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Supplementary Material

Exploring the use of the pentaphenylcyclopentadienyl ligand in uranium chemistry: the crystal structure of $(C_5Ph_5)UI_2(THF)_2$

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Table of Contents

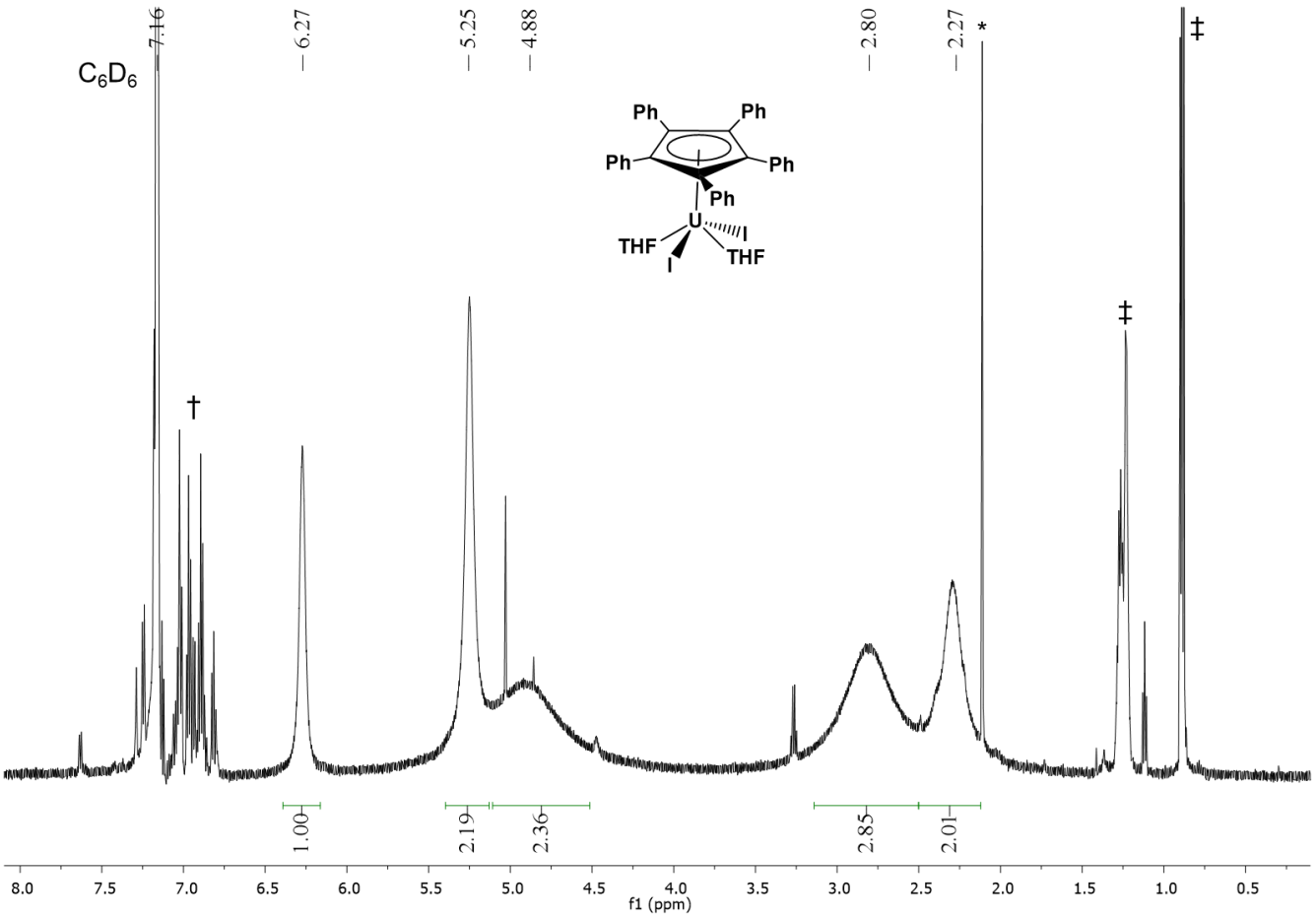

Figure S1: ^{1}H NMR spectra of $(C_5Ph_5)UI_2(THF)_2$, **1**, in C_6D_6. There were no other resonances outside this window. Impurities are marked with a symbol (†, likely HC_5Ph_5 or NaC_5Ph_5; ‡ hexane; * toluene).

