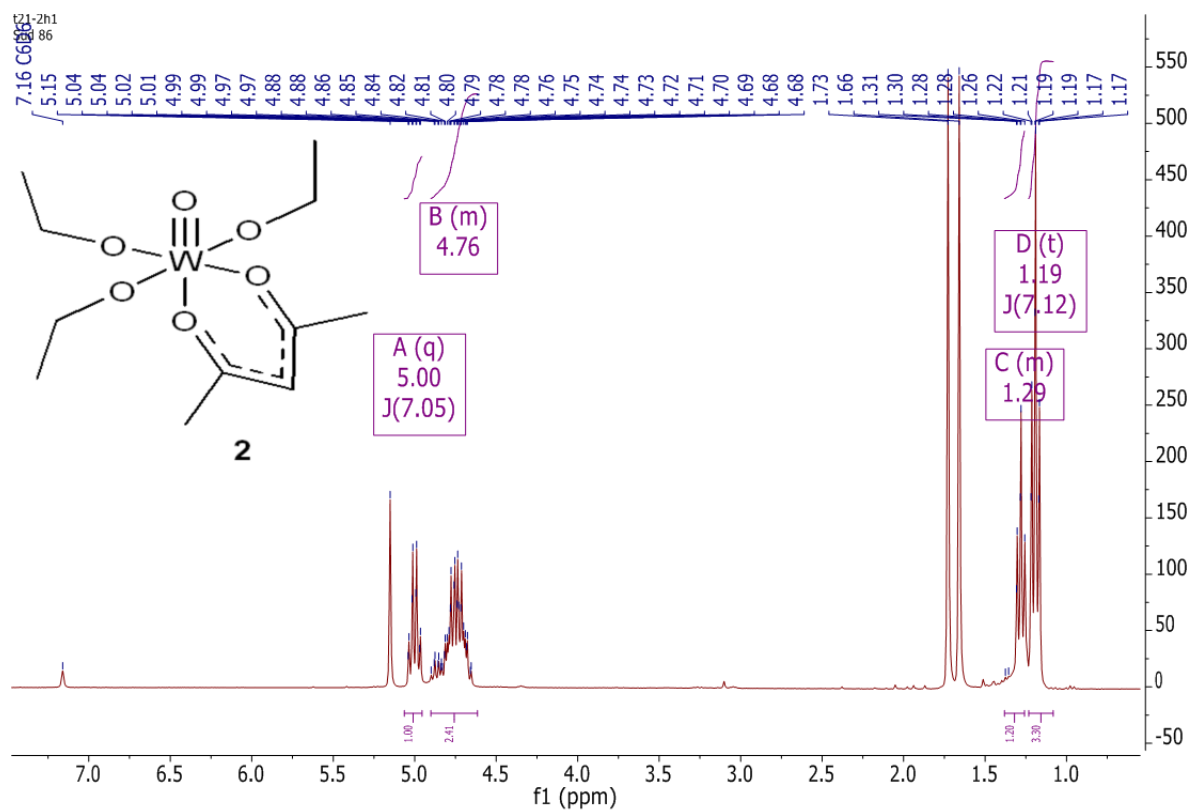


Figure S3: Room temperature ^1H NMR of **2** in C_6D_6 .

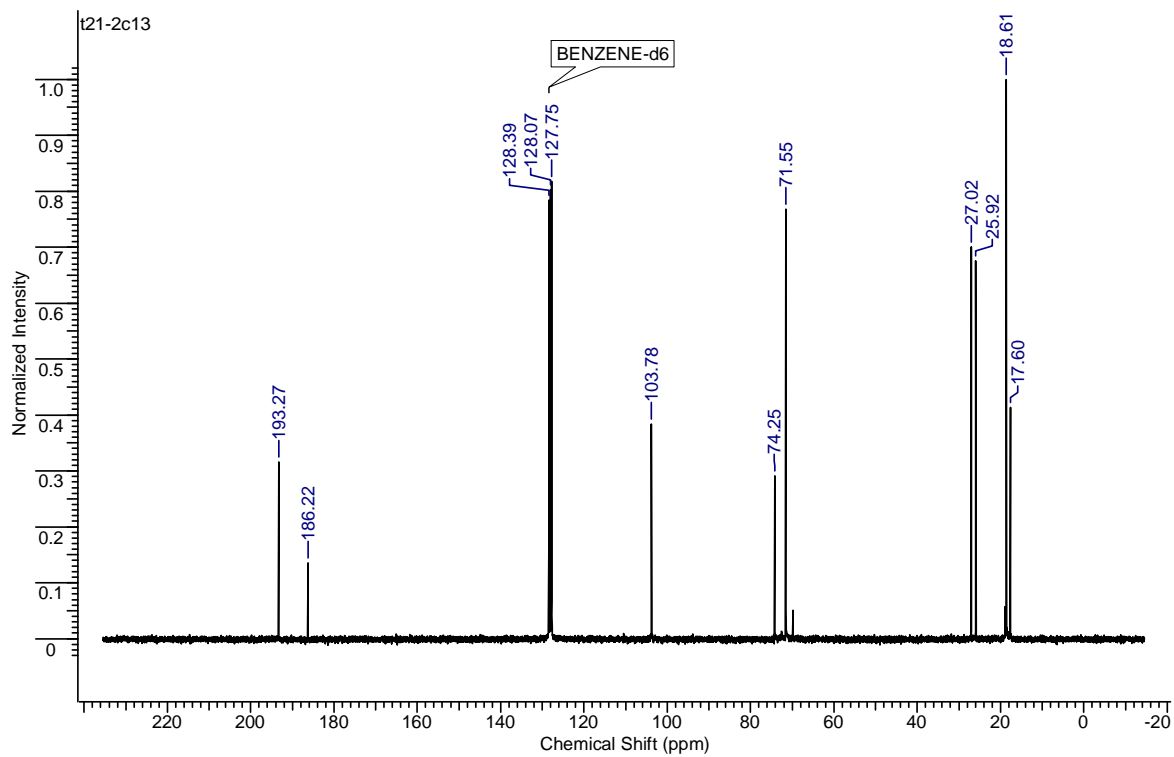


Figure S4: Room temperature ^{13}C NMR of **2** in C_6D_6 .

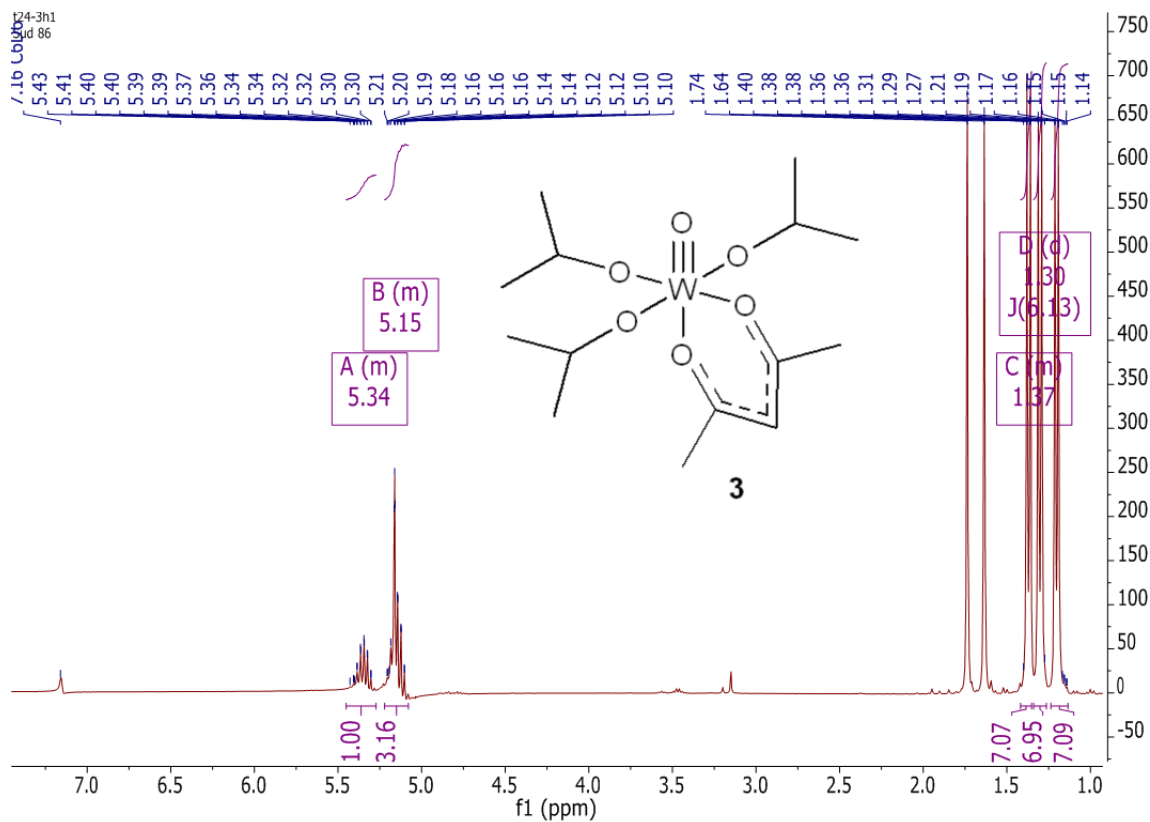


Figure S5: Room temperature ^1H NMR of **3** in C_6D_6 .

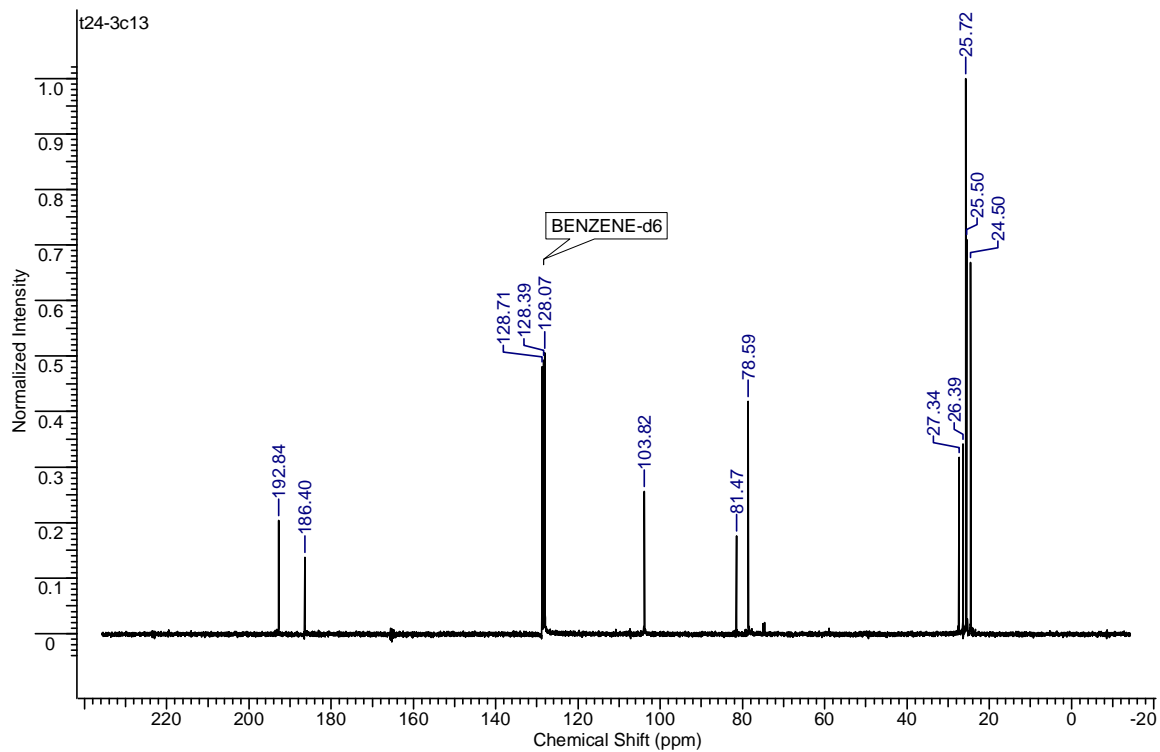


Figure S6: Room temperature ^{13}C NMR of **3** in C_6D_6 .

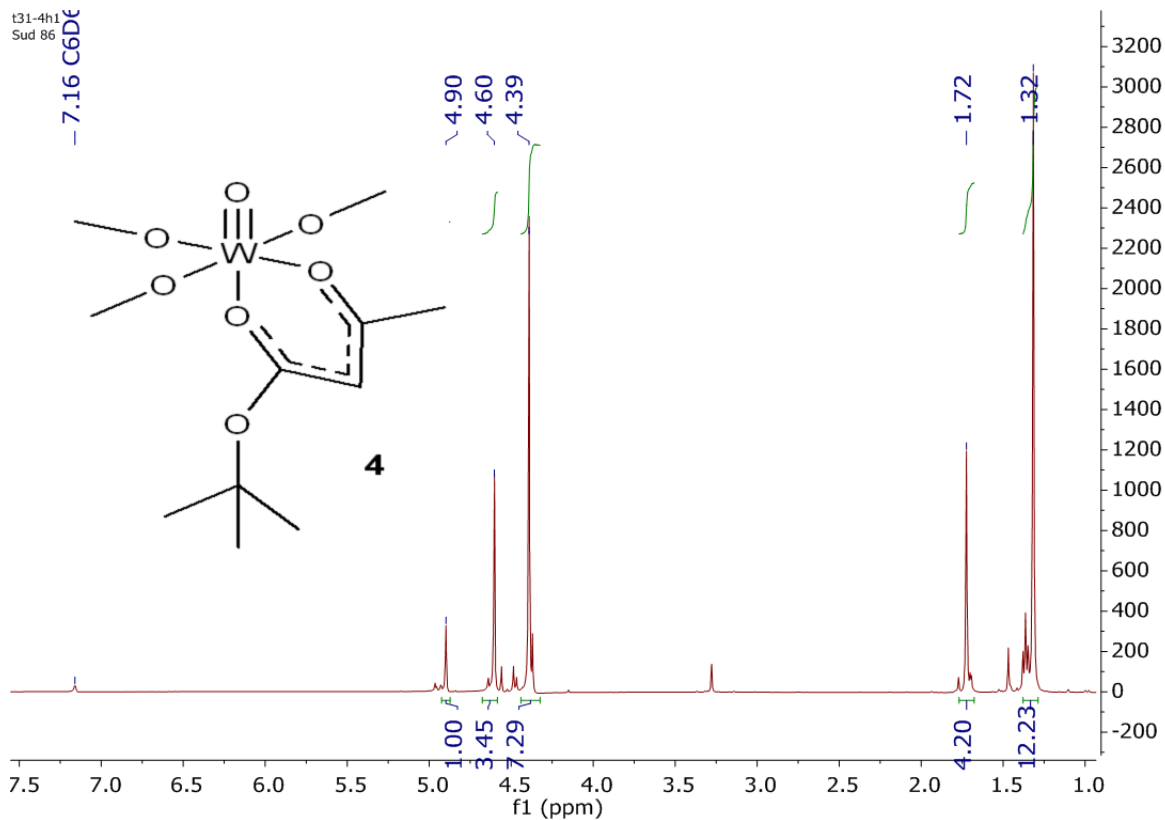


Figure S7: Room temperature ^1H NMR of **4** in C_6D_6 .

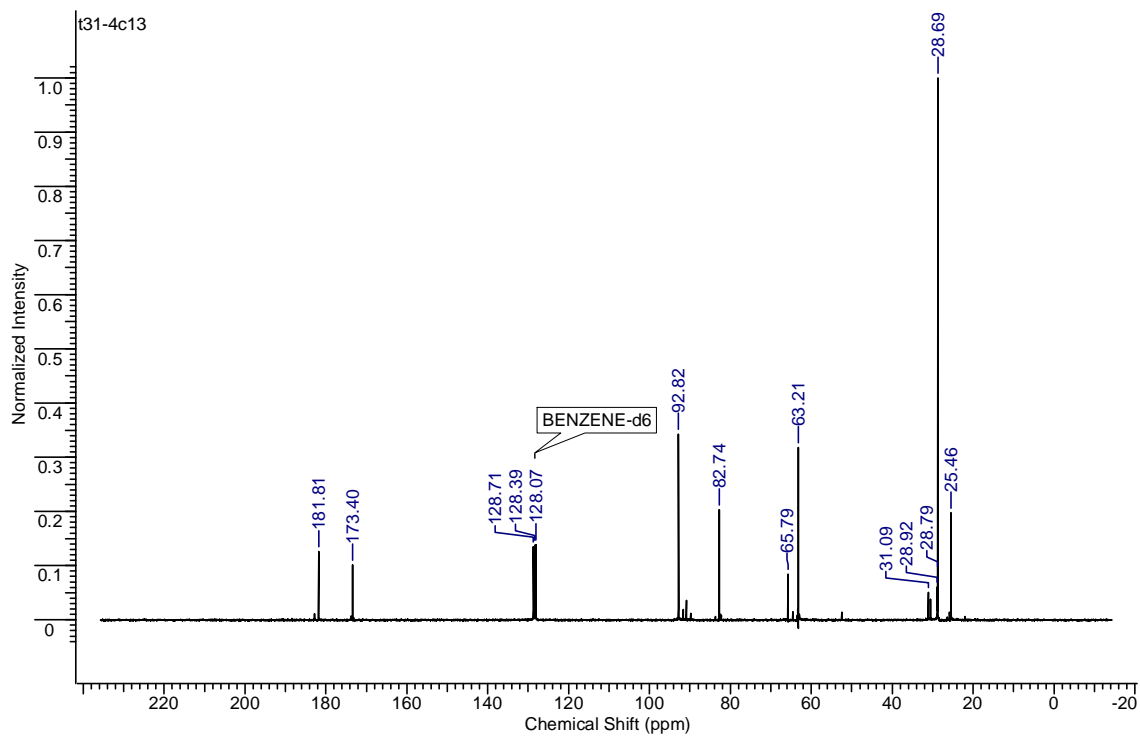


Figure S8: Room temperature ^{13}C NMR of **4** in C_6D_6 .

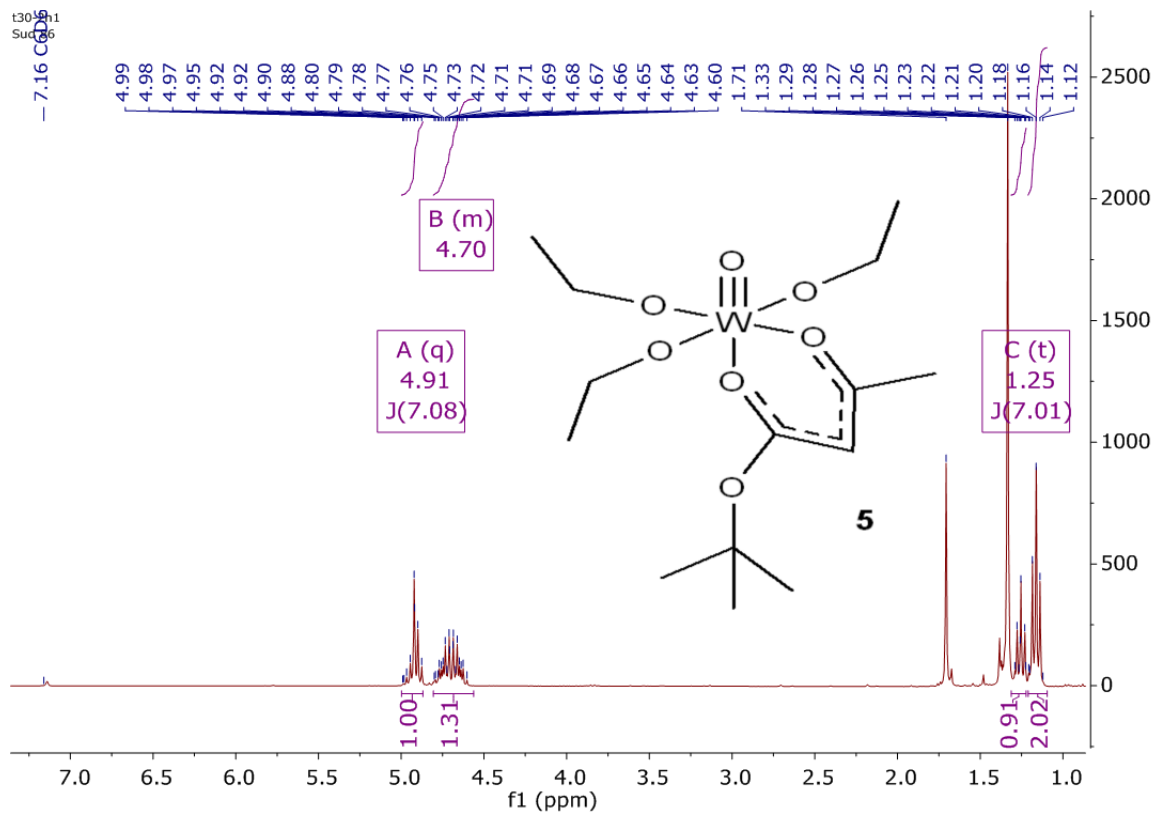


Figure S9: Room temperature ^1H NMR of **5** in C_6D_6 .

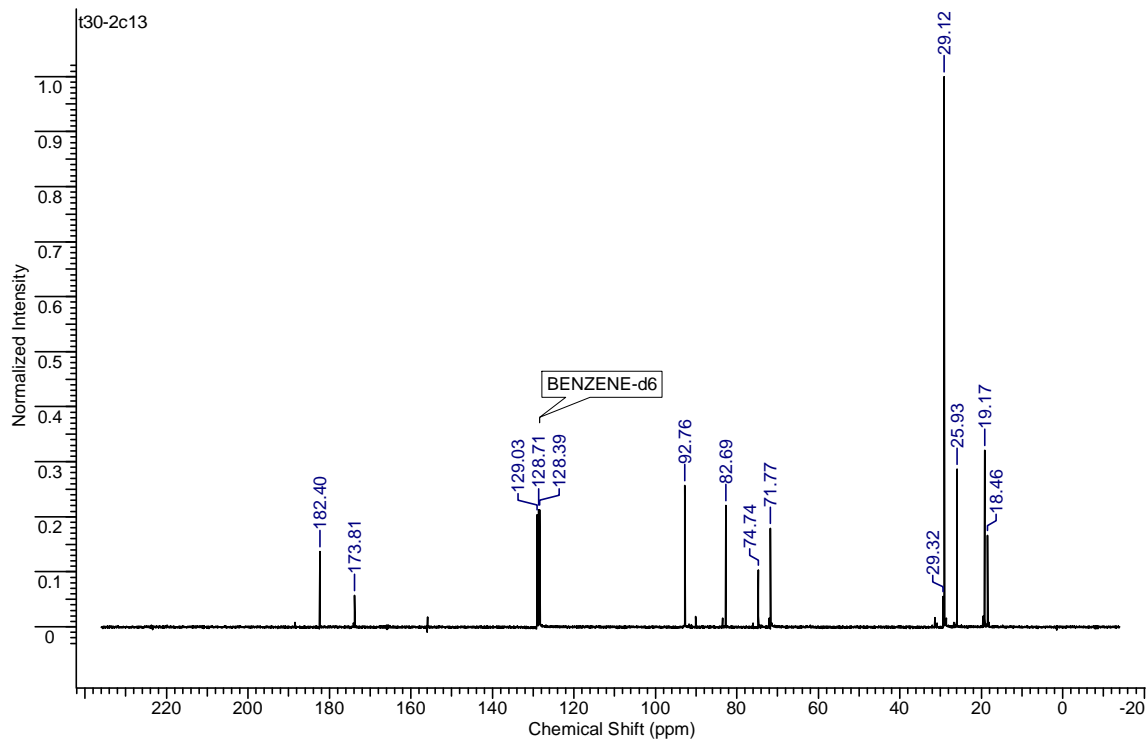


Figure S10: Room temperature ^{13}C NMR of **5** in C_6D_6 .