X-ray Data Collection, Structure Solution and Refinement for 1.

A brown crystal of approximate dimensions 0.138 x 0.214 x 0.532 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer. The APEX2[1] program package was used to determine the unit-cell parameters. Data was collected using a 15 sec/frame scan. The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program. There were

no systematic absences nor any diffraction symmetry other than the Friedel condition. The centrosymmetric triclinic space group $P\bar{1}$ was assigned and later determined to be correct.

The structure was solved by dual space methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There was one molecule of toluene solvent present.

Least-squares analysis yielded wR2 = 0.0839 and Goof = 1.044 for 492 variables refined against 11742 data (0.73 Å), R1 = 0.0352 for those 9981 data with $I > 2.0\sigma(I)$.

Table S1. Crystal data and structure refinement for **1**.

Identification code	jcw25 (Justin Wedal)	
Empirical formula	$C_{43}\ H_{41}\ I_2\ O_2\ U \bullet C_7H_8$	
Formula weight	1173.72	
Temperature	88(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.8115(7) Å	α = 77.1972(9)°.
	b = 11.5194(7) Å	β = 80.5665(9)°.
	c = 19.1426(12) Å	γ = 71.1332(9)°.
Volume	2188.9(2) $Å^3$	
Z	2	
Density (calculated)	1.781 Mg/m^3	
Absorption coefficient	5.156 mm^{-1}	
F(000)	1126	
Crystal color	brown	
Crystal size	0.532 x 0.214 x 0.138 mm^3	
Theta range for data collection	1.899 to 29.130°	
Index ranges	$-14 \le h \le 14$, $-15 \le k \le 15$, $-26 \le l \le 26$	
Reflections collected	31370	
Independent reflections	11742 [R(int) = 0.0393]	
Completeness to theta = 25.500°	99.9 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4330 and 0.2532
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11742 / 0 / 492
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I) = 9981 data]	R1 = 0.0352, wR2 = 0.0793
R indices (all data, 0.73 Å)	R1 = 0.0463, wR2 = 0.0839
Largest diff. peak and hole	2.266 and -1.398 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
U(1)	3965(1)	6345(1)	2578(1)	13(1)
I(1)	6355(1)	5954(1)	1400(1)	20(1)
I(2)	2969(1)	4387(1)	3675(1)	24(1)
O(1)	5833(3)	5799(3)	3319(2)	21(1)
O(2)	3444(3)	5201(3)	1736(2)	19(1)
C(1)	1597(4)	8082(4)	3106(2)	14(1)
C(2)	1697(4)	8309(4)	2328(2)	13(1)
C(3)	2774(4)	8814(4)	2062(2)	13(1)
C(4)	3355(4)	8878(4)	2672(2)	14(1)
C(5)	2641(4)	8408(4)	3308(2)	12(1)
C(6)	461(4)	7838(4)	3594(2)	15(1)
C(7)	590(4)	7081(4)	4273(2)	18(1)
C(8)	-505(4)	6935(4)	4736(2)	22(1)
C(9)	-1763(4)	7581(4)	4536(2)	22(1)
C(10)	-1912(4)	8349(4)	3868(2)	19(1)
C(11)	-820(4)	8477(4)	3405(2)	15(1)
C(12)	830(4)	8057(4)	1890(2)	14(1)
C(13)	422(4)	6982(4)	2100(2)	15(1)
C(14)	-374(4)	6736(4)	1691(2)	20(1)
C(15)	-776(4)	7546(4)	1062(2)	22(1)
C(16)	-399(4)	8624(4)	853(2)	20(1)
C(17)	386(4)	8887(4)	1257(2)	15(1)
C(18)	3055(4)	9408(4)	1306(2)	11(1)
C(19)	3383(4)	8757(4)	736(2)	15(1)