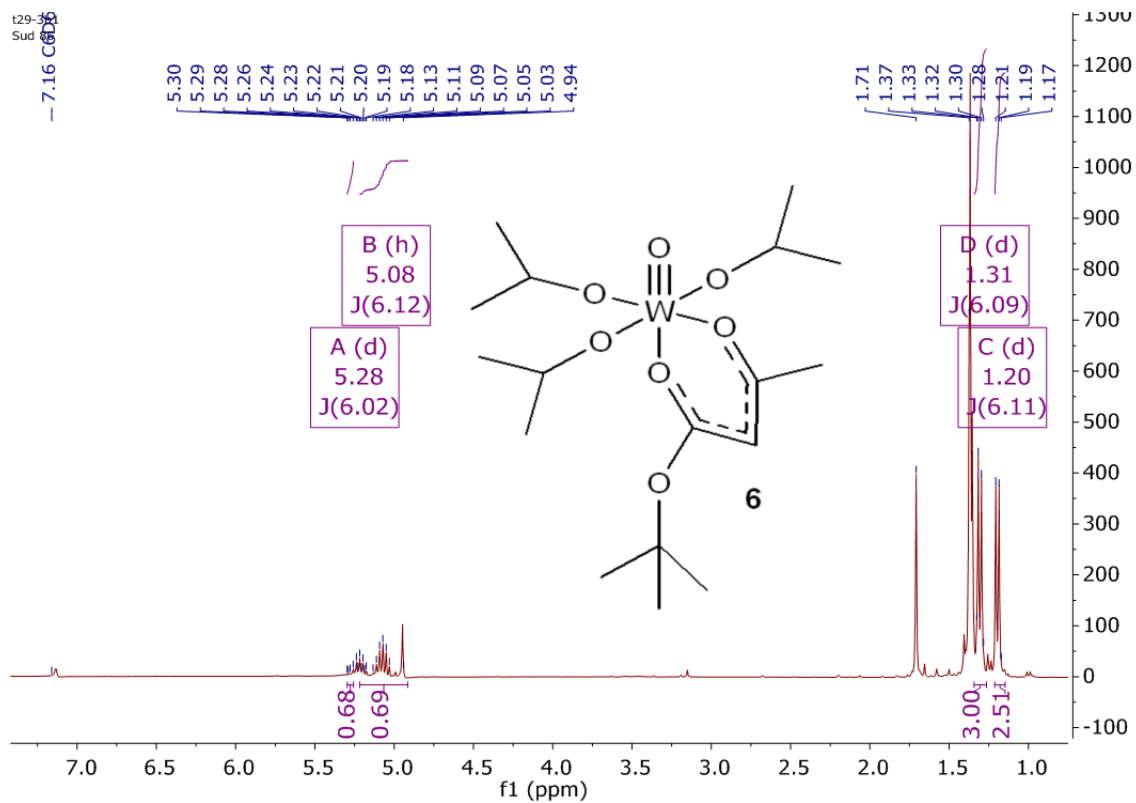


Figure S11: Room temperature ^1H NMR of **6** in C_6D_6 .

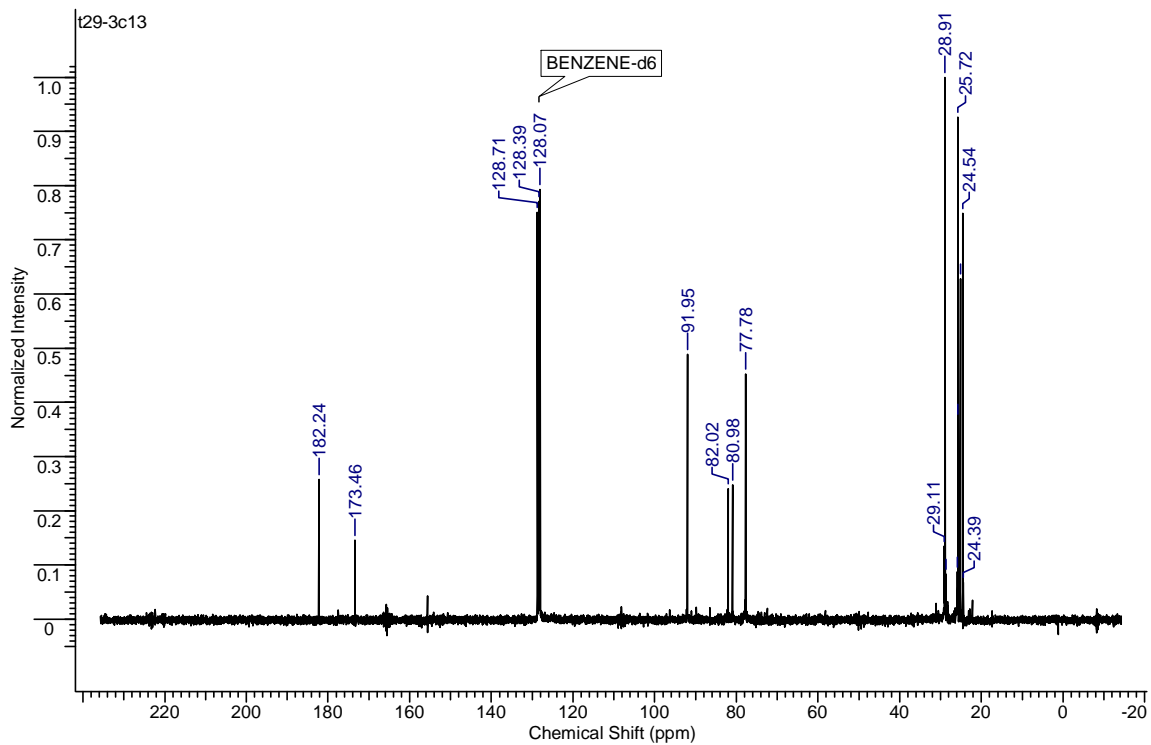


Figure S12: Room temperature ^{13}C NMR of **6** in C_6D_6 .

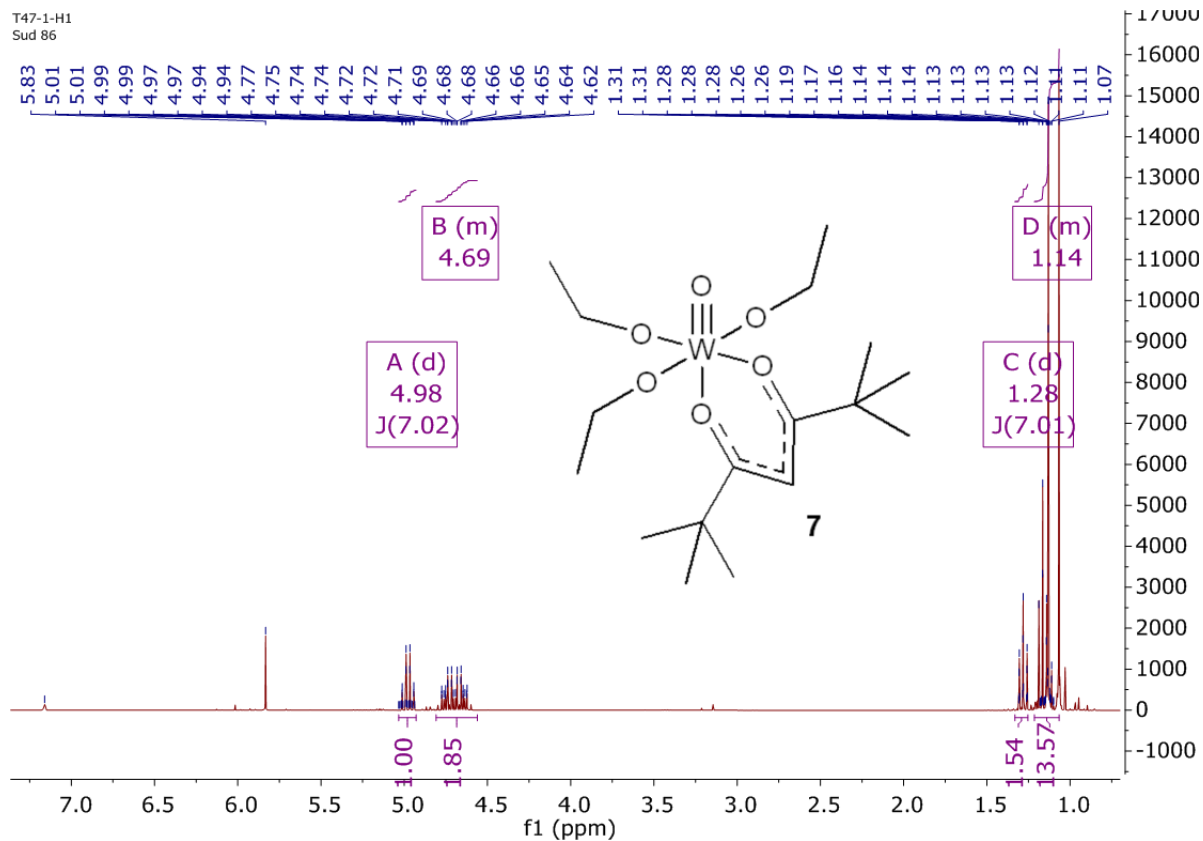


Figure S13: Room temperature ^1H NMR of **7** in C_6D_6 .

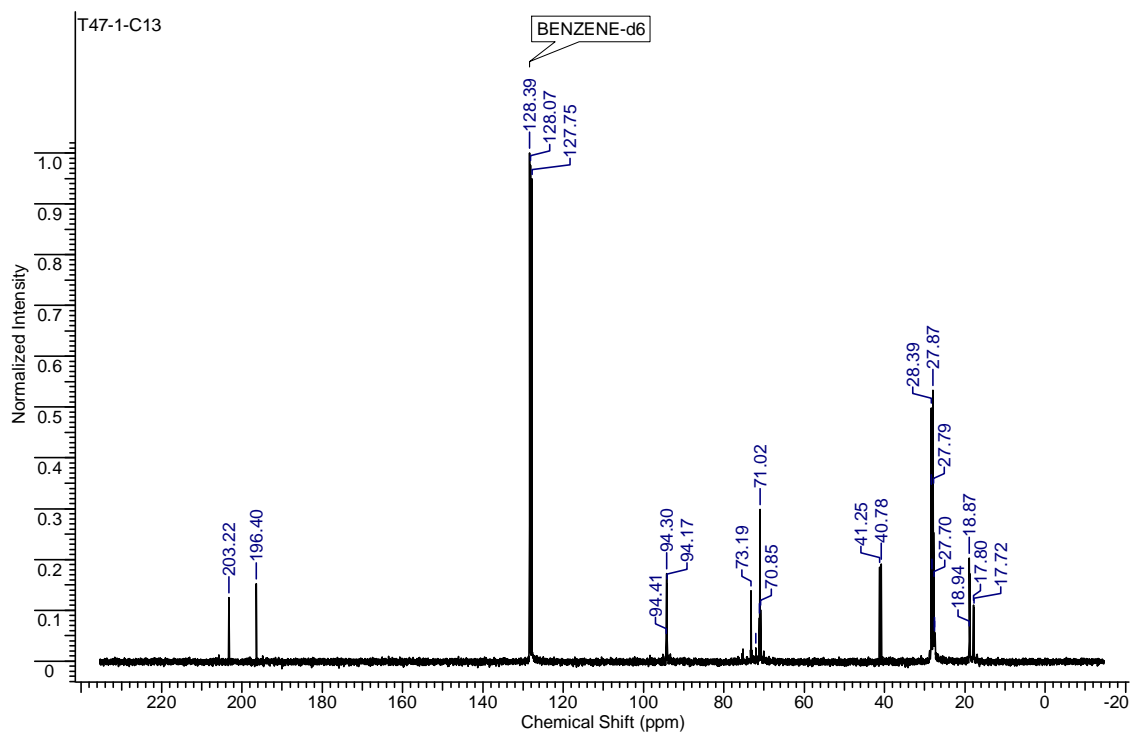


Figure S14: Room temperature ^{13}C NMR of **7** in C_6D_6 .

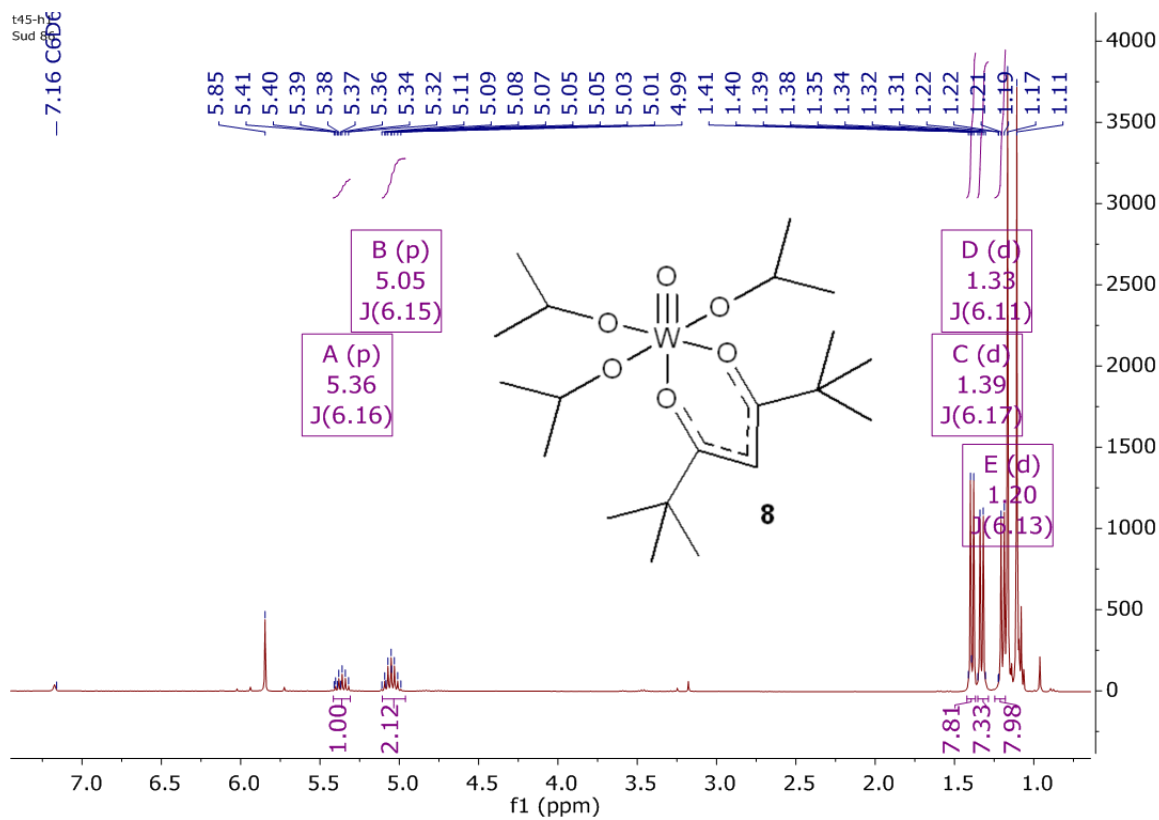


Figure S15: Room temperature ^1H NMR of **8** in C_6D_6 .

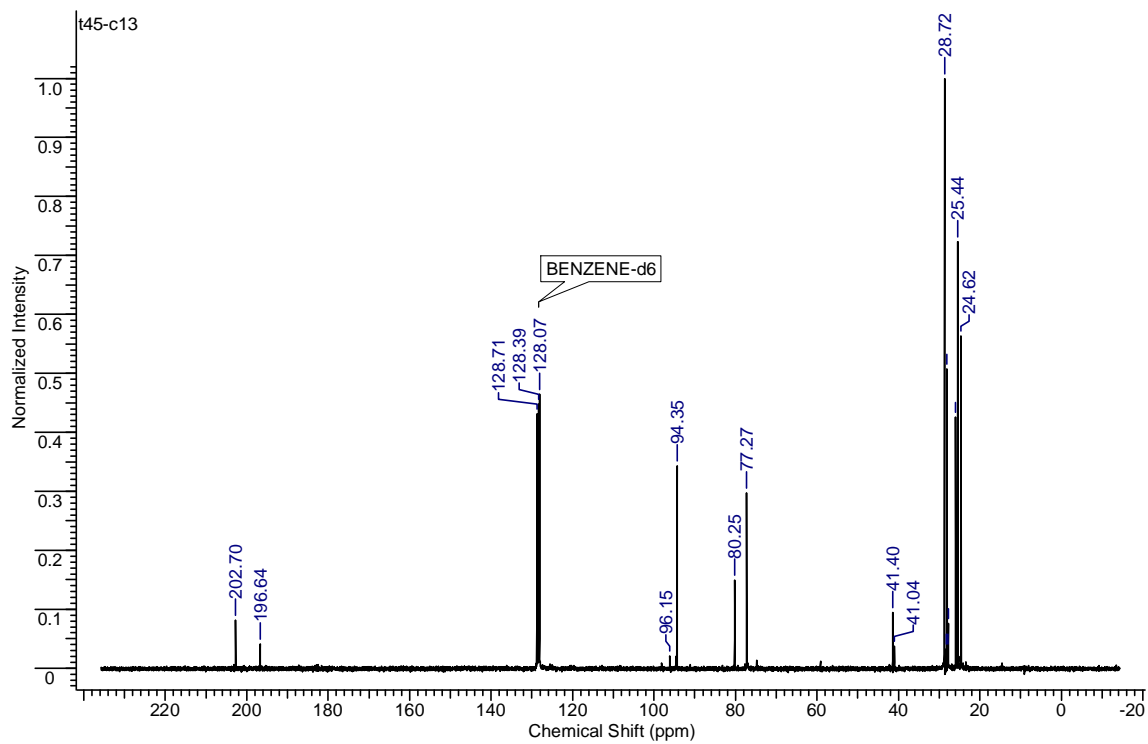


Figure S16: Room temperature ^{13}C NMR of **8** in C_6D_6 .

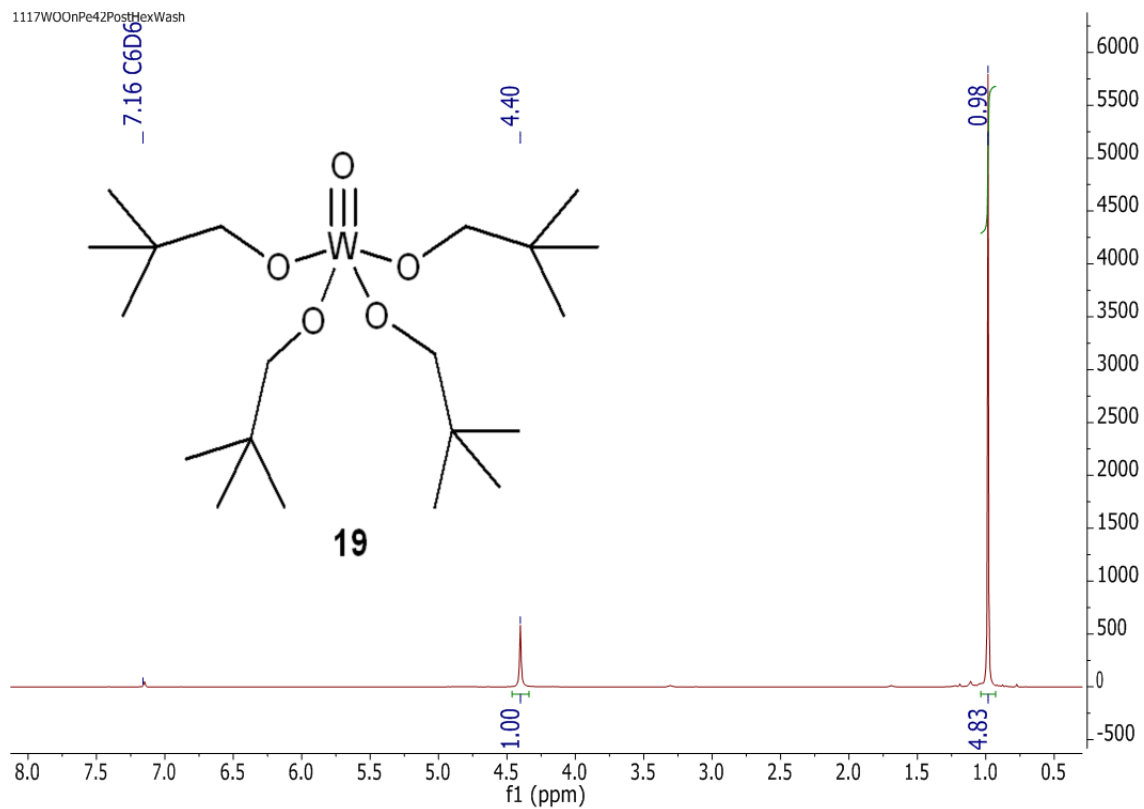


Figure S17a: Room temperature ^1H NMR of **19** in C_6D_6 .

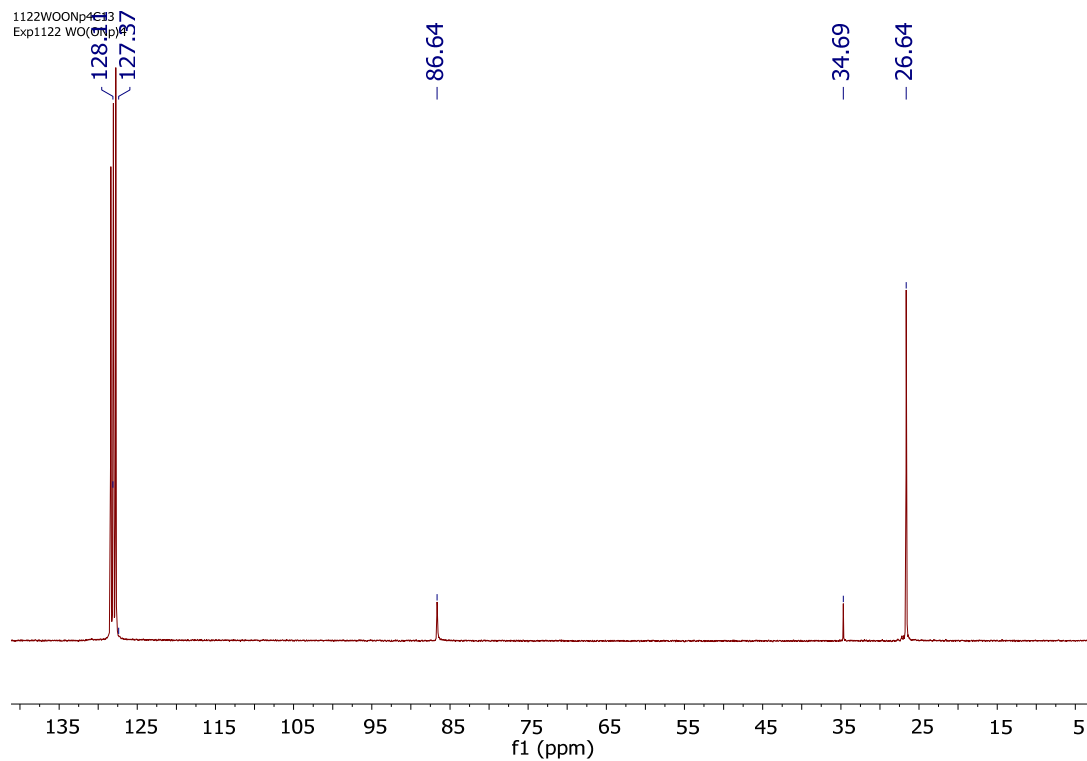


Figure S17b: Room temperature ^{13}C NMR of **19** in C_6D_6 .

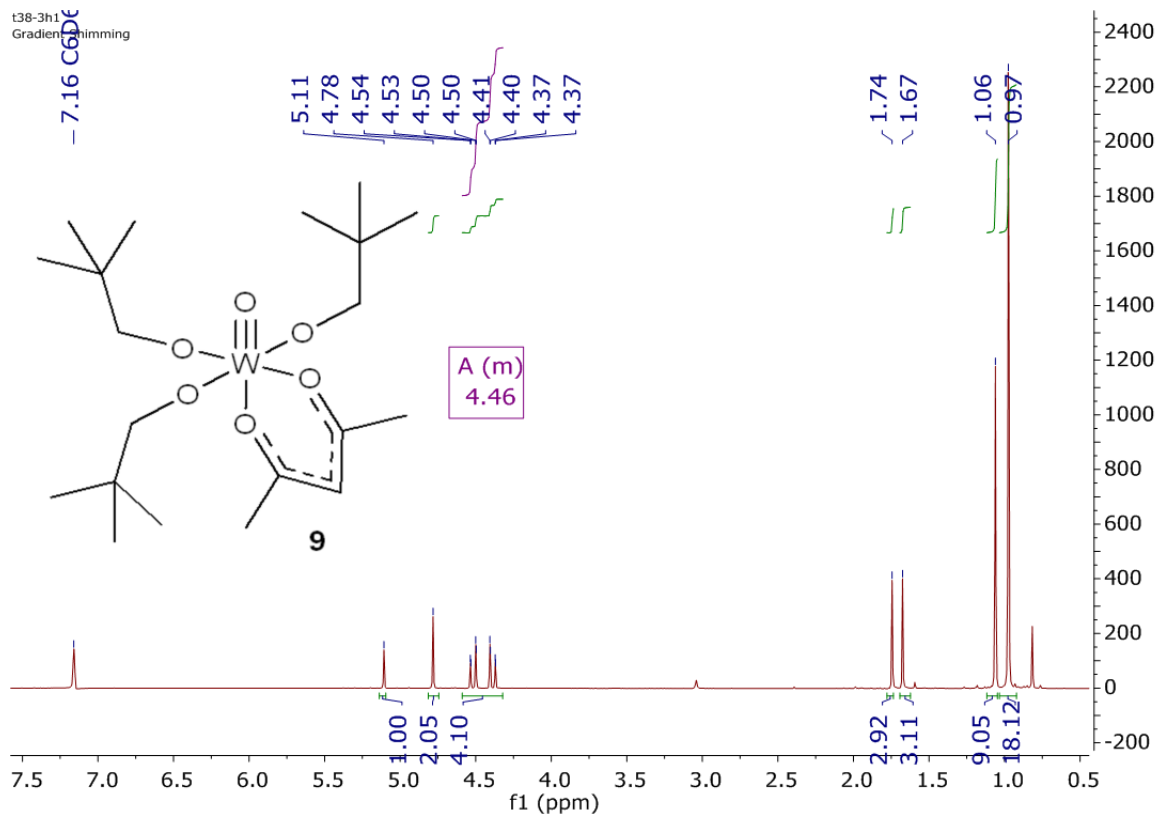


Figure S18: Room temperature ^1H NMR of **9** in C_6D_6 .

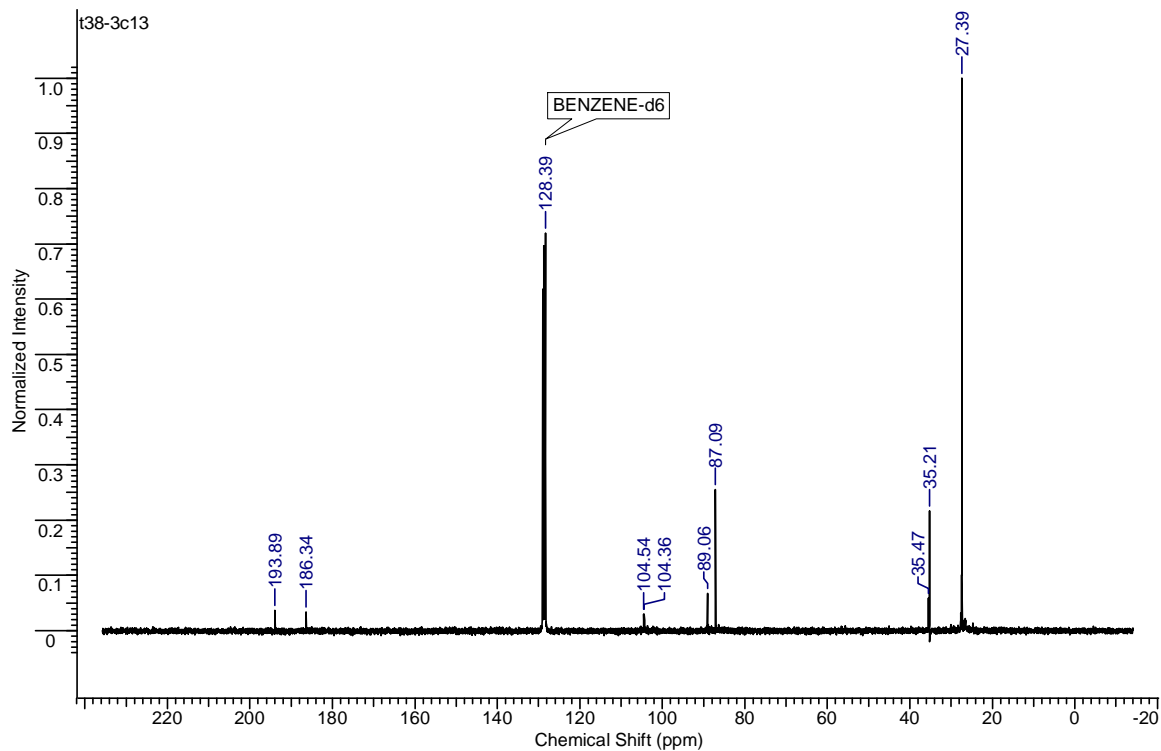


Figure S19: Room temperature ^{13}C NMR of **9** in C_6D_6 .

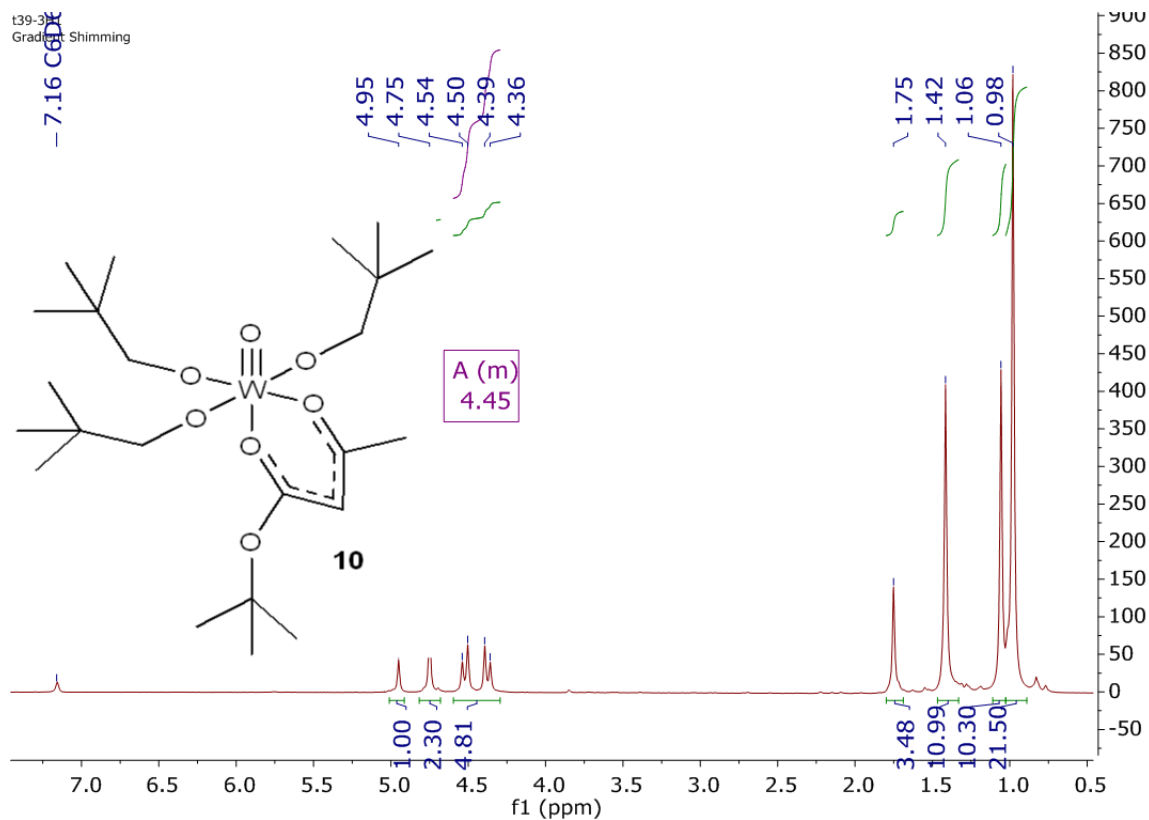


Figure S20: Room temperature ^1H NMR of **10** in C_6D_6 .

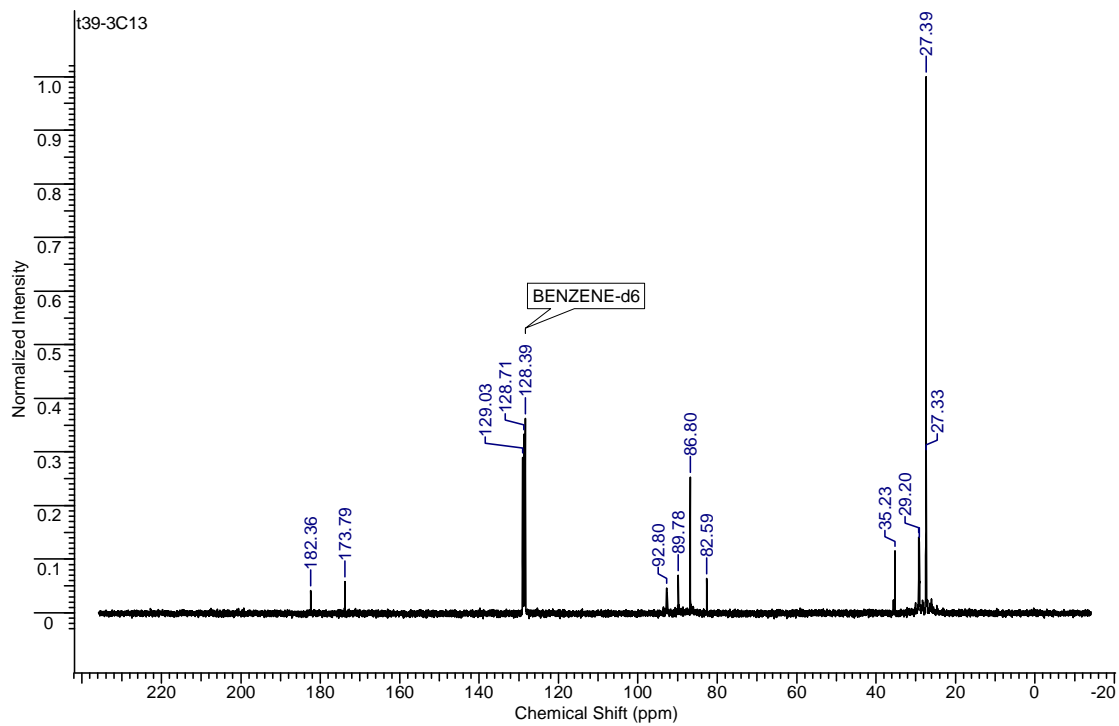


Figure S21: Room temperature ^{13}C NMR of **10** in C_6D_6 .

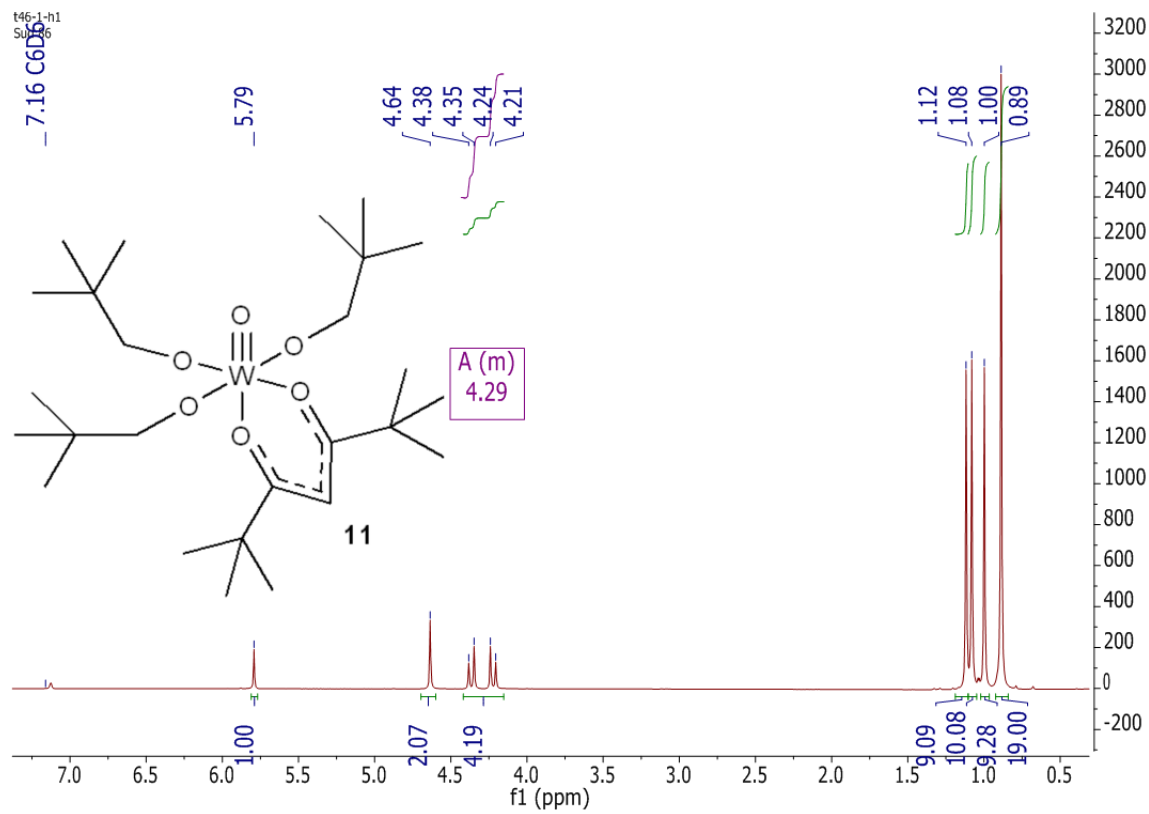


Figure S22a: Room temperature ^1H NMR of **11** in C_6D_6 .

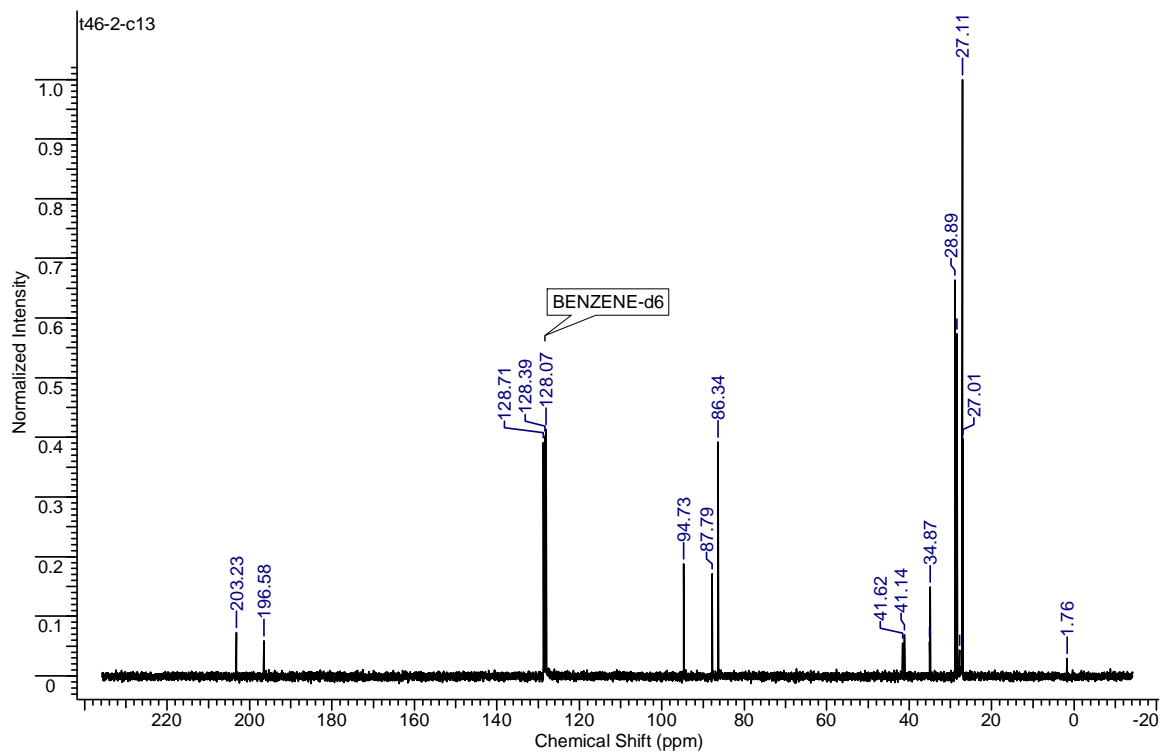


Figure S22b: Room temperature ^{13}C NMR of **11** in C_6D_6 .

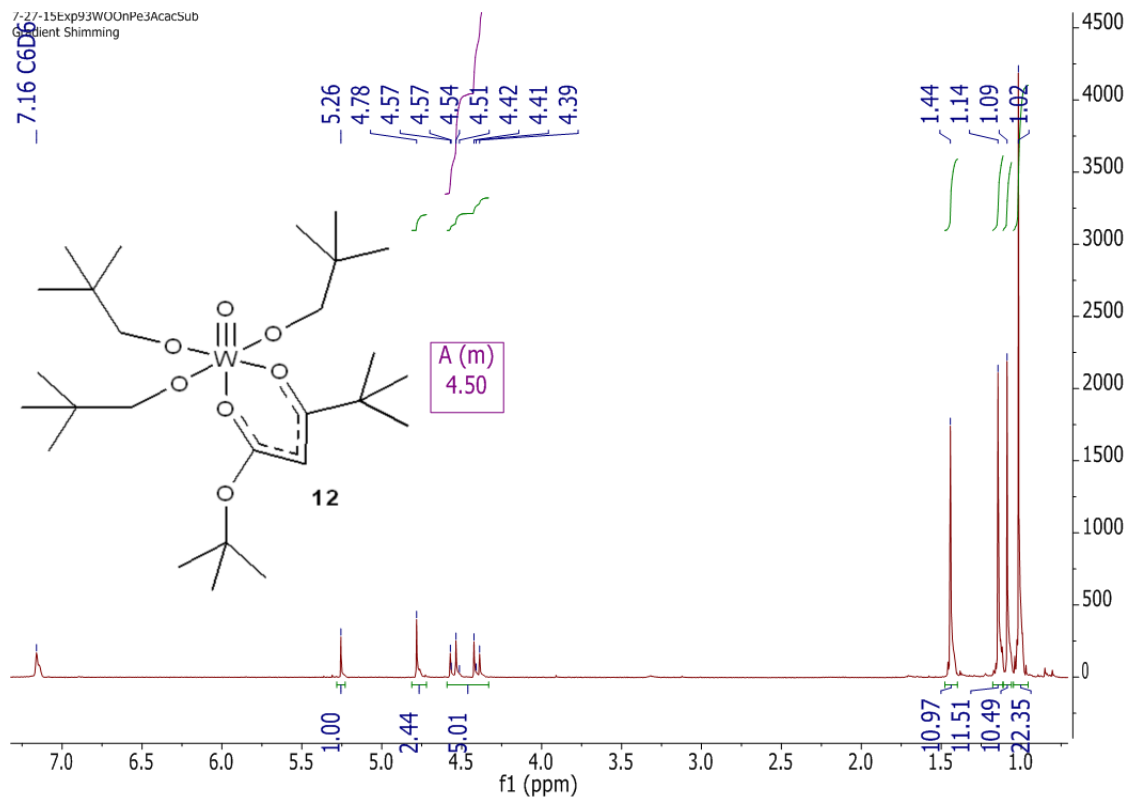


Figure S23: Room temperature ^1H NMR of **12** in C_6D_6 .

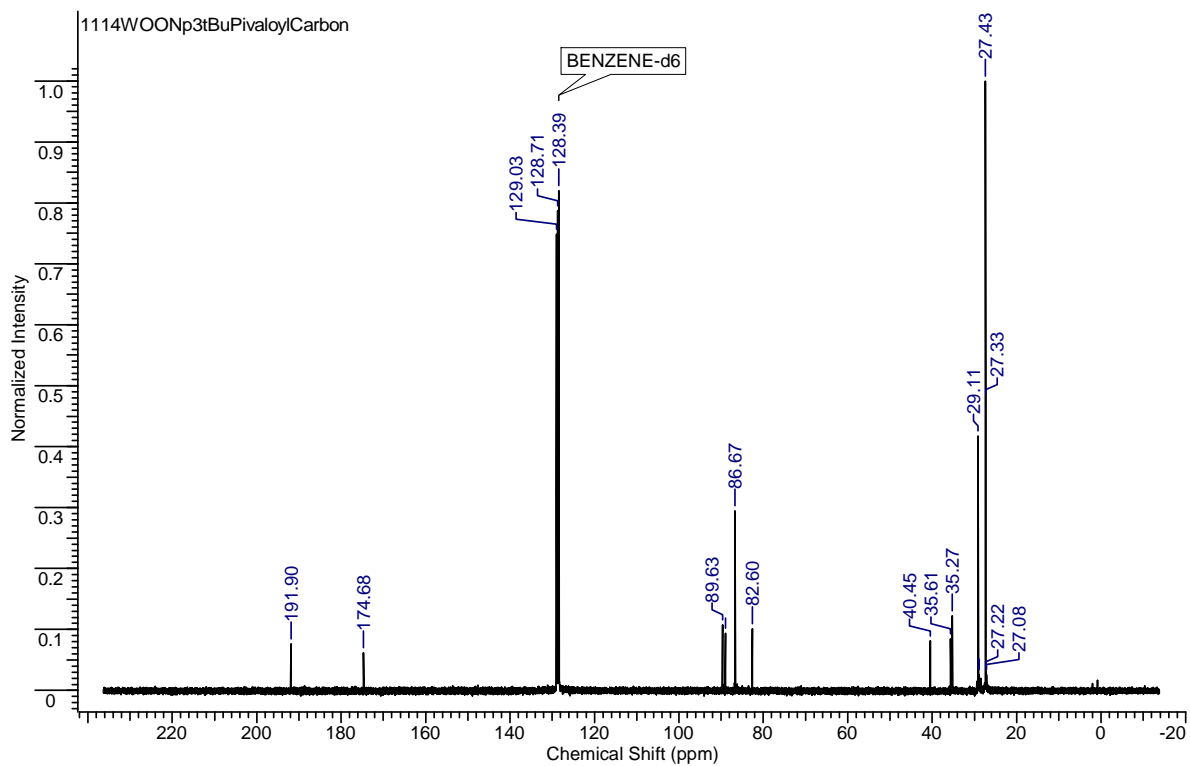


Figure S24: Room temperature ^{13}C NMR of **12** in C_6D_6 .

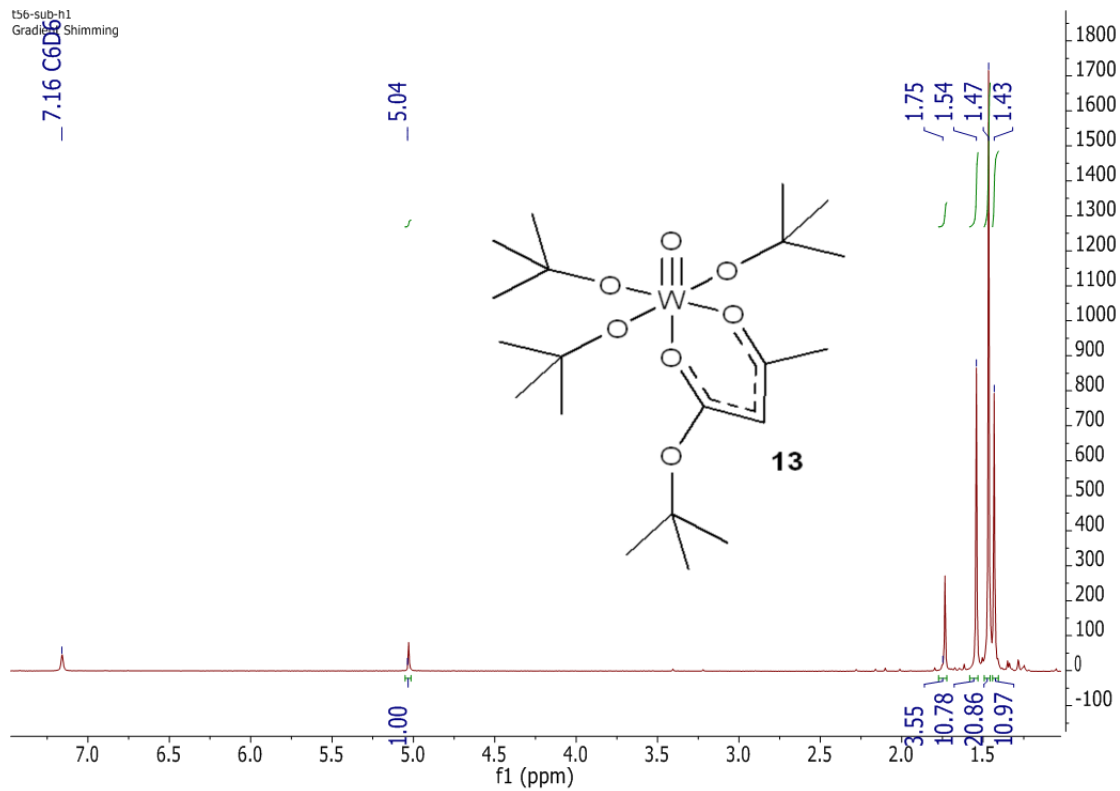


Figure S25a: Room temperature ^1H NMR of **13** in C_6D_6 .