C(20)	3541(4)	9356(4)	26(2)	18(1)
C(21)	3387(4)	10629(4)	-118(2)	20(1)
C(22)	3055(5)	11292(4)	439(2)	23(1)
C(23)	2893(4)	10691(4)	1146(2)	18(1)
C(24)	4376(4)	9498(4)	2637(2)	13(1)
C(25)	4207(4)	10363(4)	3074(2)	17(1)
C(26)	5111(4)	11016(4)	3016(2)	20(1)
C(27)	6216(4)	10796(4)	2522(2)	21(1)
C(28)	6408(4)	9929(4)	2086(2)	20(1)
C(29)	5490(4)	9288(4)	2138(2)	16(1)
C(30)	2796(4)	8477(4)	4054(2)	15(1)
C(31)	1794(4)	9278(4)	4437(2)	21(1)
C(32)	1938(5)	9445(5)	5107(2)	26(1)
C(33)	3096(5)	8809(5)	5419(2)	27(1)
C(34)	4111(5)	8018(4)	5052(2)	24(1)
C(35)	3953(4)	7844(4)	4375(2)	19(1)
C(36)	6893(4)	6386(4)	3188(3)	24(1)
C(37)	8091(5)	5350(5)	3447(3)	31(1)
C(38)	7499(5)	4618(6)	4086(3)	39(1)
C(39)	6214(5)	4654(5)	3845(3)	38(1)
C(40)	4132(5)	3849(4)	1858(3)	26(1)
C(41)	4344(6)	3470(5)	1129(3)	33(1)
C(42)	3176(5)	4409(5)	756(3)	30(1)
C(43)	3119(5)	5585(4)	992(2)	22(1)
C(44)	-540(7)	2538(7)	1591(5)	62(2)
C(45)	-460(7)	1629(7)	2133(4)	54(2)
C(46)	48(10)	1555(9)	2785(5)	96(3)
C(47)	653(7)	2345(7)	2862(5)	71(2)
C(48)	631(8)	3335(8)	2235(5)	73(2)
C(49)	16(8)	3409(8)	1620(4)	70(2)
C(50)	-1122(9)	2659(9)	911(5)	80(2)

Table S3. Bond lengths [Å] and angles [°] for 1

U(1)-Cnt1	2.539	U(1)-O(2)	2.524(3)
U(1)-O(1)	2.492(3)	U(1)-C(3)	2.744(4)

U(1)-C(2)	2.771(4)	C(21)-C(22)	1.381(6)
U(1)-C(4)	2.816(4)	C(22)-C(23)	1.388(6)
U(1)-C(5)	2.875(4)	C(24)-C(25)	1.388(6)
U(1)-C(1)	2.883(4)	C(24)-C(29)	1.400(6)
U(1)-I(2)	3.0644(3)	C(25)-C(26)	1.391(6)
U(1)-I(1)	3.1231(3)	C(26)-C(27)	1.388(6)
O(1)-C(39)	1.456(5)	C(27)-C(28)	1.384(6)
O(1)-C(36)	1.471(5)	C(28)-C(29)	1.397(6)
O(2)-C(43)	1.461(5)	C(30)-C(35)	1.391(6)
O(2)-C(40)	1.477(5)	C(30)-C(31)	1.398(6)
C(1)-C(5)	1.431(5)	C(31)-C(32)	1.379(6)
C(1)-C(2)	1.446(5)	C(32)-C(33)	1.385(7)
C(1)-C(6)	1.480(5)	C(33)-C(34)	1.383(7)
C(2)-C(3)	1.437(5)	C(34)-C(35)	1.400(6)
C(2)-C(12)	1.485(5)	C(36)-C(37)	1.515(6)
C(3)-C(4)	1.440(5)	C(37)-C(38)	1.501(7)
C(3)-C(18)	1.485(5)	C(38)-C(39)	1.520(7)
C(4)-C(5)	1.429(5)	C(40)-C(41)	1.514(7)
C(4)-C(24)	1.483(5)	C(41)-C(42)	1.531(7)
C(5)-C(30)	1.487(5)	C(42)-C(43)	1.500(6)
C(6)-C(7)	1.397(5)	C(44)-C(45)	1.291(10)
C(6)-C(11)	1.406(5)	C(44)-C(49)	1.341(11)
C(7)-C(8)	1.391(6)	C(44)-C(50)	1.498(11)
C(8)-C(9)	1.393(6)	C(45)-C(46)	1.419(11)
C(9)-C(10)	1.386(6)	C(46)-C(47)	1.324(11)
C(10)-C(11)	1.382(6)	C(47)-C(48)	1.457(11)
C(12)-C(13)	1.402(6)	C(48)-C(49)	1.418(11)
C(12)-C(17)	1.411(5)		
C(13)-C(14)	1.383(6)	Cnt1-U(1)-I(1)	121.9
C(14)-C(15)	1.387(6)	Cnt1-U(1)-I(2)	109.0
C(15)-C(16)	1.387(6)	Cnt1-U(1)-O(1)	110.7
C(16)-C(17)	1.377(6)	Cnt1-U(1)-O(2)	117.4
C(18)-C(19)	1.393(5)	O(1)-U(1)-O(2)	131.83(10)
C(18)-C(23)	1.399(6)	O(1)-U(1)-C(3)	118.56(11)
C(19)-C(20)	1.392(5)	O(2)-U(1)-C(3)	104.15(11)
C(20)-C(21)	1.390(6)	O(1)-U(1)-C(2)	136.78(11)