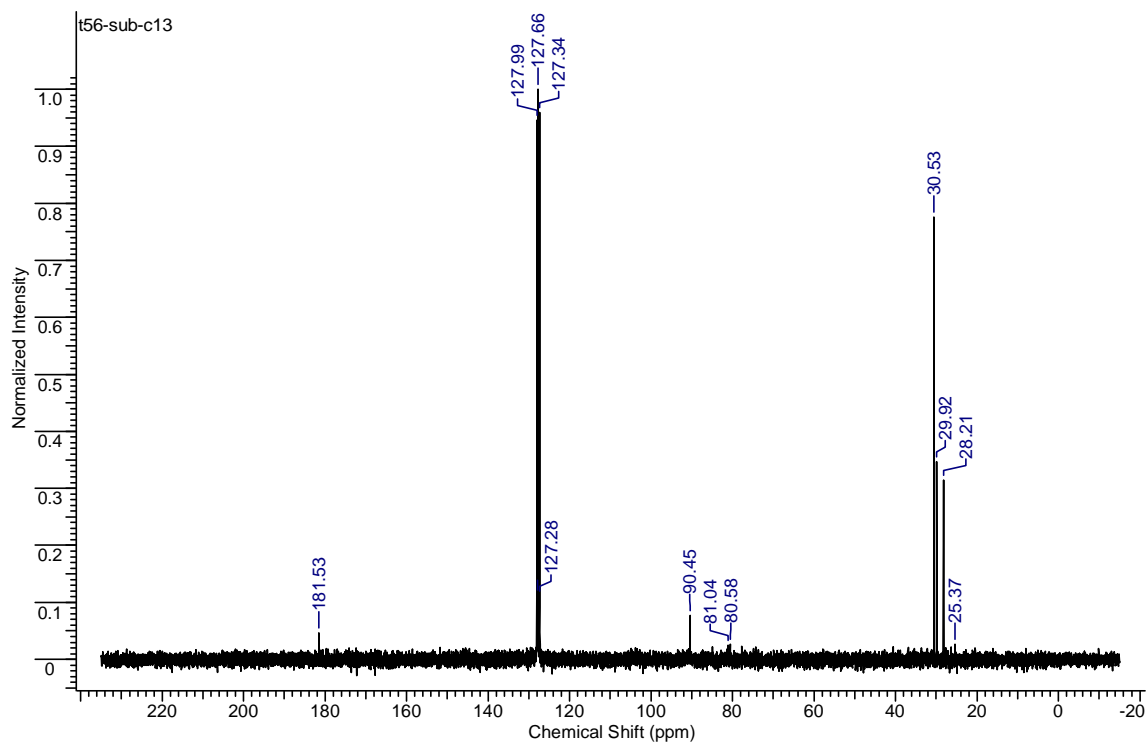


Figure S25b: Room temperature ^{13}C NMR of **13** in C_6D_6 .

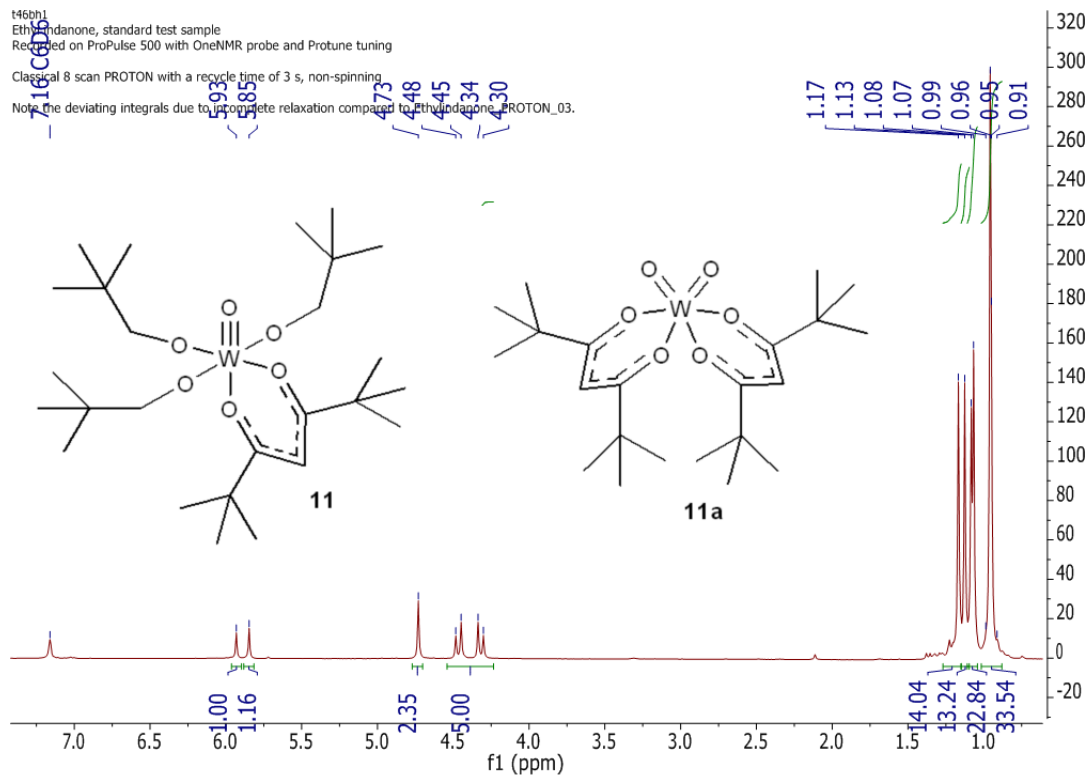


Figure S26a: Room temperature ^1H NMR of **11** and **11a** in C_6D_6 .

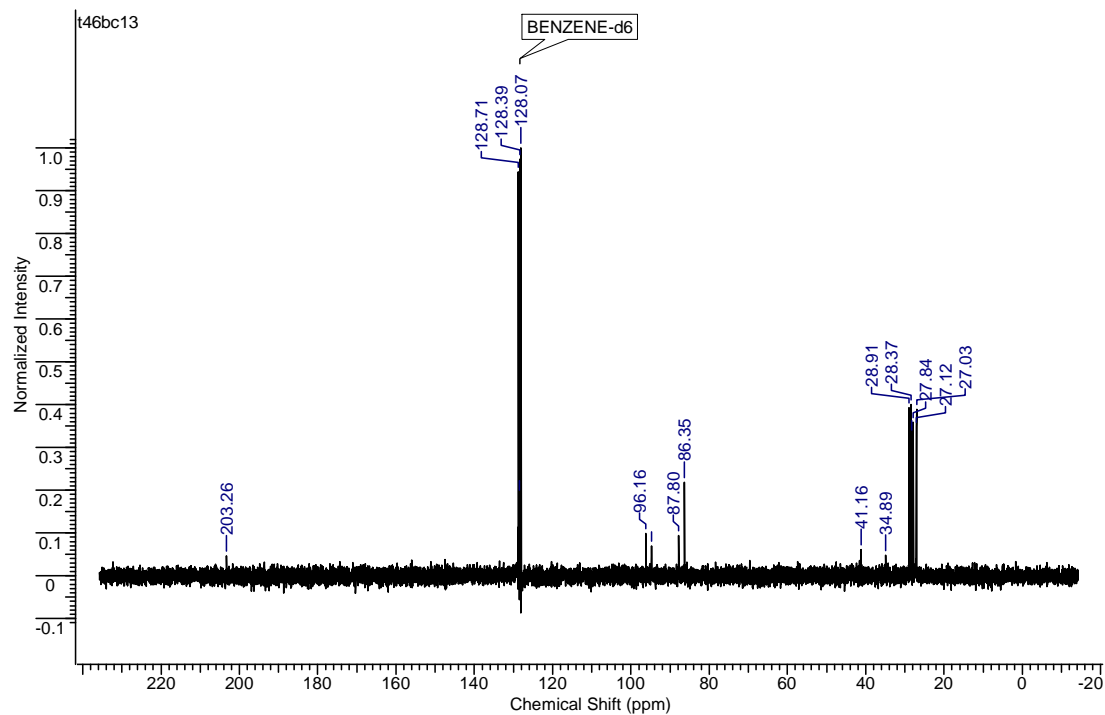


Figure S26b: Room temperature ^{13}C NMR of **11** and **11a** in C_6D_6 .

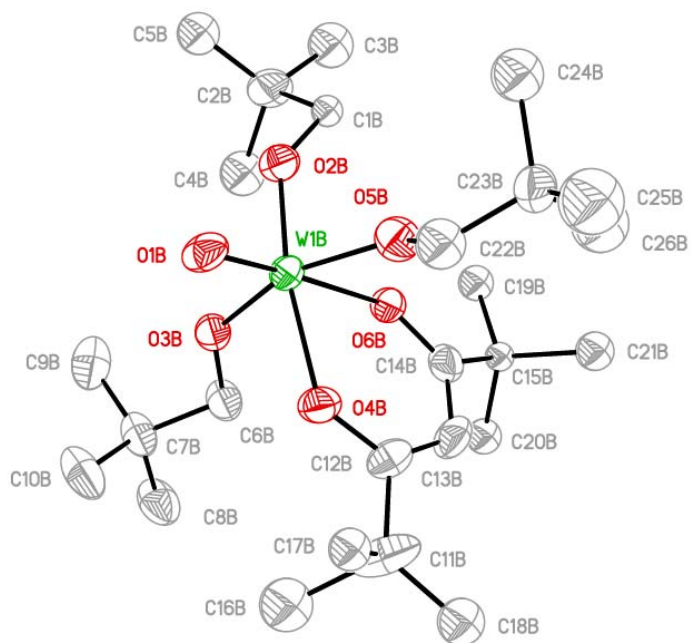
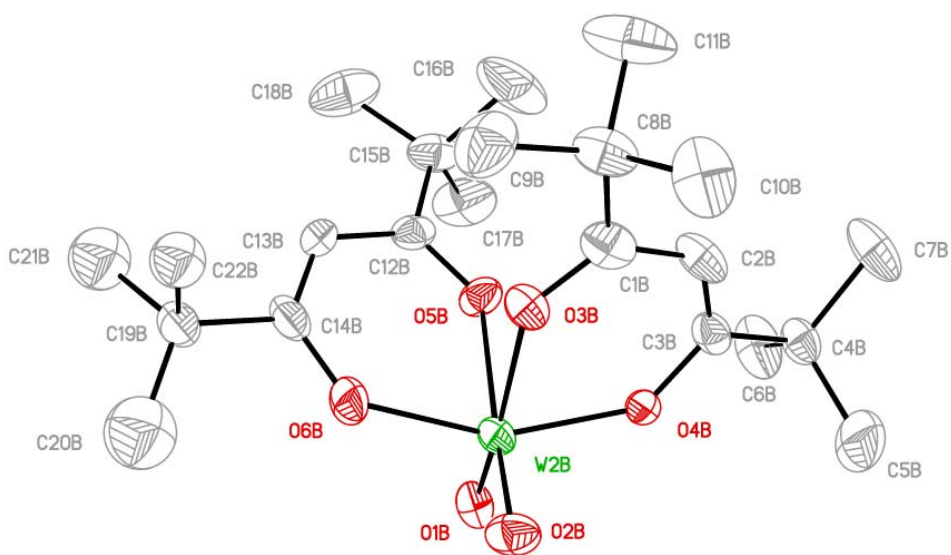
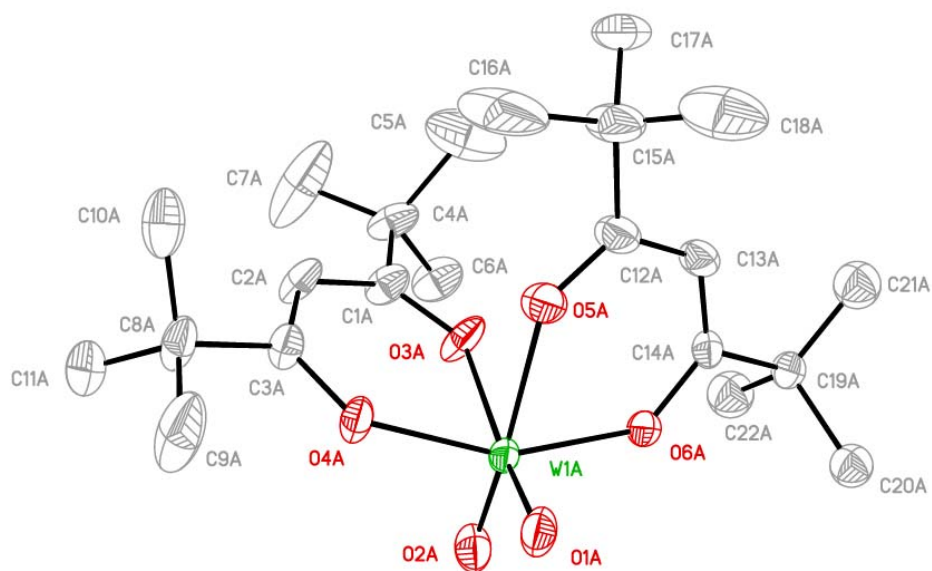


Figure S27. Molecular geometry of a second independent molecule of **11** present in the sample crystallized from toluene.



Figures S28a (top) and S28b (bottom). Molecular geometry of the two independent molecules present in the sample of **11a** crystallized from toluene.

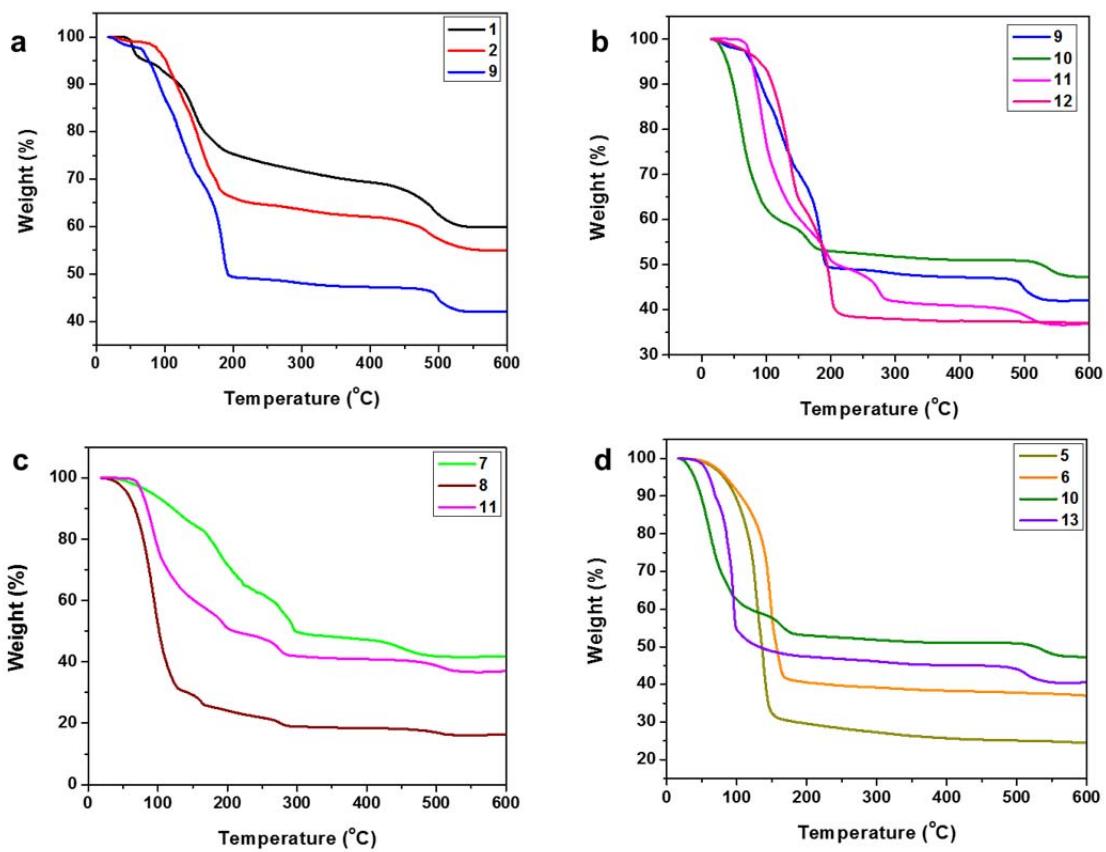


Figure S29. TGA of complexes $WO(OR)_3L$; a) 1, 2, 9, b) 9, 10, 11, 12, c) 7, 8, 11 and d) 5, 6, 10, 13.

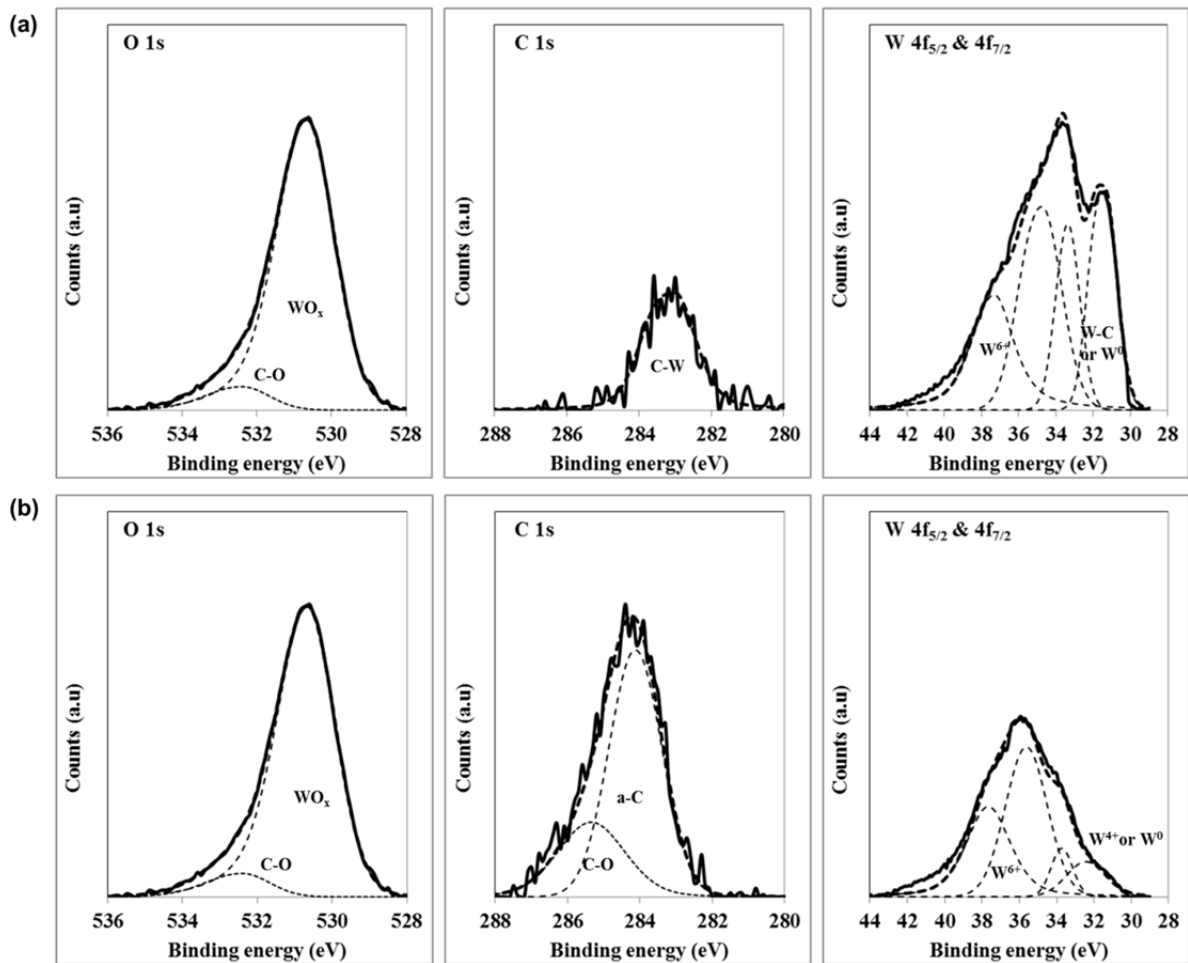


Figure S30. Deconvoluted O 1s, C 1s, and W 4f_{5/2} and 4f_{7/2} peaks of materials grown at a) 200 °C and b) 500 °C.

* The RBD Auger Scan software was used to deconvolute the XPS peaks. The Shirley base line was subtracted before peak fitting. The W 4f_{7/2} and 4f_{5/2} peak doublet area ratio was fixed to 4:3. The peak intensities for the same element show relative signal counts for each growth temperature.

Table S1: Selected properties of **1–13**.

Compound	Physical features/Characterization/Yield
1	Yellowish-orange solid, vaporizes 65-70 °C at 100-150 mTorr, melting ~ 60 °C prior to vaporization. Yield from sublimation 0.86 g; 77 %. Clean ¹ H NMR, sublimate good enough for single crystal X-ray crystallography.
2	Orange moist/semi solid, sublimed 60-65 °C at 150-200 mTorr. Yield from sublimation 0.72 g; 63%. Clean ¹ H NMR.
3	Orange liquid, distills 60-65 °C; ~ 200 mTorr. Yield 0.58 g; 53 %. Clean NMR, low viscosity.
4	Orange liquid, distills 70-75 °C; ~ 200 mTorr. Yield of distillate 0.95; 68 %. Very low viscosity. Clean ¹ H NMR.
5	Orange liquid, distills 60-65 °C; ~ 150-200 mTorr. Yield of distillate 0.66 g; 51%. Low viscosity, Clean ¹ H NMR.
6	Orange liquid, distills 60-65 °C; ~ 150-200 mTorr. Yield of distillate 0.68 g; 55 %. Low viscosity, Clean ¹ H NMR.
7	Orange liquid, distills 70-80 °C at 300-350 mTorr. Yield 0.8 g; 60 %. Low viscosity. Clean ¹ H NMR.
8	Orange liquid, distills 70-80 °C; ~ 250-300 mTorr. Yield 0.72 g; 55 %. Low viscosity. Clean ¹ H NMR.
9	Orange liquid, distills 60-65 °C; ~ 200 mTorr. Yield 0.53 g; 52 %. Clean NMR, slightly higher viscosity.
10	Pale orange waxy crystalline solid, vaporizes 55-60 °C; 150-200 mTorr. Melts ~35-40 °C prior to vaporization. Yield from sublimation 0.62 g; 55 %. Clean ¹ H NMR, sublimate good enough for single crystal X-Ray crystallography.
11	Light brown solid, sublimed 90-100 °C at 300- 350 mTorr. Yield 0.68 g; 57 %. Clean ¹ H NMR.
12	White solid, sublimed 90-105 °C at 200-250 mTorr. Yield 0.46 g; 39 %. Clean ¹ H NMR.
13	White needles, sublimed 50-65 °C at 350 mTorr. Yield 0.46 g; 39 %. Clean ¹ H NMR.

Table S2. Summary of m/z values and relative abundances for positive ion DPCI mass spectra of **1, 2, 9, 10-13**.

Compound (MW)	% rel. abundance (m/z) [ion]
1 (392)	753 (23) [M+(M-OCH ₃)] ⁺ ; 685 (1) [M+(M-acac)] ⁺ ; 421 (3) [M+C ₂ H ₅] ⁺ ; 361 (100) [M-OCH ₃] ⁺ ; 331 (2) [M-2OCH ₃] ⁺ ; 293 (31) [M-acac] ⁺ ; 101 (5) [Hacac+H] ⁺
2 (434)	823 (28) [M+(M-OC ₂ H ₅)] ⁺ ; 769 (4) [M+(M-acac)] ⁺ ; 463 (7) [M+C ₂ H ₅] ⁺ ; 389 (100) [M-OC ₂ H ₅] ⁺ ; 335 (39) [M-acac] ⁺ ; 101 (3) [Hacac+H] ⁺
9 (560)	1033 (4) [M+(M-NpO)] ⁺ ; 1021 (0.5) [M+(M-acac)] ⁺ ; 561 (3) [M+H] ⁺ ; 473 (14) [M-NpO] ⁺ ; 461 (2) [M-acac] ⁺ ; 101 (100) [Hacac+H] ⁺ ; 89 (28) [NpOH+H] ⁺ ; 71 (3) [CH ₃] ₃ CCH ₂ ⁺
10 (618)	619 (1) [M+H] ⁺ ; 531 (31) [(M+H)-NpO] ⁺ ; 477 (35) [(M-tbac)+CH ₄] ⁺ ; 461 (46) [(M+H)-tbac] ⁺ ; 391 (7) [M-2(NpO)-tbac+OH] ⁺ ; 158 (18) [Htbac+H] ⁺ ; 89 (58) [NpOH+H] ⁺ ; 71 (100) [CH ₃] ₃ CCH ₂ ⁺ ; 57 (72) [C(CH ₃) ₃] ⁺
11 (644)	673 (4) [M+C ₂ H ₅] ⁺ ; 645 (2) [M+H] ⁺ ; 557 (100) [M-NpO] ⁺ ; 461 (9) [M-dpm] ⁺ ; 185 (10) [Hdpm+H] ⁺ ; 89 (34) [NpOH+H] ⁺ ; 71 (17) [CH ₃] ₃ CCH ₂ ⁺ ; 57 (16) [C(CH ₃) ₃] ⁺
12 (660)	573 (55) [M-NpO] ⁺ ; 517 (98) [M-OR-(CH ₃) ₃ C] ⁺ ; 461 (20) [(M)-tbpa] ⁺ ; 71 (100) [CH ₂ C(CH ₃) ₃] ⁺ ; 57 (23) [C(CH ₃) ₃] ⁺
13 (576)	577 (0.6) [M+H] ⁺ ; 502 (14) [(M- ^t BuO)] ⁺ ; 419 (13) [M-tbac] ⁺ ; 103 (58) [OC(OH)CHC(CH ₃)O] ⁺ ; 57 (100) [C(CH ₃) ₃] ⁺

Table S3. Crystal data and structure refinement for **11a**.

Identification code	11a	
Empirical formula	C _{46.50} H ₈₂ O ₁₂ W ₂	
Formula weight	1200.82	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 18.4587(8) Å	α = 90°.
	b = 15.2076(7) Å	β = 104.2143(7)°.
	c = 19.5770(8) Å	γ = 90°.
Volume	5327.3(4) Å ³	
Z	4	
Density (calculated)	1.497 Mg/m ³	
Absorption coefficient	4.368 mm ⁻¹	
F(000)	2420	
Crystal size	0.171 x 0.171 x 0.158 mm ³	
Theta range for data collection	1.359 to 27.499°.	
Index ranges	-23 ≤ h ≤ 19, -19 ≤ k ≤ 19, -25 ≤ l ≤ 24	
Reflections collected	29301	
Independent reflections	11486 [R(int) = 0.0476]	
Completeness to theta = 25.242°	95.1 %	
Absorption correction	Analytical	
Max. and min. transmission	0.6458 and 0.5675	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11486 / 0 / 569	
Goodness-of-fit on F ²	0.946	
Final R indices [I > 2σ(I)]	R1 = 0.0327, wR2 = 0.0705 [8128]	
R indices (all data)	R1 = 0.0551, wR2 = 0.0763	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.911 and -1.115 e.Å ⁻³	

$$R1 = \frac{\sum(|F_o| - |F_c|)}{\sum|F_o|}$$

$$wR2 = \frac{[\sum[w(F_o^2 - F_c^2)^2] / \sum(w(F_o^2)^2)]^{1/2}}{S}$$

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

$$w = 1/[\sigma^2(F_o^2) + (m \cdot p)^2 + n \cdot p], \quad p = [\max(F_o^2, 0) + 2 \cdot F_c^2] / 3, \quad m \text{ \& \ } n \text{ are constants}$$

Table S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
W1	837(1)	7518(1)	6536(1)	10(1)
O1	101(2)	8525(1)	7305(1)	18(1)
O2	1549(2)	8600(1)	5468(1)	14(1)
O3	1773(2)	6307(1)	5465(1)	15(1)
O4	501(2)	6252(1)	7310(1)	17(1)
O5	-1370(2)	7384(1)	5655(1)	17(1)
O6	3354(2)	7567(1)	7032(1)	16(1)
C1	2274(3)	8495(2)	4630(2)	14(1)
C2	2738(3)	7494(2)	4220(2)	14(1)
C3	2432(3)	6438(2)	4638(2)	15(1)
C4	2545(4)	9577(2)	4108(2)	24(1)
C5	2855(4)	5402(2)	4088(2)	23(1)
C6	1698(4)	5319(2)	7553(2)	24(1)
C7	-1941(3)	7280(2)	4602(2)	26(1)
C8	5071(3)	7522(2)	6660(2)	21(1)

Table S5. Bond lengths [Å] and angles [°] for **1**.

W1-O1	1.7175(16)
W1-O4	1.8723(16)
W1-O5	1.8793(15)
W1-O6	1.8807(15)
W1-O2	2.0450(16)
W1-O3	2.2087(16)
O2-C1	1.305(3)
O3-C3	1.271(3)
O4-C6	1.433(3)
O5-C7	1.418(3)
O6-C8	1.415(3)
C1-C2	1.381(3)
C1-C4	1.498(3)
C2-C3	1.414(3)
C2-H2	0.9500
C3-C5	1.496(3)
C4-H4A	0.9800
C4-H4B	0.9800
C4-H4C	0.9800
C5-H5A	0.9800
C5-H5B	0.9800
C5-H5C	0.9800
C6-H6A	0.9800
C6-H6B	0.9800
C6-H6C	0.9800
C7-H7A	0.9800
C7-H7B	0.9800
C7-H7C	0.9800
C8-H8A	0.9800
C8-H8B	0.9800
C8-H8C	0.9800
O1-W1-O4	99.62(7)
O1-W1-O5	96.85(8)
O4-W1-O5	96.30(7)

O1-W1-O6	98.05(7)
O4-W1-O6	91.50(7)
O5-W1-O6	161.78(7)
O1-W1-O2	95.64(7)
O4-W1-O2	164.55(7)
O5-W1-O2	84.14(7)
O6-W1-O2	84.01(7)
O1-W1-O3	176.17(7)
O4-W1-O3	84.10(7)
O5-W1-O3	81.75(6)
O6-W1-O3	82.70(6)
O2-W1-O3	80.68(6)
C1-O2-W1	134.84(14)
C3-O3-W1	131.73(15)
C6-O4-W1	129.53(15)
C7-O5-W1	138.17(14)
C8-O6-W1	139.08(13)
O2-C1-C2	124.9(2)
O2-C1-C4	114.1(2)
C2-C1-C4	121.0(2)
C1-C2-C3	124.26(19)
C1-C2-H2	117.9
C3-C2-H2	117.9
O3-C3-C2	123.5(2)
O3-C3-C5	116.7(2)
C2-C3-C5	119.8(2)
C1-C4-H4A	109.5
C1-C4-H4B	109.5
H4A-C4-H4B	109.5
C1-C4-H4C	109.5
H4A-C4-H4C	109.5
H4B-C4-H4C	109.5
C3-C5-H5A	109.5
C3-C5-H5B	109.5
H5A-C5-H5B	109.5
C3-C5-H5C	109.5

H5A-C5-H5C	109.5
H5B-C5-H5C	109.5
O4-C6-H6A	109.5
O4-C6-H6B	109.5
H6A-C6-H6B	109.5
O4-C6-H6C	109.5
H6A-C6-H6C	109.5
H6B-C6-H6C	109.5
O5-C7-H7A	109.5
O5-C7-H7B	109.5
H7A-C7-H7B	109.5
O5-C7-H7C	109.5
H7A-C7-H7C	109.5
H7B-C7-H7C	109.5
O6-C8-H8A	109.5
O6-C8-H8B	109.5
H8A-C8-H8B	109.5
O6-C8-H8C	109.5
H8A-C8-H8C	109.5
H8B-C8-H8C	109.5

Table S6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **10**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
W(1)	5921(1)	2069(1)	9288(1)	28(1)
O(1)	4576(3)	1678(2)	8627(1)	49(1)
O(2)	5898(2)	1440(1)	10162(1)	32(1)
O(3)	4912(2)	2865(1)	9683(1)	32(1)
O(4)	6337(2)	2878(1)	8523(1)	37(1)
O(5)	7433(2)	1521(1)	9030(1)	47(1)
O(6)	7604(2)	2724(1)	10104(1)	23(1)
O(7)	8888(2)	3760(1)	10590(1)	24(1)
C(1)	5877(6)	1638(3)	10987(3)	36(2)
C(2)	5407(7)	991(4)	11427(4)	29(2)
C(3)	4049(8)	647(5)	11044(4)	56(2)
C(4)	5373(7)	1272(4)	12262(4)	50(2)
C(5)	6530(7)	317(4)	11505(4)	55(2)
C(1')	6695(8)	1182(5)	10802(4)	35(2)
C(2')	5862(10)	935(5)	11440(5)	30(2)
C(3')	4836(9)	300(5)	11124(5)	48(2)
C(4')	4942(12)	1649(7)	11586(7)	82(4)
C(5')	6871(13)	727(8)	12140(7)	92(4)
C(6)	3450(3)	3001(2)	9520(2)	42(1)
C(7)	3110(3)	3810(2)	9767(2)	40(1)
C(8)	1516(4)	3899(3)	9589(2)	64(1)
C(9)	3667(4)	3908(3)	10651(2)	51(1)
C(10)	3743(4)	4403(2)	9288(2)	51(1)
C(11)	6751(4)	4011(2)	7855(2)	47(1)
C(12)	6991(3)	3540(2)	8602(2)	30(1)
C(13)	7802(3)	3802(2)	9284(2)	25(1)
C(14)	8058(3)	3381(2)	10010(2)	22(1)
C(15)	9203(3)	3490(2)	11430(2)	25(1)
C(16)	9929(3)	2715(2)	11503(2)	33(1)
C(17)	7854(3)	3497(2)	11738(2)	30(1)
C(18)	10197(3)	4115(2)	11823(2)	34(1)

C(21)	8913(7)	1261(4)	9509(4)	37(2)
C(22)	9787(4)	1229(2)	8861(2)	44(1)
C(23)	9962(9)	2006(5)	8544(5)	62(2)
C(24)	9438(8)	600(5)	8319(5)	49(2)
C(25)	11374(8)	1040(5)	9435(5)	61(2)
C(22')	8421(7)	1790(4)	8574(4)	38(2)
C(23')	10224(9)	1300(5)	9669(5)	60(3)
C(24')	9181(10)	398(6)	8620(6)	64(3)
C(25')	10758(8)	1462(5)	8330(5)	52(2)

Table S7. Bond lengths [\AA] and angles [$^\circ$] for **10**.

W(1)-O(1)	1.699(2)
W(1)-O(2)	1.860(2)
W(1)-O(5)	1.882(2)
W(1)-O(3)	1.897(2)
W(1)-O(4)	2.021(2)
W(1)-O(6)	2.2454(19)
O(2)-C(1')	1.296(7)
O(2)-C(1)	1.466(6)
O(3)-C(6)	1.418(4)
O(4)-C(12)	1.307(3)
O(5)-C(22')	1.438(7)
O(5)-C(21)	1.580(7)
O(6)-C(14)	1.244(3)
O(7)-C(14)	1.327(3)
O(7)-C(15)	1.492(3)
C(1)-C(2)	1.477(9)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(3)	1.484(9)
C(2)-C(4)	1.524(9)
C(2)-C(5)	1.589(10)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(1')-C(2')	1.552(11)
C(1')-H(1'A)	0.9900
C(1')-H(1'B)	0.9900
C(2')-C(5')	1.442(14)

C(2')-C(3')	1.513(12)
C(2')-C(4')	1.578(14)
C(3')-H(3'A)	0.9800
C(3')-H(3'B)	0.9800
C(3')-H(3'C)	0.9800
C(4')-H(4'A)	0.9800
C(4')-H(4'B)	0.9800
C(4')-H(4'C)	0.9800
C(5')-H(5'A)	0.9800
C(5')-H(5'B)	0.9800
C(5')-H(5'C)	0.9800
C(6)-C(7)	1.520(5)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(9)	1.519(4)
C(7)-C(10)	1.524(5)
C(7)-C(8)	1.533(4)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-C(12)	1.501(4)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.358(4)
C(13)-C(14)	1.426(4)
C(13)-H(13A)	0.9500
C(15)-C(16)	1.512(4)
C(15)-C(17)	1.516(4)
C(15)-C(18)	1.519(4)

C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(21)-C(22)	1.535(7)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23')	1.378(8)
C(22)-C(24)	1.431(8)
C(22)-C(23)	1.476(8)
C(22)-C(25')	1.498(8)
C(22)-C(24')	1.579(10)
C(22)-C(22')	1.645(8)
C(22)-C(25)	1.696(9)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(22')-H(22A)	0.9900
C(22')-H(22B)	0.9900
C(23')-H(23D)	0.9800
C(23')-H(23E)	0.9800
C(23')-H(23F)	0.9800
C(24')-H(24D)	0.9800
C(24')-H(24E)	0.9800
C(24')-H(24F)	0.9800

C(25')-H(25D)	0.9800
C(25')-H(25E)	0.9800
C(25')-H(25F)	0.9800
O(1)-W(1)-O(2)	100.18(10)
O(1)-W(1)-O(5)	100.27(12)
O(2)-W(1)-O(5)	91.85(10)
O(1)-W(1)-O(3)	98.22(11)
O(2)-W(1)-O(3)	92.59(9)
O(5)-W(1)-O(3)	159.90(9)
O(1)-W(1)-O(4)	93.91(9)
O(2)-W(1)-O(4)	165.91(9)
O(5)-W(1)-O(4)	85.75(10)
O(3)-W(1)-O(4)	85.18(9)
O(1)-W(1)-O(6)	173.12(10)
O(2)-W(1)-O(6)	85.16(8)
O(5)-W(1)-O(6)	83.77(8)
O(3)-W(1)-O(6)	77.08(8)
O(4)-W(1)-O(6)	80.78(8)
C(1')-O(2)-W(1)	142.0(4)
C(1)-O(2)-W(1)	130.6(3)
C(6)-O(3)-W(1)	128.6(2)
C(12)-O(4)-W(1)	134.32(18)
C(22')-O(5)-W(1)	127.5(3)
C(21)-O(5)-W(1)	134.4(3)
C(14)-O(6)-W(1)	128.12(18)
C(14)-O(7)-C(15)	123.5(2)
O(2)-C(1)-C(2)	112.7(5)
O(2)-C(1)-H(1A)	109.0
C(2)-C(1)-H(1A)	109.0
O(2)-C(1)-H(1B)	109.0
C(2)-C(1)-H(1B)	109.0
H(1A)-C(1)-H(1B)	107.8
C(1)-C(2)-C(3)	114.8(6)
C(1)-C(2)-C(4)	108.1(5)
C(3)-C(2)-C(4)	111.2(6)

C(1)-C(2)-C(5)	108.7(6)
C(3)-C(2)-C(5)	106.4(6)
C(4)-C(2)-C(5)	107.4(5)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(2)-C(5)-H(5A)	109.5
C(2)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(2)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
O(2)-C(1')-C(2')	112.8(6)
O(2)-C(1')-H(1'A)	109.0
C(2')-C(1')-H(1'A)	109.0
O(2)-C(1')-H(1'B)	109.0
C(2')-C(1')-H(1'B)	109.0
H(1'A)-C(1')-H(1'B)	107.8
C(5')-C(2')-C(3')	114.3(9)
C(5')-C(2')-C(1')	107.0(8)
C(3')-C(2')-C(1')	110.5(7)
C(5')-C(2')-C(4')	112.2(9)
C(3')-C(2')-C(4')	105.7(8)
C(1')-C(2')-C(4')	106.9(8)
C(2')-C(3')-H(3'A)	109.5
C(2')-C(3')-H(3'B)	109.5
H(3'A)-C(3')-H(3'B)	109.5

C(2')-C(3')-H(3'C)	109.5
H(3'A)-C(3')-H(3'C)	109.5
H(3'B)-C(3')-H(3'C)	109.5
C(2')-C(4')-H(4'A)	109.5
C(2')-C(4')-H(4'B)	109.5
H(4'A)-C(4')-H(4'B)	109.5
C(2')-C(4')-H(4'C)	109.5
H(4'A)-C(4')-H(4'C)	109.5
H(4'B)-C(4')-H(4'C)	109.5
C(2')-C(5')-H(5'A)	109.5
C(2')-C(5')-H(5'B)	109.5
H(5'A)-C(5')-H(5'B)	109.5
C(2')-C(5')-H(5'C)	109.5
H(5'A)-C(5')-H(5'C)	109.5
H(5'B)-C(5')-H(5'C)	109.5
O(3)-C(6)-C(7)	111.5(3)
O(3)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
O(3)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
C(9)-C(7)-C(6)	109.2(3)
C(9)-C(7)-C(10)	111.3(3)
C(6)-C(7)-C(10)	109.6(3)
C(9)-C(7)-C(8)	109.6(3)
C(6)-C(7)-C(8)	107.8(3)
C(10)-C(7)-C(8)	109.2(3)
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5

C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(12)-C(11)-H(11A)	109.5
C(12)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(12)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(4)-C(12)-C(13)	124.9(3)
O(4)-C(12)-C(11)	113.4(3)
C(13)-C(12)-C(11)	121.7(3)
C(12)-C(13)-C(14)	123.9(3)
C(12)-C(13)-H(13A)	118.0
C(14)-C(13)-H(13A)	118.0
O(6)-C(14)-O(7)	122.3(3)
O(6)-C(14)-C(13)	125.2(3)
O(7)-C(14)-C(13)	112.4(3)
O(7)-C(15)-C(16)	111.2(2)
O(7)-C(15)-C(17)	108.1(2)
C(16)-C(15)-C(17)	113.8(3)
O(7)-C(15)-C(18)	101.5(2)
C(16)-C(15)-C(18)	110.4(3)
C(17)-C(15)-C(18)	111.2(2)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(21)-O(5)	102.4(4)
C(22)-C(21)-H(21A)	111.3
O(5)-C(21)-H(21A)	111.3
C(22)-C(21)-H(21B)	111.3
O(5)-C(21)-H(21B)	111.3
H(21A)-C(21)-H(21B)	109.2
C(24)-C(22)-C(23)	118.9(6)
C(23')-C(22)-C(25')	119.1(6)
C(24)-C(22)-C(21)	114.0(5)
C(23)-C(22)-C(21)	111.0(5)
C(23')-C(22)-C(24')	111.8(6)
C(25')-C(22)-C(24')	109.5(5)
C(23')-C(22)-C(22')	108.6(5)
C(25')-C(22)-C(22')	103.4(5)
C(24')-C(22)-C(22')	102.8(5)
C(24)-C(22)-C(25)	107.7(5)
C(23)-C(22)-C(25)	103.4(5)
C(21)-C(22)-C(25)	99.2(4)
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(25)-H(25A)	109.5
C(22)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(22)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
O(5)-C(22')-C(22)	103.7(4)
O(5)-C(22')-H(22A)	111.0
C(22)-C(22')-H(22A)	111.0
O(5)-C(22')-H(22B)	111.0
C(22)-C(22')-H(22B)	111.0
H(22A)-C(22')-H(22B)	109.0
C(22)-C(23')-H(23D)	109.5
C(22)-C(23')-H(23E)	109.5
H(23D)-C(23')-H(23E)	109.5
C(22)-C(23')-H(23F)	109.5
H(23D)-C(23')-H(23F)	109.5
H(23E)-C(23')-H(23F)	109.5
C(22)-C(24')-H(24D)	109.5
C(22)-C(24')-H(24E)	109.5
H(24D)-C(24')-H(24E)	109.5
C(22)-C(24')-H(24F)	109.5
H(24D)-C(24')-H(24F)	109.5
H(24E)-C(24')-H(24F)	109.5
C(22)-C(25')-H(25D)	109.5
C(22)-C(25')-H(25E)	109.5
H(25D)-C(25')-H(25E)	109.5
C(22)-C(25')-H(25F)	109.5
H(25D)-C(25')-H(25F)	109.5
H(25E)-C(25')-H(25F)	109.5

Table S8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
W(1A)	7978(1)	7760(1)	5936(1)	30(1)
O(1A)	7648(3)	7267(3)	6597(3)	62(2)
O(2A)	8426(2)	8456(2)	6630(3)	39(1)
O(3A)	8828(3)	7274(2)	6010(3)	48(1)
O(4A)	7589(3)	7158(2)	4964(3)	42(1)
O(5A)	7168(3)	8296(3)	5526(4)	57(1)
O(6A)	8375(2)	8323(2)	4987(3)	39(1)
C(2A)	9336(3)	9288(3)	7190(4)	38(1)
C(1A)	8615(4)	9138(4)	6618(5)	27(2)
C(3A)	9329(7)	9157(7)	8064(8)	58(3)
C(4A)	9513(6)	10038(6)	7051(7)	49(3)
C(5A)	9880(7)	8816(7)	6910(8)	63(3)
C(1C)	9012(11)	8895(11)	6450(12)	45(4)
C(3C)	9558(13)	8854(13)	7948(14)	56(6)
C(4C)	9927(13)	9717(12)	7103(15)	57(6)
C(5C)	8752(12)	9785(11)	7374(14)	52(5)
C(7A)	9799(4)	6572(4)	5795(5)	47(2)
C(6A)	9005(4)	6589(4)	5858(5)	27(2)
C(8A)	9830(5)	7030(5)	5042(6)	41(2)
C(9A)	10297(8)	6791(8)	6516(9)	58(4)
C(10A)	9927(5)	5817(5)	5555(6)	38(2)
C(6C)	9440(15)	7175(14)	5582(18)	59(7)
C(8C)	10450(20)	6560(20)	5400(20)	90(11)
C(9C)	10290(17)	6840(16)	6769(19)	48(7)
C(10C)	9590(20)	5970(20)	6010(30)	96(12)
C(11A)	7123(5)	6585(5)	3706(5)	64(2)
C(12A)	7559(3)	7181(3)	4185(4)	36(1)
C(13A)	7877(3)	7675(4)	3821(4)	38(1)
C(14A)	8276(3)	8229(3)	4236(4)	35(1)
C(15A)	8636(4)	8718(4)	3753(4)	45(2)
C(16A)	6696(7)	6271(6)	4094(8)	21(2)

C(17A)	7730(11)	6227(11)	3365(13)	56(5)
C(18A)	6706(10)	6989(9)	2837(11)	45(4)
C(16C)	6300(9)	6674(9)	3794(10)	75(4)
C(17C)	7351(10)	5897(9)	4169(11)	84(5)
C(18C)	7110(6)	6482(6)	2863(7)	39(2)
C(19A)	9096(5)	9232(4)	4330(6)	70(3)
C(20A)	8052(5)	9090(5)	3117(6)	83(3)
C(21A)	9104(4)	8319(4)	3288(4)	51(2)
C(23A)	6103(4)	8905(4)	4889(5)	48(2)
C(22A)	6444(6)	8242(5)	5249(7)	26(2)
C(24A)	5308(7)	8790(8)	4531(9)	43(3)
C(25A)	6472(8)	9139(8)	4196(9)	47(3)
C(26A)	6216(10)	9517(10)	5451(11)	47(4)
C(22C)	6760(30)	8600(30)	4900(30)	250(30)
C(24C)	5970(30)	9280(30)	4170(40)	270(30)
C(25C)	5530(30)	8490(30)	4930(40)	280(30)
C(26C)	6229(12)	9380(11)	5666(13)	60(5)
W(1B)	3513(1)	7285(1)	5122(1)	30(1)
O(1B)	3891(2)	7717(2)	4450(3)	39(1)
O(2B)	3106(2)	6560(2)	4448(3)	35(1)
O(3B)	2646(2)	7777(2)	4965(3)	36(1)
O(4B)	3835(2)	7947(2)	6066(3)	38(1)
O(5B)	4308(2)	6768(2)	5659(3)	43(1)
O(6B)	3080(2)	6766(2)	6067(2)	35(1)
C(2B)	2117(4)	5808(4)	3913(4)	49(2)
C(1B)	2835(5)	5876(4)	4480(5)	24(2)
C(3B)	1861(8)	5058(7)	4089(8)	56(3)
C(4B)	1596(7)	6323(7)	4222(8)	54(3)
C(5B)	2081(7)	5892(7)	3059(7)	46(3)
C(1D)	2487(12)	6215(12)	4576(13)	62(5)
C(3D)	1543(12)	5411(13)	3941(15)	68(6)
C(4D)	2732(12)	5279(12)	3746(14)	64(6)
C(5D)	2026(11)	6251(11)	3048(12)	52(5)
C(6B)	2191(4)	8000(3)	5466(4)	39(1)
C(7B)	1697(4)	8564(3)	5055(4)	42(2)
C(8B)	1236(4)	8776(4)	5641(5)	56(2)

C(9B)	1213(4)	8287(4)	4263(5)	56(2)
C(10B)	2121(4)	9174(4)	4864(5)	57(2)
C(12B)	3917(4)	7902(4)	6855(4)	40(1)
C(13B)	3665(4)	7367(4)	7241(4)	40(2)
C(14B)	3233(4)	6832(3)	6829(4)	38(1)
C(11B)	4260(5)	8552(5)	7296(5)	64(2)
C(16B)	3646(7)	9181(7)	6953(8)	61(3)
C(17B)	4792(6)	8822(5)	6923(6)	34(2)
C(18B)	4390(6)	8564(6)	8178(7)	47(2)
C(16D)	3735(13)	8905(13)	7566(15)	59(6)
C(17D)	5054(15)	8636(15)	7058(17)	64(7)
C(18D)	4764(11)	8187(11)	8239(12)	47(5)
C(15B)	2800(6)	6324(5)	7275(6)	22(2)
C(19B)	2316(7)	5829(6)	6700(7)	34(2)
C(20B)	2346(8)	6762(8)	7716(9)	34(3)
C(21B)	3366(7)	5926(6)	7904(8)	38(3)
C(15D)	3058(9)	6339(8)	7417(10)	35(4)
C(19D)	2654(10)	5757(9)	6869(11)	51(4)
C(20D)	2526(11)	6693(11)	7830(13)	45(5)
C(21D)	3666(10)	6060(10)	8061(11)	51(4)
C(23B)	5427(4)	6198(4)	6219(4)	47(2)
C(22B)	5013(8)	6827(8)	5917(10)	49(3)
C(24B)	5272(8)	5623(8)	5520(10)	53(4)
C(25B)	6180(10)	6306(11)	6552(13)	76(5)
C(26B)	5068(11)	5875(10)	6900(12)	69(5)
C(22D)	4977(8)	6590(8)	5501(10)	50(3)
C(24D)	6131(10)	6041(10)	5944(12)	72(5)
C(25D)	5695(10)	6798(10)	6912(11)	68(5)
C(26D)	5094(12)	5663(12)	6509(15)	84(6)

Table S9. Bond lengths [\AA] and angles [$^\circ$] for **11**.