O(2)-U(1)-C(2)	91.40(11)	C(43)-O(2)-U(1)	131.9(2)
C(3)-U(1)-C(2)	30.21(11)	C(40)-O(2)-U(1)	113.7(2)
O(1)-U(1)-C(4)	90.62(11)	C(5)-C(1)-C(2)	107.4(3)
O(2)-U(1)-C(4)	134.13(10)	C(5)-C(1)-C(6)	125.6(3)
C(3)-U(1)-C(4)	29.98(11)	C(2)-C(1)-C(6)	125.7(3)
C(2)-U(1)-C(4)	49.23(11)	C(5)-C(1)-U(1)	75.3(2)
O(1)-U(1)-C(5)	89.04(10)	C(2)-C(1)-U(1)	70.9(2)
O(2)-U(1)-C(5)	138.19(10)	C(6)-C(1)-U(1)	129.6(3)
C(3)-U(1)-C(5)	48.64(11)	C(3)-C(2)-C(1)	108.0(3)
C(2)-U(1)-C(5)	48.45(11)	C(3)-C(2)-C(12)	126.7(4)
C(4)-U(1)-C(5)	29.06(11)	C(1)-C(2)-C(12)	125.4(3)
O(1)-U(1)-C(1)	114.20(11)	C(3)-C(2)-U(1)	73.8(2)
O(2)-U(1)-C(1)	110.27(10)	C(1)-C(2)-U(1)	79.5(2)
C(3)-U(1)-C(1)	48.89(11)	C(12)-C(2)-U(1)	113.0(3)
C(2)-U(1)-C(1)	29.54(11)	C(2)-C(3)-C(4)	108.0(3)
C(4)-U(1)-C(1)	48.19(11)	C(2)-C(3)-C(18)	125.5(3)
C(5)-U(1)-C(1)	28.79(11)	C(4)-C(3)-C(18)	125.4(3)
O(1)-U(1)-I(2)	86.92(7)	C(2)-C(3)-U(1)	75.9(2)
O(2)-U(1)-I(2)	79.97(7)	C(4)-C(3)-U(1)	77.8(2)
C(3)-U(1)-I(2)	131.84(8)	C(18)-C(3)-U(1)	122.2(3)
C(2)-U(1)-I(2)	103.18(8)	C(5)-C(4)-C(3)	107.7(3)
C(4)-U(1)-I(2)	125.60(8)	C(5)-C(4)-C(24)	126.5(3)
C(5)-U(1)-I(2)	96.54(8)	C(3)-C(4)-C(24)	125.2(3)
C(1)-U(1)-I(2)	84.14(8)	C(5)-C(4)-U(1)	77.8(2)
O(1)-U(1)-I(1)	78.80(7)	C(3)-C(4)-U(1)	72.2(2)
O(2)-U(1)-I(1)	74.54(7)	C(24)-C(4)-U(1)	122.7(3)
C(3)-U(1)-I(1)	97.25(8)	C(4)-C(5)-C(1)	108.9(3)
C(2)-U(1)-I(1)	120.61(8)	C(4)-C(5)-C(30)	125.1(3)
C(4)-U(1)-I(1)	103.45(8)	C(1)-C(5)-C(30)	125.1(3)
C(5)-U(1)-I(1)	131.36(8)	C(4)-C(5)-U(1)	73.2(2)
C(1)-U(1)-I(1)	146.14(8)	C(1)-C(5)-U(1)	75.9(2)
I(2)-U(1)-I(1)	129.011(9)	C(30)-C(5)-U(1)	126.0(3)
C(39)-O(1)-C(36)	108.4(3)	C(7)-C(6)-C(11)	117.4(4)
C(39)-O(1)-U(1)	123.8(3)	C(7)-C(6)-C(1)	122.8(4)
C(36)-O(1)-U(1)	126.3(2)	C(11)-C(6)-C(1)	119.5(3)
C(43)-O(2)-C(40)	108.1(3)	C(8)-C(7)-C(6)	121.3(4)