W(1A)-O(1A)	1.702(5)
W(1A)-O(2A)	1.866(4)
W(1A)-O(5A)	1.877(5)
W(1A)-O(3A)	1.877(5)
W(1A)-O(4A)	2.008(4)
W(1A)-O(6A)	2.217(4)
O(2A)-C(1A)	1.380(9)
O(2A)-C(1C)	1.51(2)
O(3A)-C(6A)	1.419(9)
O(3A)-C(6C)	1.54(3)
O(4A)-C(12A)	1.296(7)
O(5A)-C(22C)	1.30(6)
O(5A)-C(22A)	1.373(12)
O(6A)-C(14A)	1.243(7)
C(2A)-C(4C)	1.45(2)
C(2A)-C(1C)	1.47(2)
C(2A)-C(3A)	1.494(14)
C(2A)-C(3C)	1.51(2)
C(2A)-C(1A)	1.526(10)
C(2A)-C(4A)	1.534(13)
C(2A)-C(5A)	1.552(14)
C(2A)-C(5C)	1.58(2)
C(1A)-H(1AA)	0.9900
C(1A)-H(1AB)	0.9900
C(3A)-H(3AA)	0.9800
C(3A)-H(3AB)	0.9800
C(3A)-H(3AC)	0.9800
C(4A)-H(4AA)	0.9800
C(4A)-H(4AB)	0.9800
C(4A)-H(4AC)	0.9800
C(5A)-H(5AA)	0.9800
C(5A)-H(5AB)	0.9800
C(5A)-H(5AC)	0.9800
C(1C)-H(1CA)	0.9900

C(1C)-H(1CB)	0.9900
C(3C)-H(3CA)	0.9800
C(3C)-H(3CB)	0.9800
C(3C)-H(3CC)	0.9800
C(4C)-H(4CA)	0.9800
C(4C)-H(4CB)	0.9800
C(4C)-H(4CC)	0.9800
C(5C)-H(5CA)	0.9800
C(5C)-H(5CB)	0.9800
C(5C)-H(5CC)	0.9800
C(7A)-C(10C)	1.32(4)
C(7A)-C(6C)	1.37(3)
C(7A)-C(9A)	1.425(16)
C(7A)-C(8C)	1.55(4)
C(7A)-C(8A)	1.561(11)
C(7A)-C(10A)	1.561(11)
C(7A)-C(6A)	1.566(10)
C(7A)-C(9C)	1.77(3)
C(6A)-H(6AA)	0.9900
C(6A)-H(6AB)	0.9900
C(8A)-H(8AA)	0.9800
C(8A)-H(8AB)	0.9800
C(8A)-H(8AC)	0.9800
C(9A)-H(9AA)	0.9800
C(9A)-H(9AB)	0.9800
C(9A)-H(9AC)	0.9800
C(10A)-H(10A)	0.9800
C(10A)-H(10B)	0.9800
C(10A)-H(10C)	0.9800
C(6C)-H(6CA)	0.9900
C(6C)-H(6CB)	0.9900
C(8C)-H(8CA)	0.9800
C(8C)-H(8CB)	0.9800
C(8C)-H(8CC)	0.9800
C(9C)-H(9CA)	0.9800
C(9C)-H(9CB)	0.9800

C(9C)-H(9CC)	0.9800
C(10C)-H(10D)	0.9800
C(10C)-H(10E)	0.9800
C(10C)-H(10F)	0.9800
C(11A)-C(16A)	1.318(15)
C(11A)-C(18C)	1.424(13)
C(11A)-C(12A)	1.548(10)
C(11A)-C(17C)	1.560(19)
C(11A)-C(17A)	1.58(2)
C(11A)-C(16C)	1.645(18)
C(11A)-C(18A)	1.689(19)
C(12A)-C(13A)	1.362(9)
C(13A)-C(14A)	1.414(9)
C(13A)-H(13A)	0.9500
C(14A)-C(15A)	1.524(8)
C(15A)-C(19A)	1.526(12)
C(15A)-C(21A)	1.539(10)
C(15A)-C(20A)	1.542(10)
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17A)-H(17A)	0.9800
C(17A)-H(17B)	0.9800
C(17A)-H(17C)	0.9800
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(16C)-H(16D)	0.9800
C(16C)-H(16E)	0.9800
C(16C)-H(16F)	0.9800
C(17C)-H(17D)	0.9800
C(17C)-H(17E)	0.9800
C(17C)-H(17F)	0.9800
C(18C)-H(18D)	0.9800
C(18C)-H(18E)	0.9800
C(18C)-H(18F)	0.9800

C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(23A)-C(25C)	1.38(6)
C(23A)-C(24C)	1.39(6)
C(23A)-C(22C)	1.39(5)
C(23A)-C(26A)	1.506(19)
C(23A)-C(22A)	1.513(13)
C(23A)-C(24A)	1.531(16)
C(23A)-C(25A)	1.570(17)
C(23A)-C(26C)	1.57(2)
C(22A)-H(22A)	0.9900
C(22A)-H(22B)	0.9900
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(25A)-H(25A)	0.9800
C(25A)-H(25B)	0.9800
C(25A)-H(25C)	0.9800
C(26A)-H(26A)	0.9800
C(26A)-H(26B)	0.9800
C(26A)-H(26C)	0.9800
C(22C)-H(22C)	0.9900
C(22C)-H(22D)	0.9900
C(24C)-H(24D)	0.9800
C(24C)-H(24E)	0.9800
C(24C)-H(24F)	0.9800
C(25C)-H(25D)	0.9800
C(25C)-H(25E)	0.9800
C(25C)-H(25F)	0.9800

C(26C)-H(26D)	0.9800
C(26C)-H(26E)	0.9800
C(26C)-H(26F)	0.9800
W(1B)-O(1B)	1.704(4)
W(1B)-O(2B)	1.866(4)
W(1B)-O(5B)	1.883(5)
W(1B)-O(3B)	1.898(4)
W(1B)-O(4B)	2.027(4)
W(1B)-O(6B)	2.208(4)
O(2B)-C(1D)	1.43(2)
O(2B)-C(1B)	1.440(9)
O(3B)-C(6B)	1.422(7)
O(4B)-C(12B)	1.301(7)
O(5B)-C(22B)	1.336(15)
O(5B)-C(22D)	1.424(16)
O(6B)-C(14B)	1.251(7)
C(2B)-C(3D)	1.36(2)
C(2B)-C(1D)	1.42(2)
C(2B)-C(5B)	1.430(14)
C(2B)-C(1B)	1.495(11)
C(2B)-C(3B)	1.593(15)
C(2B)-C(4B)	1.594(15)
C(2B)-C(4D)	1.65(2)
C(2B)-C(5D)	1.66(2)
C(1B)-H(1BA)	0.9900
C(1B)-H(1BB)	0.9900
C(3B)-H(3BA)	0.9800
C(3B)-H(3BB)	0.9800
C(3B)-H(3BC)	0.9800
C(4B)-H(4BA)	0.9800
C(4B)-H(4BB)	0.9800
C(4B)-H(4BC)	0.9800
C(5B)-H(5BA)	0.9800
C(5B)-H(5BB)	0.9800
C(5B)-H(5BC)	0.9800
C(1D)-H(1DA)	0.9900

C(1D)-H(1DB)	0.9900
C(3D)-H(3DA)	0.9800
C(3D)-H(3DB)	0.9800
C(3D)-H(3DC)	0.9800
C(4D)-H(4DA)	0.9800
C(4D)-H(4DB)	0.9800
C(4D)-H(4DC)	0.9800
C(5D)-H(5DA)	0.9800
C(5D)-H(5DB)	0.9800
C(5D)-H(5DC)	0.9800
C(6B)-C(7B)	1.515(8)
C(6B)-H(6BA)	0.9900
C(6B)-H(6BB)	0.9900
C(7B)-C(10B)	1.522(10)
C(7B)-C(8B)	1.532(9)
C(7B)-C(9B)	1.535(11)
C(8B)-H(8BA)	0.9800
C(8B)-H(8BB)	0.9800
C(8B)-H(8BC)	0.9800
C(9B)-H(9BA)	0.9800
C(9B)-H(9BB)	0.9800
C(9B)-H(9BC)	0.9800
C(10B)-H(10G)	0.9800
C(10B)-H(10H)	0.9800
C(10B)-H(10I)	0.9800
C(12B)-C(13B)	1.379(9)
C(12B)-C(11B)	1.538(10)
C(13B)-C(14B)	1.412(9)
C(13B)-H(13B)	0.9500
C(14B)-C(15D)	1.474(16)
C(14B)-C(15B)	1.594(12)
C(11B)-C(16D)	1.39(2)
C(11B)-C(17B)	1.425(12)
C(11B)-C(18B)	1.444(13)
C(11B)-C(17D)	1.68(3)
C(11B)-C(16B)	1.712(16)

C(11B)-C(18D)	1.80(2)
C(16B)-H(16G)	0.9800
C(16B)-H(16H)	0.9800
C(16B)-H(16I)	0.9800
C(17B)-H(17G)	0.9800
C(17B)-H(17H)	0.9800
C(17B)-H(17I)	0.9800
C(18B)-H(18G)	0.9800
C(18B)-H(18H)	0.9800
C(18B)-H(18I)	0.9800
C(16D)-H(16J)	0.9800
C(16D)-H(16K)	0.9800
C(16D)-H(16L)	0.9800
C(17D)-H(17J)	0.9800
C(17D)-H(17K)	0.9800
C(17D)-H(17L)	0.9800
C(18D)-H(18J)	0.9800
C(18D)-H(18K)	0.9800
C(18D)-H(18L)	0.9800
C(15B)-C(19B)	1.523(16)
C(15B)-C(20B)	1.534(18)
C(15B)-C(21B)	1.541(16)
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(15D)-C(21D)	1.50(2)
C(15D)-C(20D)	1.53(3)
C(15D)-C(19D)	1.55(2)
C(19D)-H(19G)	0.9800
C(19D)-H(19H)	0.9800

C(19D)-H(19I)	0.9800
C(20D)-H(20G)	0.9800
C(20D)-H(20H)	0.9800
C(20D)-H(20I)	0.9800
C(21D)-H(21G)	0.9800
C(21D)-H(21H)	0.9800
C(21D)-H(21I)	0.9800
C(23B)-C(26D)	1.37(2)
C(23B)-C(25B)	1.45(2)
C(23B)-C(22B)	1.487(16)
C(23B)-C(22D)	1.518(16)
C(23B)-C(24D)	1.57(2)
C(23B)-C(24B)	1.600(17)
C(23B)-C(26B)	1.60(2)
C(23B)-C(25D)	1.645(19)
C(22B)-H(22E)	0.9900
C(22B)-H(22H)	0.9900
C(24B)-H(24G)	0.9800
C(24B)-H(24H)	0.9800
C(24B)-H(24I)	0.9800
C(25B)-H(25G)	0.9800
C(25B)-H(25H)	0.9800
C(25B)-H(25I)	0.9800
C(26B)-H(26G)	0.9800
C(26B)-H(26H)	0.9800
C(26B)-H(26I)	0.9800
C(22D)-H(22F)	0.9900
C(22D)-H(22G)	0.9900
C(24D)-H(24J)	0.9800
C(24D)-H(24K)	0.9800
C(24D)-H(24L)	0.9800
C(25D)-H(25J)	0.9800
C(25D)-H(25K)	0.9800
C(25D)-H(25L)	0.9800
C(26D)-H(26J)	0.9800
C(26D)-H(26K)	0.9800

C(26D)-H(26L)	0.9800
O(1A)-W(1A)-O(2A)	101.2(2)
O(1A)-W(1A)-O(5A)	98.3(3)
O(2A)-W(1A)-O(5A)	92.7(2)
O(1A)-W(1A)-O(3A)	97.4(3)
O(2A)-W(1A)-O(3A)	93.1(2)
O(5A)-W(1A)-O(3A)	161.8(3)
O(1A)-W(1A)-O(4A)	94.2(2)
O(2A)-W(1A)-O(4A)	164.58(18)
O(5A)-W(1A)-O(4A)	84.6(2)
O(3A)-W(1A)-O(4A)	85.1(2)
O(1A)-W(1A)-O(6A)	174.5(2)
O(2A)-W(1A)-O(6A)	84.24(18)
O(5A)-W(1A)-O(6A)	82.0(2)
O(3A)-W(1A)-O(6A)	81.5(2)
O(4A)-W(1A)-O(6A)	80.35(16)
C(1A)-O(2A)-W(1A)	141.1(5)
C(1C)-O(2A)-W(1A)	123.3(8)
C(6A)-O(3A)-W(1A)	135.1(5)
C(6C)-O(3A)-W(1A)	142.5(11)
C(12A)-O(4A)-W(1A)	136.0(4)
C(22C)-O(5A)-W(1A)	148(3)
C(22A)-O(5A)-W(1A)	141.2(6)
C(14A)-O(6A)-W(1A)	131.3(4)
C(4C)-C(2A)-C(1C)	114.0(13)
C(4C)-C(2A)-C(3C)	109.5(14)
C(1C)-C(2A)-C(3C)	113.7(13)
C(3A)-C(2A)-C(1A)	111.6(7)
C(3A)-C(2A)-C(4A)	111.5(8)
C(1A)-C(2A)-C(4A)	106.9(7)
C(3A)-C(2A)-C(5A)	111.1(8)
C(1A)-C(2A)-C(5A)	106.4(7)
C(4A)-C(2A)-C(5A)	109.2(8)
C(4C)-C(2A)-C(5C)	106.4(13)
C(1C)-C(2A)-C(5C)	107.6(12)

C(3C)-C(2A)-C(5C)	104.8(13)
O(2A)-C(1A)-C(2A)	112.5(6)
O(2A)-C(1A)-H(1AA)	109.1
C(2A)-C(1A)-H(1AA)	109.1
O(2A)-C(1A)-H(1AB)	109.1
C(2A)-C(1A)-H(1AB)	109.1
H(1AA)-C(1A)-H(1AB)	107.8
C(2A)-C(3A)-H(3AA)	109.5
C(2A)-C(3A)-H(3AB)	109.5
H(3AA)-C(3A)-H(3AB)	109.5
C(2A)-C(3A)-H(3AC)	109.5
H(3AA)-C(3A)-H(3AC)	109.5
H(3AB)-C(3A)-H(3AC)	109.5
C(2A)-C(4A)-H(4AA)	109.5
C(2A)-C(4A)-H(4AB)	109.5
H(4AA)-C(4A)-H(4AB)	109.5
C(2A)-C(4A)-H(4AC)	109.5
H(4AA)-C(4A)-H(4AC)	109.5
H(4AB)-C(4A)-H(4AC)	109.5
C(2A)-C(5A)-H(5AA)	109.5
C(2A)-C(5A)-H(5AB)	109.5
H(5AA)-C(5A)-H(5AB)	109.5
C(2A)-C(5A)-H(5AC)	109.5
H(5AA)-C(5A)-H(5AC)	109.5
H(5AB)-C(5A)-H(5AC)	109.5
C(2A)-C(1C)-O(2A)	108.7(13)
C(2A)-C(1C)-H(1CA)	110.0
O(2A)-C(1C)-H(1CA)	110.0
C(2A)-C(1C)-H(1CB)	110.0
O(2A)-C(1C)-H(1CB)	110.0
H(1CA)-C(1C)-H(1CB)	108.3
C(2A)-C(3C)-H(3CA)	109.5
C(2A)-C(3C)-H(3CB)	109.5
H(3CA)-C(3C)-H(3CB)	109.5
C(2A)-C(3C)-H(3CC)	109.5
H(3CA)-C(3C)-H(3CC)	109.5

H(3CB)-C(3C)-H(3CC)	109.5
C(2A)-C(4C)-H(4CA)	109.5
C(2A)-C(4C)-H(4CB)	109.5
H(4CA)-C(4C)-H(4CB)	109.5
C(2A)-C(4C)-H(4CC)	109.5
H(4CA)-C(4C)-H(4CC)	109.5
H(4CB)-C(4C)-H(4CC)	109.5
C(2A)-C(5C)-H(5CA)	109.5
C(2A)-C(5C)-H(5CB)	109.5
H(5CA)-C(5C)-H(5CB)	109.5
C(2A)-C(5C)-H(5CC)	109.5
H(5CA)-C(5C)-H(5CC)	109.5
H(5CB)-C(5C)-H(5CC)	109.5
C(10C)-C(7A)-C(6C)	131(2)
C(10C)-C(7A)-C(8C)	116(2)
C(6C)-C(7A)-C(8C)	108.0(19)
C(9A)-C(7A)-C(8A)	111.7(8)
C(9A)-C(7A)-C(10A)	112.7(8)
C(8A)-C(7A)-C(10A)	107.0(7)
C(9A)-C(7A)-C(6A)	114.5(8)
C(8A)-C(7A)-C(6A)	105.5(6)
C(10A)-C(7A)-C(6A)	104.8(6)
C(10C)-C(7A)-C(9C)	98(2)
C(6C)-C(7A)-C(9C)	96.7(16)
C(8C)-C(7A)-C(9C)	95.2(18)
O(3A)-C(6A)-C(7A)	108.3(6)
O(3A)-C(6A)-H(6AA)	110.0
C(7A)-C(6A)-H(6AA)	110.0
O(3A)-C(6A)-H(6AB)	110.0
C(7A)-C(6A)-H(6AB)	110.0
H(6AA)-C(6A)-H(6AB)	108.4
C(7A)-C(8A)-H(8AA)	109.5
C(7A)-C(8A)-H(8AB)	109.5
H(8AA)-C(8A)-H(8AB)	109.5
C(7A)-C(8A)-H(8AC)	109.5
H(8AA)-C(8A)-H(8AC)	109.5

H(8AB)-C(8A)-H(8AC)	109.5
C(7A)-C(9A)-H(9AA)	109.5
C(7A)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(7A)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
C(7A)-C(10A)-H(10A)	109.5
C(7A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(7A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
C(7A)-C(6C)-O(3A)	112.7(19)
C(7A)-C(6C)-H(6CA)	109.1
O(3A)-C(6C)-H(6CA)	109.1
C(7A)-C(6C)-H(6CB)	109.1
O(3A)-C(6C)-H(6CB)	109.1
H(6CA)-C(6C)-H(6CB)	107.8
C(7A)-C(8C)-H(8CA)	109.5
C(7A)-C(8C)-H(8CB)	109.5
H(8CA)-C(8C)-H(8CB)	109.5
C(7A)-C(8C)-H(8CC)	109.5
H(8CA)-C(8C)-H(8CC)	109.5
H(8CB)-C(8C)-H(8CC)	109.5
C(7A)-C(9C)-H(9CA)	109.5
C(7A)-C(9C)-H(9CB)	109.5
H(9CA)-C(9C)-H(9CB)	109.5
C(7A)-C(9C)-H(9CC)	109.5
H(9CA)-C(9C)-H(9CC)	109.5
H(9CB)-C(9C)-H(9CC)	109.5
C(7A)-C(10C)-H(10D)	109.5
C(7A)-C(10C)-H(10E)	109.5
H(10D)-C(10C)-H(10E)	109.5
C(7A)-C(10C)-H(10F)	109.5
H(10D)-C(10C)-H(10F)	109.5

H(10E)-C(10C)-H(10F) 109.5
C(16A)-C(11A)-C(12A) 114.9(8)
C(18C)-C(11A)-C(12A) 120.2(8)
C(18C)-C(11A)-C(17C) 108.1(10)
C(12A)-C(11A)-C(17C) 109.4(9)
C(16A)-C(11A)-C(17A) 125.4(11)
C(12A)-C(11A)-C(17A) 99.1(9)
C(18C)-C(11A)-C(16C) 108.2(9)
C(12A)-C(11A)-C(16C) 107.2(8)
C(17C)-C(11A)-C(16C) 102.3(11)
C(16A)-C(11A)-C(18A) 114.6(10)
C(12A)-C(11A)-C(18A) 101.0(9)
C(17A)-C(11A)-C(18A) 98.0(11)
O(4A)-C(12A)-C(13A) 124.1(6)
O(4A)-C(12A)-C(11A) 112.8(6)
C(13A)-C(12A)-C(11A) 123.1(6)
C(12A)-C(13A)-C(14A) 124.8(5)
C(12A)-C(13A)-H(13A) 117.6
C(14A)-C(13A)-H(13A) 117.6
O(6A)-C(14A)-C(13A) 123.3(5)
O(6A)-C(14A)-C(15A) 117.9(6)
C(13A)-C(14A)-C(15A) 118.8(6)
C(14A)-C(15A)-C(19A) 110.1(6)
C(14A)-C(15A)-C(21A) 110.5(6)
C(19A)-C(15A)-C(21A) 109.2(6)
C(14A)-C(15A)-C(20A) 108.1(6)
C(19A)-C(15A)-C(20A) 110.8(7)
C(21A)-C(15A)-C(20A) 108.0(6)
C(11A)-C(16A)-H(16A) 109.5
C(11A)-C(16A)-H(16B) 109.5
H(16A)-C(16A)-H(16B) 109.5
C(11A)-C(16A)-H(16C) 109.5
H(16A)-C(16A)-H(16C) 109.5
H(16B)-C(16A)-H(16C) 109.5
C(11A)-C(17A)-H(17A) 109.5
C(11A)-C(17A)-H(17B) 109.5

H(17A)-C(17A)-H(17B) 109.5
C(11A)-C(17A)-H(17C) 109.5
H(17A)-C(17A)-H(17C) 109.5
H(17B)-C(17A)-H(17C) 109.5
C(11A)-C(18A)-H(18A) 109.5
C(11A)-C(18A)-H(18B) 109.5
H(18A)-C(18A)-H(18B) 109.5
C(11A)-C(18A)-H(18C) 109.5
H(18A)-C(18A)-H(18C) 109.5
H(18B)-C(18A)-H(18C) 109.5
C(11A)-C(16C)-H(16D) 109.5
C(11A)-C(16C)-H(16E) 109.5
H(16D)-C(16C)-H(16E) 109.5
C(11A)-C(16C)-H(16F) 109.5
H(16D)-C(16C)-H(16F) 109.5
H(16E)-C(16C)-H(16F) 109.5
C(11A)-C(17C)-H(17D) 109.5
C(11A)-C(17C)-H(17E) 109.5
H(17D)-C(17C)-H(17E) 109.5
C(11A)-C(17C)-H(17F) 109.5
H(17D)-C(17C)-H(17F) 109.5
H(17E)-C(17C)-H(17F) 109.5
C(11A)-C(18C)-H(18D) 109.5
C(11A)-C(18C)-H(18E) 109.5
H(18D)-C(18C)-H(18E) 109.5
C(11A)-C(18C)-H(18F) 109.5
H(18D)-C(18C)-H(18F) 109.5
H(18E)-C(18C)-H(18F) 109.5
C(15A)-C(19A)-H(19A) 109.5
C(15A)-C(19A)-H(19B) 109.5
H(19A)-C(19A)-H(19B) 109.5
C(15A)-C(19A)-H(19C) 109.5
H(19A)-C(19A)-H(19C) 109.5
H(19B)-C(19A)-H(19C) 109.5
C(15A)-C(20A)-H(20A) 109.5
C(15A)-C(20A)-H(20B) 109.5