C(7)-C(8)-C(9)	120.2(4)	C(27)-C(28)-C(29)	120.2(4)
C(10)-C(9)-C(8)	119.4(4)	C(28)-C(29)-C(24)	120.6(4)
C(11)-C(10)-C(9)	120.2(4)	C(35)-C(30)-C(31)	117.6(4)
C(10)-C(11)-C(6)	121.5(4)	C(35)-C(30)-C(5)	122.5(4)
C(13)-C(12)-C(17)	118.1(4)	C(31)-C(30)-C(5)	119.7(4)
C(13)-C(12)-C(2)	120.4(3)	C(32)-C(31)-C(30)	121.7(4)
C(17)-C(12)-C(2)	121.5(4)	C(31)-C(32)-C(33)	120.0(4)
C(14)-C(13)-C(12)	120.7(4)	C(34)-C(33)-C(32)	119.8(4)
C(13)-C(14)-C(15)	120.5(4)	C(33)-C(34)-C(35)	119.8(4)
C(16)-C(15)-C(14)	119.5(4)	C(30)-C(35)-C(34)	121.1(4)
C(17)-C(16)-C(15)	120.7(4)	O(1)-C(36)-C(37)	104.9(4)
C(16)-C(17)-C(12)	120.5(4)	C(38)-C(37)-C(36)	101.9(4)
C(19)-C(18)-C(23)	118.1(4)	C(37)-C(38)-C(39)	103.3(4)
C(19)-C(18)-C(3)	122.6(4)	O(1)-C(39)-C(38)	106.0(4)
C(23)-C(18)-C(3)	119.2(4)	O(2)-C(40)-C(41)	105.6(4)
C(20)-C(19)-C(18)	121.5(4)	C(40)-C(41)-C(42)	102.2(4)
C(21)-C(20)-C(19)	119.3(4)	C(43)-C(42)-C(41)	101.4(4)
C(22)-C(21)-C(20)	120.1(4)	O(2)-C(43)-C(42)	105.3(4)
C(21)-C(22)-C(23)	120.4(4)	C(45)-C(44)-C(49)	117.3(8)
C(22)-C(23)-C(18)	120.7(4)	C(45)-C(44)-C(50)	125.6(8)
C(25)-C(24)-C(29)	118.3(4)	C(49)-C(44)-C(50)	116.9(8)
C(25)-C(24)-C(4)	120.3(4)	C(44)-C(45)-C(46)	124.8(8)
C(29)-C(24)-C(4)	121.3(4)	C(47)-C(46)-C(45)	122.3(8)
C(24)-C(25)-C(26)	121.2(4)	C(46)-C(47)-C(48)	112.8(8)
C(27)-C(26)-C(25)	120.1(4)	C(49)-C(48)-C(47)	122.0(9)
C(28)-C(27)-C(26)	119.6(4)	C(44)-C(49)-C(48)	120.4(8)

X-ray Data Collection, Structure Solution and Refinement for 2.