H(20A)-C(20A)-H(20B) 109.5
C(15A)-C(20A)-H(20C) 109.5
H(20A)-C(20A)-H(20C) 109.5
H(20B)-C(20A)-H(20C) 109.5
C(15A)-C(21A)-H(21A) 109.5
C(15A)-C(21A)-H(21B) 109.5
H(21A)-C(21A)-H(21B) 109.5
C(15A)-C(21A)-H(21C) 109.5
H(21A)-C(21A)-H(21C) 109.5
H(21B)-C(21A)-H(21C) 109.5
C(25C)-C(23A)-C(24C) 111(3)
C(25C)-C(23A)-C(22C) 119(3)
C(24C)-C(23A)-C(22C) 102(3)
C(26A)-C(23A)-C(22A) 116.2(10)
C(26A)-C(23A)-C(24A) 110.3(10)
C(22A)-C(23A)-C(24A) 109.7(9)
C(26A)-C(23A)-C(25A) 102.1(10)
C(22A)-C(23A)-C(25A) 108.2(8)
C(24A)-C(23A)-C(25A) 109.9(9)
C(25C)-C(23A)-C(26C) 106(3)
C(24C)-C(23A)-C(26C) 112(3)
C(22C)-C(23A)-C(26C) 106(3)
O(5A)-C(22A)-C(23A) 112.6(8)
O(5A)-C(22A)-H(22A) 109.1
C(23A)-C(22A)-H(22A) 109.1
O(5A)-C(22A)-H(22B) 109.1
C(23A)-C(22A)-H(22B) 109.1
H(22A)-C(22A)-H(22B) 107.8
C(23A)-C(24A)-H(24A) 109.5
C(23A)-C(24A)-H(24B) 109.5
H(24A)-C(24A)-H(24B) 109.5
C(23A)-C(24A)-H(24C) 109.5
H(24A)-C(24A)-H(24C) 109.5
H(24B)-C(24A)-H(24C) 109.5
C(23A)-C(25A)-H(25A) 109.5
C(23A)-C(25A)-H(25B) 109.5

H(25A)-C(25A)-H(25B)	109.5
C(23A)-C(25A)-H(25C)	109.5
H(25A)-C(25A)-H(25C)	109.5
H(25B)-C(25A)-H(25C)	109.5
C(23A)-C(26A)-H(26A)	109.5
C(23A)-C(26A)-H(26B)	109.5
H(26A)-C(26A)-H(26B)	109.5
C(23A)-C(26A)-H(26C)	109.5
H(26A)-C(26A)-H(26C)	109.5
H(26B)-C(26A)-H(26C)	109.5
O(5A)-C(22C)-C(23A)	126(4)
O(5A)-C(22C)-H(22C)	105.8
C(23A)-C(22C)-H(22C)	105.8
O(5A)-C(22C)-H(22D)	105.8
C(23A)-C(22C)-H(22D)	105.8
H(22C)-C(22C)-H(22D)	106.2
C(23A)-C(24C)-H(24D)	109.5
C(23A)-C(24C)-H(24E)	109.5
H(24D)-C(24C)-H(24E)	109.5
C(23A)-C(24C)-H(24F)	109.5
H(24D)-C(24C)-H(24F)	109.5
H(24E)-C(24C)-H(24F)	109.5
C(23A)-C(25C)-H(25D)	109.5
C(23A)-C(25C)-H(25E)	109.5
H(25D)-C(25C)-H(25E)	109.5
C(23A)-C(25C)-H(25F)	109.5
H(25D)-C(25C)-H(25F)	109.5
H(25E)-C(25C)-H(25F)	109.5
C(23A)-C(26C)-H(26D)	109.5
C(23A)-C(26C)-H(26E)	109.5
H(26D)-C(26C)-H(26E)	109.5
C(23A)-C(26C)-H(26F)	109.5
H(26D)-C(26C)-H(26F)	109.5
H(26E)-C(26C)-H(26F)	109.5
O(1B)-W(1B)-O(2B)	99.16(19)
O(1B)-W(1B)-O(5B)	98.8(2)

O(2B)-W(1B)-O(5B)	93.7(2)
O(1B)-W(1B)-O(3B)	99.2(2)
O(2B)-W(1B)-O(3B)	93.75(19)
O(5B)-W(1B)-O(3B)	159.07(19)
O(1B)-W(1B)-O(4B)	95.87(19)
O(2B)-W(1B)-O(4B)	164.97(18)
O(5B)-W(1B)-O(4B)	84.28(19)
O(3B)-W(1B)-O(4B)	83.44(19)
O(1B)-W(1B)-O(6B)	175.71(19)
O(2B)-W(1B)-O(6B)	84.86(17)
O(5B)-W(1B)-O(6B)	79.35(18)
O(3B)-W(1B)-O(6B)	81.90(17)
O(4B)-W(1B)-O(6B)	80.13(16)
C(1D)-O(2B)-W(1B)	120.9(9)
C(1B)-O(2B)-W(1B)	141.8(5)
C(6B)-O(3B)-W(1B)	136.3(4)
C(12B)-O(4B)-W(1B)	134.1(4)
C(22B)-O(5B)-W(1B)	140.0(7)
C(22D)-O(5B)-W(1B)	135.8(7)
C(14B)-O(6B)-W(1B)	130.6(4)
C(3D)-C(2B)-C(1D)	123.8(15)
C(5B)-C(2B)-C(1B)	116.6(8)
C(5B)-C(2B)-C(3B)	110.4(8)
C(1B)-C(2B)-C(3B)	104.3(8)
C(5B)-C(2B)-C(4B)	111.6(9)
C(1B)-C(2B)-C(4B)	107.5(7)
C(3B)-C(2B)-C(4B)	105.7(9)
C(3D)-C(2B)-C(4D)	106.1(14)
C(1D)-C(2B)-C(4D)	103.4(13)
C(3D)-C(2B)-C(5D)	113.9(13)
C(1D)-C(2B)-C(5D)	109.0(13)
C(4D)-C(2B)-C(5D)	96.3(12)
O(2B)-C(1B)-C(2B)	110.6(7)
O(2B)-C(1B)-H(1BA)	109.5
C(2B)-C(1B)-H(1BA)	109.5
O(2B)-C(1B)-H(1BB)	109.5

C(2B)-C(1B)-H(1BB)	109.5
H(1BA)-C(1B)-H(1BB)	108.1
C(2B)-C(3B)-H(3BA)	109.5
C(2B)-C(3B)-H(3BB)	109.5
H(3BA)-C(3B)-H(3BB)	109.5
C(2B)-C(3B)-H(3BC)	109.5
H(3BA)-C(3B)-H(3BC)	109.5
H(3BB)-C(3B)-H(3BC)	109.5
C(2B)-C(4B)-H(4BA)	109.5
C(2B)-C(4B)-H(4BB)	109.5
H(4BA)-C(4B)-H(4BB)	109.5
C(2B)-C(4B)-H(4BC)	109.5
H(4BA)-C(4B)-H(4BC)	109.5
H(4BB)-C(4B)-H(4BC)	109.5
C(2B)-C(5B)-H(5BA)	109.5
C(2B)-C(5B)-H(5BB)	109.5
H(5BA)-C(5B)-H(5BB)	109.5
C(2B)-C(5B)-H(5BC)	109.5
H(5BA)-C(5B)-H(5BC)	109.5
H(5BB)-C(5B)-H(5BC)	109.5
C(2B)-C(1D)-O(2B)	115.6(16)
C(2B)-C(1D)-H(1DA)	108.4
O(2B)-C(1D)-H(1DA)	108.4
C(2B)-C(1D)-H(1DB)	108.4
O(2B)-C(1D)-H(1DB)	108.4
H(1DA)-C(1D)-H(1DB)	107.5
C(2B)-C(3D)-H(3DA)	109.5
C(2B)-C(3D)-H(3DB)	109.5
H(3DA)-C(3D)-H(3DB)	109.5
C(2B)-C(3D)-H(3DC)	109.5
H(3DA)-C(3D)-H(3DC)	109.5
H(3DB)-C(3D)-H(3DC)	109.5
C(2B)-C(4D)-H(4DA)	109.5
C(2B)-C(4D)-H(4DB)	109.5
H(4DA)-C(4D)-H(4DB)	109.5
C(2B)-C(4D)-H(4DC)	109.5

H(4DA)-C(4D)-H(4DC)	109.5
H(4DB)-C(4D)-H(4DC)	109.5
C(2B)-C(5D)-H(5DA)	109.5
C(2B)-C(5D)-H(5DB)	109.5
H(5DA)-C(5D)-H(5DB)	109.5
C(2B)-C(5D)-H(5DC)	109.5
H(5DA)-C(5D)-H(5DC)	109.5
H(5DB)-C(5D)-H(5DC)	109.5
O(3B)-C(6B)-C(7B)	111.5(5)
O(3B)-C(6B)-H(6BA)	109.3
C(7B)-C(6B)-H(6BA)	109.3
O(3B)-C(6B)-H(6BB)	109.3
C(7B)-C(6B)-H(6BB)	109.3
H(6BA)-C(6B)-H(6BB)	108.0
C(6B)-C(7B)-C(10B)	110.5(6)
C(6B)-C(7B)-C(8B)	107.8(5)
C(10B)-C(7B)-C(8B)	110.4(6)
C(6B)-C(7B)-C(9B)	109.3(6)
C(10B)-C(7B)-C(9B)	110.0(6)
C(8B)-C(7B)-C(9B)	108.9(6)
C(7B)-C(8B)-H(8BA)	109.5
C(7B)-C(8B)-H(8BB)	109.5
H(8BA)-C(8B)-H(8BB)	109.5
C(7B)-C(8B)-H(8BC)	109.5
H(8BA)-C(8B)-H(8BC)	109.5
H(8BB)-C(8B)-H(8BC)	109.5
C(7B)-C(9B)-H(9BA)	109.5
C(7B)-C(9B)-H(9BB)	109.5
H(9BA)-C(9B)-H(9BB)	109.5
C(7B)-C(9B)-H(9BC)	109.5
H(9BA)-C(9B)-H(9BC)	109.5
H(9BB)-C(9B)-H(9BC)	109.5
C(7B)-C(10B)-H(10G)	109.5
C(7B)-C(10B)-H(10H)	109.5
H(10G)-C(10B)-H(10H)	109.5
C(7B)-C(10B)-H(10I)	109.5

H(10G)-C(10B)-H(10I)	109.5
H(10H)-C(10B)-H(10I)	109.5
O(4B)-C(12B)-C(13B)	124.0(6)
O(4B)-C(12B)-C(11B)	111.7(6)
C(13B)-C(12B)-C(11B)	124.0(6)
C(12B)-C(13B)-C(14B)	124.3(6)
C(12B)-C(13B)-H(13B)	117.8
C(14B)-C(13B)-H(13B)	117.8
O(6B)-C(14B)-C(13B)	123.2(6)
O(6B)-C(14B)-C(15D)	125.7(9)
C(13B)-C(14B)-C(15D)	110.9(8)
O(6B)-C(14B)-C(15B)	113.2(7)
C(13B)-C(14B)-C(15B)	123.0(6)
C(17B)-C(11B)-C(18B)	118.4(8)
C(16D)-C(11B)-C(12B)	107.4(12)
C(17B)-C(11B)-C(12B)	111.6(7)
C(18B)-C(11B)-C(12B)	117.3(8)
C(16D)-C(11B)-C(17D)	143.9(16)
C(12B)-C(11B)-C(17D)	106.3(11)
C(17B)-C(11B)-C(16B)	96.0(8)
C(18B)-C(11B)-C(16B)	105.8(8)
C(12B)-C(11B)-C(16B)	103.9(7)
C(16D)-C(11B)-C(18D)	101.2(13)
C(12B)-C(11B)-C(18D)	100.4(9)
C(17D)-C(11B)-C(18D)	84.9(13)
C(11B)-C(16B)-H(16G)	109.5
C(11B)-C(16B)-H(16H)	109.5
H(16G)-C(16B)-H(16H)	109.5
C(11B)-C(16B)-H(16I)	109.5
H(16G)-C(16B)-H(16I)	109.5
H(16H)-C(16B)-H(16I)	109.5
C(11B)-C(17B)-H(17G)	109.5
C(11B)-C(17B)-H(17H)	109.5
H(17G)-C(17B)-H(17H)	109.5
C(11B)-C(17B)-H(17I)	109.5
H(17G)-C(17B)-H(17I)	109.5

H(17H)-C(17B)-H(17I) 109.5
C(11B)-C(18B)-H(18G) 109.5
C(11B)-C(18B)-H(18H) 109.5
H(18G)-C(18B)-H(18H) 109.5
C(11B)-C(18B)-H(18I) 109.5
H(18G)-C(18B)-H(18I) 109.5
H(18H)-C(18B)-H(18I) 109.5
C(11B)-C(16D)-H(16J) 109.5
C(11B)-C(16D)-H(16K) 109.5
H(16J)-C(16D)-H(16K) 109.5
C(11B)-C(16D)-H(16L) 109.5
H(16J)-C(16D)-H(16L) 109.5
H(16K)-C(16D)-H(16L) 109.5
C(11B)-C(17D)-H(17J) 109.5
C(11B)-C(17D)-H(17K) 109.5
H(17J)-C(17D)-H(17K) 109.5
C(11B)-C(17D)-H(17L) 109.5
H(17J)-C(17D)-H(17L) 109.5
H(17K)-C(17D)-H(17L) 109.5
C(11B)-C(18D)-H(18J) 109.5
C(11B)-C(18D)-H(18K) 109.5
H(18J)-C(18D)-H(18K) 109.5
C(11B)-C(18D)-H(18L) 109.5
H(18J)-C(18D)-H(18L) 109.5
H(18K)-C(18D)-H(18L) 109.5
C(19B)-C(15B)-C(20B) 108.8(10)
C(19B)-C(15B)-C(21B) 110.3(9)
C(20B)-C(15B)-C(21B) 110.2(10)
C(19B)-C(15B)-C(14B) 114.1(8)
C(20B)-C(15B)-C(14B) 107.8(9)
C(21B)-C(15B)-C(14B) 105.5(9)
C(15B)-C(19B)-H(19D) 109.5
C(15B)-C(19B)-H(19E) 109.5
H(19D)-C(19B)-H(19E) 109.5
C(15B)-C(19B)-H(19F) 109.5
H(19D)-C(19B)-H(19F) 109.5

H(19E)-C(19B)-H(19F) 109.5
C(15B)-C(20B)-H(20D) 109.5
C(15B)-C(20B)-H(20E) 109.5
H(20D)-C(20B)-H(20E) 109.5
C(15B)-C(20B)-H(20F) 109.5
H(20D)-C(20B)-H(20F) 109.5
H(20E)-C(20B)-H(20F) 109.5
C(15B)-C(21B)-H(21D) 109.5
C(15B)-C(21B)-H(21E) 109.5
H(21D)-C(21B)-H(21E) 109.5
C(15B)-C(21B)-H(21F) 109.5
H(21D)-C(21B)-H(21F) 109.5
H(21E)-C(21B)-H(21F) 109.5
C(14B)-C(15D)-C(21D) 117.0(14)
C(14B)-C(15D)-C(20D) 107.1(13)
C(21D)-C(15D)-C(20D) 109.5(14)
C(14B)-C(15D)-C(19D) 104.0(12)
C(21D)-C(15D)-C(19D) 111.3(14)
C(20D)-C(15D)-C(19D) 107.5(15)
C(15D)-C(19D)-H(19G) 109.5
C(15D)-C(19D)-H(19H) 109.5
H(19G)-C(19D)-H(19H) 109.5
C(15D)-C(19D)-H(19I) 109.5
H(19G)-C(19D)-H(19I) 109.5
H(19H)-C(19D)-H(19I) 109.5
C(15D)-C(20D)-H(20G) 109.5
C(15D)-C(20D)-H(20H) 109.5
H(20G)-C(20D)-H(20H) 109.5
C(15D)-C(20D)-H(20I) 109.5
H(20G)-C(20D)-H(20I) 109.5
H(20H)-C(20D)-H(20I) 109.5
C(15D)-C(21D)-H(21G) 109.5
C(15D)-C(21D)-H(21H) 109.5
H(21G)-C(21D)-H(21H) 109.5
C(15D)-C(21D)-H(21I) 109.5
H(21G)-C(21D)-H(21I) 109.5

H(21H)-C(21D)-H(21I)	109.5
C(25B)-C(23B)-C(22B)	115.2(12)
C(26D)-C(23B)-C(22D)	115.8(13)
C(26D)-C(23B)-C(24D)	117.9(13)
C(22D)-C(23B)-C(24D)	103.9(10)
C(25B)-C(23B)-C(24B)	112.5(11)
C(22B)-C(23B)-C(24B)	109.6(9)
C(25B)-C(23B)-C(26B)	110.3(12)
C(22B)-C(23B)-C(26B)	106.2(10)
C(24B)-C(23B)-C(26B)	102.1(11)
C(26D)-C(23B)-C(25D)	112.7(13)
C(22D)-C(23B)-C(25D)	103.4(10)
C(24D)-C(23B)-C(25D)	101.3(11)
O(5B)-C(22B)-C(23B)	117.8(11)
O(5B)-C(22B)-H(22E)	107.9
C(23B)-C(22B)-H(22E)	107.9
O(5B)-C(22B)-H(22H)	107.9
C(23B)-C(22B)-H(22H)	107.9
H(22E)-C(22B)-H(22H)	107.2
C(23B)-C(24B)-H(24G)	109.5
C(23B)-C(24B)-H(24H)	109.5
H(24G)-C(24B)-H(24H)	109.5
C(23B)-C(24B)-H(24I)	109.5
H(24G)-C(24B)-H(24I)	109.5
H(24H)-C(24B)-H(24I)	109.5
C(23B)-C(25B)-H(25G)	109.5
C(23B)-C(25B)-H(25H)	109.5
H(25G)-C(25B)-H(25H)	109.5
C(23B)-C(25B)-H(25I)	109.5
H(25G)-C(25B)-H(25I)	109.5
H(25H)-C(25B)-H(25I)	109.5
C(23B)-C(26B)-H(26G)	109.5
C(23B)-C(26B)-H(26H)	109.5
H(26G)-C(26B)-H(26H)	109.5
C(23B)-C(26B)-H(26I)	109.5
H(26G)-C(26B)-H(26I)	109.5

H(26H)-C(26B)-H(26I) 109.5
O(5B)-C(22D)-C(23B) 110.6(11)
O(5B)-C(22D)-H(22F) 109.5
C(23B)-C(22D)-H(22F) 109.5
O(5B)-C(22D)-H(22G) 109.5
C(23B)-C(22D)-H(22G) 109.5
H(22F)-C(22D)-H(22G) 108.1
C(23B)-C(24D)-H(24J) 109.5
C(23B)-C(24D)-H(24K) 109.5
H(24J)-C(24D)-H(24K) 109.5
C(23B)-C(24D)-H(24L) 109.5
H(24J)-C(24D)-H(24L) 109.5
H(24K)-C(24D)-H(24L) 109.5
C(23B)-C(25D)-H(25J) 109.5
C(23B)-C(25D)-H(25K) 109.5
H(25J)-C(25D)-H(25K) 109.5
C(23B)-C(25D)-H(25L) 109.5
H(25J)-C(25D)-H(25L) 109.5
H(25K)-C(25D)-H(25L) 109.5
C(23B)-C(26D)-H(26J) 109.5
C(23B)-C(26D)-H(26K) 109.5
H(26J)-C(26D)-H(26K) 109.5
C(23B)-C(26D)-H(26L) 109.5
H(26J)-C(26D)-H(26L) 109.5
H(26K)-C(26D)-H(26L) 109.5

Table S10. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **11a**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
W(1A)	1540(1)	2796(1)	6801(1)	23(1)
O(1A)	1781(2)	1836(2)	7265(2)	32(1)
O(2A)	637(2)	2985(2)	6855(2)	36(1)
O(3A)	1541(2)	4022(2)	6257(2)	38(1)
O(4A)	2090(2)	3538(2)	7598(1)	29(1)
O(5A)	2624(2)	2821(2)	6546(2)	35(1)
O(6A)	1262(2)	2324(2)	5833(2)	27(1)
C(1A)	1811(3)	4763(3)	6444(2)	31(1)
C(2A)	2254(3)	4931(3)	7133(2)	32(1)
C(3A)	2369(3)	4327(3)	7667(2)	27(1)
C(4A)	1658(3)	5473(3)	5872(2)	36(1)
C(5A)	2172(4)	5261(4)	5355(3)	75(2)
C(6A)	862(3)	5382(3)	5438(3)	44(1)
C(7A)	1790(4)	6374(3)	6141(3)	96(3)
C(8A)	2834(3)	4550(3)	8409(2)	34(1)
C(9A)	2891(4)	3751(3)	8895(3)	69(2)
C(10A)	3622(3)	4816(3)	8358(2)	41(1)
C(11A)	2460(3)	5322(3)	8689(3)	44(1)
C(12A)	2819(3)	2734(3)	5980(2)	33(1)
C(13A)	2300(3)	2477(3)	5346(2)	28(1)
C(14A)	1577(3)	2286(2)	5298(2)	23(1)
C(15A)	3640(3)	2877(4)	6004(3)	49(2)
C(16A)	4045(4)	3234(6)	6735(3)	111(3)
C(17A)	3725(3)	3523(4)	5430(3)	58(2)
C(18A)	3976(3)	1988(5)	5864(4)	68(2)
C(19A)	1021(3)	2002(3)	4617(2)	27(1)
C(20A)	702(3)	1094(4)	4733(3)	34(2)
C(21A)	1335(4)	1982(4)	3982(3)	43(2)
C(22A)	361(4)	2675(4)	4489(4)	44(2)
C(20C)	1026(18)	2688(17)	4079(16)	50(8)
C(21C)	1421(16)	1192(17)	4318(14)	45(7)

C(22C)	360(18)	1730(20)	4709(17)	61(10)
W(2B)	3194(1)	2242(1)	3293(1)	27(1)
O(1B)	2666(2)	3153(2)	3363(2)	36(1)
O(2B)	3221(2)	1675(2)	4059(2)	38(1)
O(3B)	3864(2)	1195(2)	2966(2)	34(1)
O(4B)	2388(2)	1581(2)	2654(2)	28(1)
O(5B)	3348(2)	2704(2)	2291(2)	33(1)
O(6B)	4197(2)	2762(2)	3618(2)	37(1)
C(1B)	3696(3)	596(3)	2517(2)	36(1)
C(2B)	2947(3)	477(3)	2109(2)	36(1)
C(3B)	2354(3)	955(3)	2177(2)	29(1)
C(4B)	1565(3)	842(3)	1727(2)	33(1)
C(5B)	1086(4)	491(5)	2206(3)	76(2)
C(6B)	1268(3)	1729(3)	1439(3)	52(2)
C(7B)	1528(3)	204(3)	1112(3)	52(2)
C(8B)	4312(3)	-27(3)	2426(3)	41(1)
C(9B)	5066(3)	265(4)	2865(3)	57(2)
C(10B)	4121(3)	-949(3)	2653(3)	57(2)
C(11B)	4334(4)	-39(4)	1646(3)	75(2)
C(12B)	3893(3)	3035(3)	2108(2)	30(1)
C(13B)	4587(3)	3185(4)	2609(3)	43(1)
C(14B)	4703(3)	3049(3)	3312(3)	38(1)
C(15B)	3768(3)	3275(3)	1332(3)	40(1)
C(16B)	3719(5)	2416(4)	935(3)	81(2)
C(17B)	3067(3)	3805(4)	1128(3)	64(2)
C(18B)	4414(3)	3812(4)	1189(3)	63(2)
C(19B)	5458(3)	3216(4)	3837(3)	58(2)
C(20B)	5367(7)	3494(8)	4500(6)	84(4)
C(21B)	5843(6)	4054(6)	3484(5)	66(3)
C(22B)	5934(5)	2483(6)	3838(5)	46(2)
C(20D)	5405(7)	3974(7)	4303(6)	18(3)
C(21D)	6106(11)	3023(12)	3617(10)	72(6)
C(22D)	5517(10)	2330(9)	4453(8)	53(5)
C(23)	3647(8)	-226(9)	5054(7)	73(4)
C(24)	3997(11)	-397(12)	4559(10)	74(5)
C(25)	4651(11)	89(17)	4730(10)	125(7)

C(26)	5079(9)	532(10)	5077(9)	75(4)
C(27)	6037(13)	661(15)	5271(13)	119(9)

Table S11. Bond lengths [\AA] and angles [$^\circ$] for **11a**.

W(1A)-O(1A)	1.719(3)
W(1A)-O(2A)	1.721(3)
W(1A)-O(6A)	1.974(3)
W(1A)-O(4A)	1.989(3)
W(1A)-O(3A)	2.147(3)
W(1A)-O(5A)	2.177(3)
O(3A)-C(1A)	1.250(5)
O(4A)-C(3A)	1.300(5)
O(5A)-C(12A)	1.255(5)
O(6A)-C(14A)	1.316(5)
C(1A)-C(2A)	1.419(6)
C(1A)-C(4A)	1.531(6)
C(2A)-C(3A)	1.368(6)
C(2A)-H(2AA)	0.9500
C(3A)-C(8A)	1.533(6)
C(4A)-C(7A)	1.467(7)
C(4A)-C(6A)	1.513(6)
C(4A)-C(5A)	1.580(8)
C(5A)-H(5AA)	0.9800
C(5A)-H(5AB)	0.9800
C(5A)-H(5AC)	0.9800
C(6A)-H(6AA)	0.9800
C(6A)-H(6AB)	0.9800
C(6A)-H(6AC)	0.9800
C(7A)-H(7AA)	0.9800
C(7A)-H(7AB)	0.9800
C(7A)-H(7AC)	0.9800
C(8A)-C(11A)	1.530(7)
C(8A)-C(9A)	1.531(6)
C(8A)-C(10A)	1.536(7)
C(9A)-H(9AA)	0.9800
C(9A)-H(9AB)	0.9800
C(9A)-H(9AC)	0.9800
C(10A)-H(10A)	0.9800

C(10A)-H(10B)	0.9800
C(10A)-H(10C)	0.9800
C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-C(13A)	1.424(6)
C(12A)-C(15A)	1.519(7)
C(13A)-C(14A)	1.346(6)
C(13A)-H(13A)	0.9500
C(14A)-C(19A)	1.532(6)
C(15A)-C(17A)	1.530(7)
C(15A)-C(18A)	1.540(8)
C(15A)-C(16A)	1.542(7)
C(16A)-H(16A)	0.9800
C(16A)-H(16B)	0.9800
C(16A)-H(16C)	0.9800
C(17A)-H(17A)	0.9800
C(17A)-H(17B)	0.9800
C(17A)-H(17C)	0.9800
C(18A)-H(18A)	0.9800
C(18A)-H(18B)	0.9800
C(18A)-H(18C)	0.9800
C(19A)-C(22C)	1.34(3)
C(19A)-C(20C)	1.48(3)
C(19A)-C(21A)	1.496(8)
C(19A)-C(20A)	1.540(7)
C(19A)-C(22A)	1.563(8)
C(19A)-C(21C)	1.62(3)
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(22A)-H(22A)	0.9800
C(22A)-H(22B)	0.9800

C(22A)-H(22C)	0.9800
C(20C)-H(20D)	0.9800
C(20C)-H(20E)	0.9800
C(20C)-H(20F)	0.9800
C(21C)-H(21D)	0.9800
C(21C)-H(21E)	0.9800
C(21C)-H(21F)	0.9800
C(22C)-H(22D)	0.9800
C(22C)-H(22E)	0.9800
C(22C)-H(22F)	0.9800
W(2B)-O(1B)	1.719(3)
W(2B)-O(2B)	1.720(3)
W(2B)-O(4B)	1.968(3)
W(2B)-O(6B)	1.970(3)
W(2B)-O(5B)	2.167(3)
W(2B)-O(3B)	2.205(3)
O(3B)-C(1B)	1.250(5)
O(4B)-C(3B)	1.324(5)
O(5B)-C(12B)	1.252(5)
O(6B)-C(14B)	1.302(6)
C(1B)-C(2B)	1.428(7)
C(1B)-C(8B)	1.524(7)
C(2B)-C(3B)	1.347(6)
C(2B)-H(2BA)	0.9500
C(3B)-C(4B)	1.515(6)
C(4B)-C(6B)	1.512(6)
C(4B)-C(5B)	1.535(7)
C(4B)-C(7B)	1.536(6)
C(5B)-H(5BA)	0.9800
C(5B)-H(5BB)	0.9800
C(5B)-H(5BC)	0.9800
C(6B)-H(6BA)	0.9800
C(6B)-H(6BB)	0.9800
C(6B)-H(6BC)	0.9800
C(7B)-H(7BA)	0.9800
C(7B)-H(7BB)	0.9800

C(7B)-H(7BC)	0.9800
C(8B)-C(9B)	1.512(7)
C(8B)-C(10B)	1.537(7)
C(8B)-C(11B)	1.538(7)
C(9B)-H(9BA)	0.9800
C(9B)-H(9BB)	0.9800
C(9B)-H(9BC)	0.9800
C(10B)-H(10D)	0.9800
C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(12B)-C(13B)	1.428(7)
C(12B)-C(15B)	1.524(6)
C(13B)-C(14B)	1.355(7)
C(13B)-H(13B)	0.9500
C(14B)-C(19B)	1.537(7)
C(15B)-C(17B)	1.492(7)
C(15B)-C(16B)	1.511(7)
C(15B)-C(18B)	1.527(7)
C(16B)-H(16D)	0.9800
C(16B)-H(16E)	0.9800
C(16B)-H(16F)	0.9800
C(17B)-H(17D)	0.9800
C(17B)-H(17E)	0.9800
C(17B)-H(17F)	0.9800
C(18B)-H(18D)	0.9800
C(18B)-H(18E)	0.9800
C(18B)-H(18F)	0.9800
C(19B)-C(21D)	1.397(19)
C(19B)-C(20B)	1.414(12)
C(19B)-C(22B)	1.419(10)
C(19B)-C(20D)	1.490(11)
C(19B)-C(21B)	1.686(11)
C(19B)-C(22D)	1.793(16)

C(20B)-H(20G)	0.9800
C(20B)-H(20H)	0.9800
C(20B)-H(20I)	0.9800
C(21B)-H(21G)	0.9800
C(21B)-H(21H)	0.9800
C(21B)-H(21I)	0.9800
C(22B)-H(22G)	0.9800
C(22B)-H(22H)	0.9800
C(22B)-H(22I)	0.9800
C(20D)-H(20J)	0.9800
C(20D)-H(20K)	0.9800
C(20D)-H(20L)	0.9800
C(21D)-H(21J)	0.9800
C(21D)-H(21K)	0.9800
C(21D)-H(21L)	0.9800
C(22D)-H(22J)	0.9800
C(22D)-H(22K)	0.9800
C(22D)-H(22L)	0.9800
C(23)-C(24)	1.32(2)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.39(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.129(18)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.72(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
O(1A)-W(1A)-O(2A)	103.74(15)

O(1A)-W(1A)-O(6A)	99.86(12)
O(2A)-W(1A)-O(6A)	95.29(13)
O(1A)-W(1A)-O(4A)	92.91(12)
O(2A)-W(1A)-O(4A)	99.97(14)
O(6A)-W(1A)-O(4A)	157.18(12)
O(1A)-W(1A)-O(3A)	165.47(14)
O(2A)-W(1A)-O(3A)	90.22(14)
O(6A)-W(1A)-O(3A)	82.57(11)
O(4A)-W(1A)-O(3A)	80.51(11)
O(1A)-W(1A)-O(5A)	90.19(14)
O(2A)-W(1A)-O(5A)	165.88(14)
O(6A)-W(1A)-O(5A)	79.81(12)
O(4A)-W(1A)-O(5A)	81.33(12)
O(3A)-W(1A)-O(5A)	76.07(13)
C(1A)-O(3A)-W(1A)	133.3(3)
C(3A)-O(4A)-W(1A)	135.8(3)
C(12A)-O(5A)-W(1A)	132.8(3)
C(14A)-O(6A)-W(1A)	135.9(3)
O(3A)-C(1A)-C(2A)	122.4(4)
O(3A)-C(1A)-C(4A)	115.7(4)
C(2A)-C(1A)-C(4A)	121.9(4)
C(3A)-C(2A)-C(1A)	123.4(4)
C(3A)-C(2A)-H(2AA)	118.3
C(1A)-C(2A)-H(2AA)	118.3
O(4A)-C(3A)-C(2A)	123.9(4)
O(4A)-C(3A)-C(8A)	114.7(4)
C(2A)-C(3A)-C(8A)	121.4(4)
C(7A)-C(4A)-C(6A)	109.8(5)
C(7A)-C(4A)-C(1A)	114.3(4)
C(6A)-C(4A)-C(1A)	108.9(4)
C(7A)-C(4A)-C(5A)	110.4(5)
C(6A)-C(4A)-C(5A)	106.0(5)
C(1A)-C(4A)-C(5A)	107.0(4)
C(4A)-C(5A)-H(5AA)	109.5
C(4A)-C(5A)-H(5AB)	109.5
H(5AA)-C(5A)-H(5AB)	109.5

C(4A)-C(5A)-H(5AC)	109.5
H(5AA)-C(5A)-H(5AC)	109.5
H(5AB)-C(5A)-H(5AC)	109.5
C(4A)-C(6A)-H(6AA)	109.5
C(4A)-C(6A)-H(6AB)	109.5
H(6AA)-C(6A)-H(6AB)	109.5
C(4A)-C(6A)-H(6AC)	109.5
H(6AA)-C(6A)-H(6AC)	109.5
H(6AB)-C(6A)-H(6AC)	109.5
C(4A)-C(7A)-H(7AA)	109.5
C(4A)-C(7A)-H(7AB)	109.5
H(7AA)-C(7A)-H(7AB)	109.5
C(4A)-C(7A)-H(7AC)	109.5
H(7AA)-C(7A)-H(7AC)	109.5
H(7AB)-C(7A)-H(7AC)	109.5
C(11A)-C(8A)-C(9A)	110.8(4)
C(11A)-C(8A)-C(3A)	108.2(4)
C(9A)-C(8A)-C(3A)	110.5(4)
C(11A)-C(8A)-C(10A)	109.8(4)
C(9A)-C(8A)-C(10A)	109.1(4)
C(3A)-C(8A)-C(10A)	108.4(4)
C(8A)-C(9A)-H(9AA)	109.5
C(8A)-C(9A)-H(9AB)	109.5
H(9AA)-C(9A)-H(9AB)	109.5
C(8A)-C(9A)-H(9AC)	109.5
H(9AA)-C(9A)-H(9AC)	109.5
H(9AB)-C(9A)-H(9AC)	109.5
C(8A)-C(10A)-H(10A)	109.5
C(8A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(8A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
C(8A)-C(11A)-H(11A)	109.5
C(8A)-C(11A)-H(11B)	109.5
H(11A)-C(11A)-H(11B)	109.5

C(8A)-C(11A)-H(11C) 109.5
H(11A)-C(11A)-H(11C) 109.5
H(11B)-C(11A)-H(11C) 109.5
O(5A)-C(12A)-C(13A) 121.5(4)
O(5A)-C(12A)-C(15A) 117.2(4)
C(13A)-C(12A)-C(15A) 121.3(4)
C(14A)-C(13A)-C(12A) 124.3(4)
C(14A)-C(13A)-H(13A) 117.9
C(12A)-C(13A)-H(13A) 117.9
O(6A)-C(14A)-C(13A) 124.0(4)
O(6A)-C(14A)-C(19A) 111.9(4)
C(13A)-C(14A)-C(19A) 124.2(4)
C(12A)-C(15A)-C(17A) 110.5(5)
C(12A)-C(15A)-C(18A) 108.2(4)
C(17A)-C(15A)-C(18A) 108.3(5)
C(12A)-C(15A)-C(16A) 109.4(4)
C(17A)-C(15A)-C(16A) 109.9(5)
C(18A)-C(15A)-C(16A) 110.5(6)
C(15A)-C(16A)-H(16A) 109.5
C(15A)-C(16A)-H(16B) 109.5
H(16A)-C(16A)-H(16B) 109.5
C(15A)-C(16A)-H(16C) 109.5
H(16A)-C(16A)-H(16C) 109.5
H(16B)-C(16A)-H(16C) 109.5
C(15A)-C(17A)-H(17A) 109.5
C(15A)-C(17A)-H(17B) 109.5
H(17A)-C(17A)-H(17B) 109.5
C(15A)-C(17A)-H(17C) 109.5
H(17A)-C(17A)-H(17C) 109.5
H(17B)-C(17A)-H(17C) 109.5
C(15A)-C(18A)-H(18A) 109.5
C(15A)-C(18A)-H(18B) 109.5
H(18A)-C(18A)-H(18B) 109.5
C(15A)-C(18A)-H(18C) 109.5
H(18A)-C(18A)-H(18C) 109.5
H(18B)-C(18A)-H(18C) 109.5

C(22C)-C(19A)-C(20C) 118.5(19)
C(22C)-C(19A)-C(14A) 114.1(14)
C(20C)-C(19A)-C(14A) 107.5(12)
C(21A)-C(19A)-C(14A) 114.6(4)
C(21A)-C(19A)-C(20A) 110.1(4)
C(14A)-C(19A)-C(20A) 108.9(4)
C(21A)-C(19A)-C(22A) 109.0(5)
C(14A)-C(19A)-C(22A) 106.6(4)
C(20A)-C(19A)-C(22A) 107.4(4)
C(22C)-C(19A)-C(21C) 108.8(17)
C(20C)-C(19A)-C(21C) 101.3(15)
C(14A)-C(19A)-C(21C) 105.2(10)
C(19A)-C(20A)-H(20A) 109.5
C(19A)-C(20A)-H(20B) 109.5
H(20A)-C(20A)-H(20B) 109.5
C(19A)-C(20A)-H(20C) 109.5
H(20A)-C(20A)-H(20C) 109.5
H(20B)-C(20A)-H(20C) 109.5
C(19A)-C(21A)-H(21A) 109.5
C(19A)-C(21A)-H(21B) 109.5
H(21A)-C(21A)-H(21B) 109.5
C(19A)-C(21A)-H(21C) 109.5
H(21A)-C(21A)-H(21C) 109.5
H(21B)-C(21A)-H(21C) 109.5
C(19A)-C(22A)-H(22A) 109.5
C(19A)-C(22A)-H(22B) 109.5
H(22A)-C(22A)-H(22B) 109.5
C(19A)-C(22A)-H(22C) 109.5
H(22A)-C(22A)-H(22C) 109.5
H(22B)-C(22A)-H(22C) 109.5
C(19A)-C(20C)-H(20D) 109.5
C(19A)-C(20C)-H(20E) 109.5
H(20D)-C(20C)-H(20E) 109.5
C(19A)-C(20C)-H(20F) 109.5
H(20D)-C(20C)-H(20F) 109.5
H(20E)-C(20C)-H(20F) 109.5

C(19A)-C(21C)-H(21D)	109.5
C(19A)-C(21C)-H(21E)	109.5
H(21D)-C(21C)-H(21E)	109.5
C(19A)-C(21C)-H(21F)	109.5
H(21D)-C(21C)-H(21F)	109.5
H(21E)-C(21C)-H(21F)	109.5
C(19A)-C(22C)-H(22D)	109.5
C(19A)-C(22C)-H(22E)	109.5
H(22D)-C(22C)-H(22E)	109.5
C(19A)-C(22C)-H(22F)	109.5
H(22D)-C(22C)-H(22F)	109.5
H(22E)-C(22C)-H(22F)	109.5
O(1B)-W(2B)-O(2B)	103.23(15)
O(1B)-W(2B)-O(4B)	96.18(13)
O(2B)-W(2B)-O(4B)	98.87(14)
O(1B)-W(2B)-O(6B)	98.99(14)
O(2B)-W(2B)-O(6B)	95.51(14)
O(4B)-W(2B)-O(6B)	156.10(13)
O(1B)-W(2B)-O(5B)	90.80(13)
O(2B)-W(2B)-O(5B)	165.90(14)
O(4B)-W(2B)-O(5B)	80.62(12)
O(6B)-W(2B)-O(5B)	80.81(12)
O(1B)-W(2B)-O(3B)	167.09(13)
O(2B)-W(2B)-O(3B)	89.64(13)
O(4B)-W(2B)-O(3B)	80.62(11)
O(6B)-W(2B)-O(3B)	80.48(13)
O(5B)-W(2B)-O(3B)	76.35(12)
C(1B)-O(3B)-W(2B)	132.1(3)
C(3B)-O(4B)-W(2B)	135.5(3)
C(12B)-O(5B)-W(2B)	133.0(3)
C(14B)-O(6B)-W(2B)	135.1(3)
O(3B)-C(1B)-C(2B)	121.6(5)
O(3B)-C(1B)-C(8B)	118.2(5)
C(2B)-C(1B)-C(8B)	120.2(4)
C(3B)-C(2B)-C(1B)	125.1(4)
C(3B)-C(2B)-H(2BA)	117.4

C(1B)-C(2B)-H(2BA)	117.4
O(4B)-C(3B)-C(2B)	123.9(4)
O(4B)-C(3B)-C(4B)	111.3(4)
C(2B)-C(3B)-C(4B)	124.8(4)
C(6B)-C(4B)-C(3B)	108.9(4)
C(6B)-C(4B)-C(5B)	109.2(5)
C(3B)-C(4B)-C(5B)	107.5(4)
C(6B)-C(4B)-C(7B)	109.2(4)
C(3B)-C(4B)-C(7B)	112.2(4)
C(5B)-C(4B)-C(7B)	109.7(4)
C(4B)-C(5B)-H(5BA)	109.5
C(4B)-C(5B)-H(5BB)	109.5
H(5BA)-C(5B)-H(5BB)	109.5
C(4B)-C(5B)-H(5BC)	109.5
H(5BA)-C(5B)-H(5BC)	109.5
H(5BB)-C(5B)-H(5BC)	109.5
C(4B)-C(6B)-H(6BA)	109.5
C(4B)-C(6B)-H(6BB)	109.5
H(6BA)-C(6B)-H(6BB)	109.5
C(4B)-C(6B)-H(6BC)	109.5
H(6BA)-C(6B)-H(6BC)	109.5
H(6BB)-C(6B)-H(6BC)	109.5
C(4B)-C(7B)-H(7BA)	109.5
C(4B)-C(7B)-H(7BB)	109.5
H(7BA)-C(7B)-H(7BB)	109.5
C(4B)-C(7B)-H(7BC)	109.5
H(7BA)-C(7B)-H(7BC)	109.5
H(7BB)-C(7B)-H(7BC)	109.5
C(9B)-C(8B)-C(1B)	111.0(4)
C(9B)-C(8B)-C(10B)	110.4(4)
C(1B)-C(8B)-C(10B)	107.6(5)
C(9B)-C(8B)-C(11B)	108.8(5)
C(1B)-C(8B)-C(11B)	109.0(4)
C(10B)-C(8B)-C(11B)	110.0(5)
C(8B)-C(9B)-H(9BA)	109.5
C(8B)-C(9B)-H(9BB)	109.5

H(9BA)-C(9B)-H(9BB)	109.5
C(8B)-C(9B)-H(9BC)	109.5
H(9BA)-C(9B)-H(9BC)	109.5
H(9BB)-C(9B)-H(9BC)	109.5
C(8B)-C(10B)-H(10D)	109.5
C(8B)-C(10B)-H(10E)	109.5
H(10D)-C(10B)-H(10E)	109.5
C(8B)-C(10B)-H(10F)	109.5
H(10D)-C(10B)-H(10F)	109.5
H(10E)-C(10B)-H(10F)	109.5
C(8B)-C(11B)-H(11D)	109.5
C(8B)-C(11B)-H(11E)	109.5
H(11D)-C(11B)-H(11E)	109.5
C(8B)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
O(5B)-C(12B)-C(13B)	121.0(4)
O(5B)-C(12B)-C(15B)	116.5(4)
C(13B)-C(12B)-C(15B)	122.5(4)
C(14B)-C(13B)-C(12B)	124.3(5)
C(14B)-C(13B)-H(13B)	117.8
C(12B)-C(13B)-H(13B)	117.8
O(6B)-C(14B)-C(13B)	124.5(5)
O(6B)-C(14B)-C(19B)	112.5(5)
C(13B)-C(14B)-C(19B)	123.0(5)
C(17B)-C(15B)-C(16B)	113.0(5)
C(17B)-C(15B)-C(12B)	107.7(4)
C(16B)-C(15B)-C(12B)	106.3(4)
C(17B)-C(15B)-C(18B)	109.1(4)
C(16B)-C(15B)-C(18B)	108.6(5)
C(12B)-C(15B)-C(18B)	112.2(5)
C(15B)-C(16B)-H(16D)	109.5
C(15B)-C(16B)-H(16E)	109.5
H(16D)-C(16B)-H(16E)	109.5
C(15B)-C(16B)-H(16F)	109.5
H(16D)-C(16B)-H(16F)	109.5

H(16E)-C(16B)-H(16F) 109.5
C(15B)-C(17B)-H(17D) 109.5
C(15B)-C(17B)-H(17E) 109.5
H(17D)-C(17B)-H(17E) 109.5
C(15B)-C(17B)-H(17F) 109.5
H(17D)-C(17B)-H(17F) 109.5
H(17E)-C(17B)-H(17F) 109.5
C(15B)-C(18B)-H(18D) 109.5
C(15B)-C(18B)-H(18E) 109.5
H(18D)-C(18B)-H(18E) 109.5
C(15B)-C(18B)-H(18F) 109.5
H(18D)-C(18B)-H(18F) 109.5
H(18E)-C(18B)-H(18F) 109.5
C(20B)-C(19B)-C(22B) 116.5(8)
C(21D)-C(19B)-C(20D) 122.8(10)
C(21D)-C(19B)-C(14B) 117.6(9)
C(20B)-C(19B)-C(14B) 111.8(6)
C(22B)-C(19B)-C(14B) 109.3(5)
C(20D)-C(19B)-C(14B) 110.6(6)
C(20B)-C(19B)-C(21B) 107.9(7)
C(22B)-C(19B)-C(21B) 105.8(6)
C(14B)-C(19B)-C(21B) 104.8(6)
C(21D)-C(19B)-C(22D) 97.8(10)
C(20D)-C(19B)-C(22D) 99.9(7)
C(14B)-C(19B)-C(22D) 102.7(7)
C(19B)-C(20B)-H(20G) 109.5
C(19B)-C(20B)-H(20H) 109.5
H(20G)-C(20B)-H(20H) 109.5
C(19B)-C(20B)-H(20I) 109.5
H(20G)-C(20B)-H(20I) 109.5
H(20H)-C(20B)-H(20I) 109.5
C(19B)-C(21B)-H(21G) 109.5
C(19B)-C(21B)-H(21H) 109.5
H(21G)-C(21B)-H(21H) 109.5
C(19B)-C(21B)-H(21I) 109.5
H(21G)-C(21B)-H(21I) 109.5

H(21H)-C(21B)-H(21I)	109.5
C(19B)-C(22B)-H(22G)	109.5
C(19B)-C(22B)-H(22H)	109.5
H(22G)-C(22B)-H(22H)	109.5
C(19B)-C(22B)-H(22I)	109.5
H(22G)-C(22B)-H(22I)	109.5
H(22H)-C(22B)-H(22I)	109.5
C(19B)-C(20D)-H(20J)	109.5
C(19B)-C(20D)-H(20K)	109.5
H(20J)-C(20D)-H(20K)	109.5
C(19B)-C(20D)-H(20L)	109.5
H(20J)-C(20D)-H(20L)	109.5
H(20K)-C(20D)-H(20L)	109.5
C(19B)-C(21D)-H(21J)	109.5
C(19B)-C(21D)-H(21K)	109.5
H(21J)-C(21D)-H(21K)	109.5
C(19B)-C(21D)-H(21L)	109.5
H(21J)-C(21D)-H(21L)	109.5
H(21K)-C(21D)-H(21L)	109.5
C(19B)-C(22D)-H(22J)	109.5
C(19B)-C(22D)-H(22K)	109.5
H(22J)-C(22D)-H(22K)	109.5
C(19B)-C(22D)-H(22L)	109.5
H(22J)-C(22D)-H(22L)	109.5
H(22K)-C(22D)-H(22L)	109.5
C(24)-C(23)-H(23A)	109.5
C(24)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(24)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(23)-C(24)-C(25)	105.9(17)
C(23)-C(24)-H(24A)	110.6
C(25)-C(24)-H(24A)	110.6
C(23)-C(24)-H(24B)	110.6
C(25)-C(24)-H(24B)	110.6

H(24A)-C(24)-H(24B)	108.7
C(26)-C(25)-C(24)	155(2)
C(26)-C(25)-H(25A)	97.8
C(24)-C(25)-H(25A)	97.8
C(26)-C(25)-H(25B)	97.8
C(24)-C(25)-H(25B)	97.8
H(25A)-C(25)-H(25B)	103.7
C(25)-C(26)-C(27)	136.7(19)
C(25)-C(26)-H(26A)	103.0
C(27)-C(26)-H(26A)	103.0
C(25)-C(26)-H(26B)	103.0
C(27)-C(26)-H(26B)	103.0
H(26A)-C(26)-H(26B)	105.1
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

Reference:

- (1) SHELXTL2013; Bruker-AXS: Madison, Wisconsin, 2013.