A colorless crystal of approximate dimensions 0.146 x 0.178 x 0.359 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer system. The APEX2[1] program package was used to determine the unit-cell parameters. Data was collected using a 60 sec/frame scan. The raw frame data was processed using SAINT2 and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program

package. The diffraction symmetry was *mmm* and the systematic absences were consistent with the orthorhombic space group $P2_12_12_1$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

Least-squares analysis yielded wR2 = 0.1110 and Goof = 1.027 for 461 variables refined against 9383 data (0.75 Å), R1 = 0.0495 for those 7658 with $I > 2.0\sigma(I)$. The absolute structure could not be assigned by refinement of the Flack parameter.[6] The structure was refined as a two-component inversion twin.

Table S4. Crystal data and structure refinement for 2.

Identification code	jcw26	
Empirical formula	C_{47} H_{49} Na O_3	
Formula weight	684.85	
Temperature	93(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 9.0566(8) Å	α= 90°.
	b = 19.3468(16) Å	β= 90°.
	c = 21.5360(18) Å	γ = 90°.
Volume	3773.5(6) $Å^3$	
Z	4	
Density (calculated)	1.205 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1464	
Crystal color	colorless	
Crystal size	0.146 x 0.178 x 0.359 mm^3	
Theta range for data collection	1.415 to 28.311°	
Index ranges	$-12 \le h \le 11$, $-25 \le k \le 25$, $-28 \le l \le 28$	

Reflections collected	47533
Independent reflections	9383 [R(int) = 0.0791]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8621 and 0.7833
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9383 / 0 / 461
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I) = 7658 data]	R1 = 0.0495, wR2 = 0.1023
R indices (all data, 0.75 Å)	R1 = 0.0690, wR2 = 0.1110
Largest diff. peak and hole	0.406 and -0.224 e.$Å^{-3}$

Table S5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Na(1)	6160(1)	9895(1)	970(1)	19(1)
O(1)	4828(2)	10088(1)	43(1)	30(1)
O(2)	4201(2)	9275(1)	1413(1)	26(1)
O(3)	5328(2)	10958(1)	1394(1)	21(1)
C(1)	8859(3)	9467(1)	589(1)	13(1)
C(2)	8571(3)	8958(1)	1054(1)	13(1)
C(3)	8685(3)	9282(1)	1646(1)	14(1)
C(4)	9058(3)	9986(1)	1548(1)	13(1)
C(5)	9156(3)	10107(1)	897(1)	13(1)
C(6)	8798(3)	9337(1)	-90(1)	13(1)
C(7)	9783(3)	9646(1)	-506(1)	16(1)
C(8)	9713(3)	9514(1)	-1140(1)	18(1)
C(9)	8656(3)	9064(1)	-1376(1)	19(1)
C(10)	7677(3)	8748(1)	-971(1)	18(1)
C(11)	7738(3)	8889(1)	-342(1)	16(1)
C(12)	8271(3)	8215(1)	930(1)	13(1)
C(13)	7016(3)	7887(1)	1170(1)	17(1)
C(14)	6690(3)	7207(1)	1018(1)	21(1)
C(15)	7605(3)	6834(1)	625(1)	21(1)
C(16)	8877(3)	7149(1)	397(1)	19(1)

C(17)	9202(3)	7827(1)	546(1)	16(1)
C(18)	8502(3)	8966(1)	2266(1)	14(1)
C(19)	7721(3)	9316(1)	2733(1)	15(1)
C(20)	7605(3)	9050(1)	3330(1)	18(1)
C(21)	8269(3)	8428(1)	3475(1)	21(1)
C(22)	9012(3)	8064(1)	3019(1)	20(1)
C(23)	9116(3)	8328(1)	2420(1)	16(1)
C(24)	9420(3)	10493(1)	2044(1)	13(1)
C(25)	10564(3)	10362(1)	2462(1)	16(1)
C(26)	10983(3)	10852(1)	2899(1)	18(1)
C(27)	10261(3)	11482(1)	2937(1)	18(1)
C(28)	9096(3)	11613(1)	2535(1)	16(1)
C(29)	8689(3)	11125(1)	2093(1)	14(1)
C(30)	9542(3)	10787(1)	628(1)	13(1)
C(31)	10724(3)	11167(1)	876(1)	14(1)
C(32)	11080(3)	11818(1)	659(1)	17(1)
C(33)	10299(3)	12109(1)	175(1)	21(1)
C(34)	9151(3)	11740(1)	-85(1)	23(1)
C(35)	8765(3)	11090(1)	138(1)	18(1)
C(36)	4955(3)	9977(2)	-621(1)	25(1)
C(37)	3791(3)	10431(2)	-935(1)	26(1)
C(38)	3303(4)	10921(2)	-416(1)	29(1)
C(39)	3479(3)	10465(2)	149(1)	29(1)
C(40)	2907(3)	9006(2)	1103(1)	28(1)
C(41)	2732(4)	8286(2)	1362(2)	31(1)
C(42)	3281(4)	8354(2)	2022(2)	44(1)
C(43)	4119(3)	9034(2)	2040(1)	26(1)
C(44)	5423(4)	11656(2)	1174(1)	27(1)
C(45)	5151(4)	12108(2)	1738(2)	31(1)
C(46)	4003(4)	11687(2)	2094(1)	31(1)
C(47)	4431(3)	10945(2)	1954(1)	25(1)

Table S6. Bond lengths [Å] and angles [°] for 2.

Na-cnt	2.563	Na(1)-O(3)	2.374(2)
Na(1)-O(2)	2.345(2)	Na(1)-C(1)	2.708(3)
Na(1)-O(1)	2.362(2)	Na(1)-C(5)	2.749(3)

Na(1)-C(2)	2.844(3)	C(22)-C(23)	1.390(4)
Na(1)-C(4)	2.911(3)	C(24)-C(29)	1.394(4)
Na(1)-C(3)	2.960(3)	C(24)-C(25)	1.395(4)
O(1)-C(39)	1.442(3)	C(25)-C(26)	1.390(4)
O(1)-C(36)	1.450(3)	C(26)-C(27)	1.385(4)
C(1)-C(2)	1.428(3)	C(27)-C(28)	1.388(4)
C(1)-C(5)	1.431(3)	C(28)-C(29)	1.390(4)
C(1)-C(6)	1.486(3)	C(30)-C(35)	1.398(4)
O(2)-C(43)	1.431(3)	C(30)-C(31)	1.405(4)
O(2)-C(40)	1.445(4)	C(31)-C(32)	1.381(4)
C(2)-C(3)	1.424(3)	C(32)-C(33)	1.379(4)
C(2)-C(12)	1.486(3)	C(33)-C(34)	1.379(4)
O(3)-C(44)	1.433(3)	C(34)-C(35)	1.391(4)
O(3)-C(47)	1.454(3)	C(36)-C(37)	1.530(4)
C(3)-C(4)	1.419(3)	C(37)-C(38)	1.530(4)
C(3)-C(18)	1.478(3)	C(38)-C(39)	1.512(4)
C(4)-C(5)	1.425(3)	C(40)-C(41)	1.510(4)
C(4)-C(24)	1.486(3)	C(41)-C(42)	1.512(5)
C(5)-C(30)	1.479(3)	C(42)-C(43)	1.521(5)
C(6)-C(7)	1.398(4)	C(44)-C(45)	1.515(4)
C(6)-C(11)	1.402(4)	C(45)-C(46)	1.527(5)
C(7)-C(8)	1.390(3)	C(46)-C(47)	1.517(4)
C(8)-C(9)	1.391(4)		
C(9)-C(10)	1.387(4)	O(2)-Na(1)-O(1)	92.20(8)
C(10)-C(11)	1.383(4)	O(2)-Na(1)-O(3)	92.64(8)
C(12)-C(17)	1.399(4)	O(1)-Na(1)-O(3)	91.51(8)
C(12)-C(13)	1.401(4)	O(2)-Na(1)-C(1)	130.51(8)
C(13)-C(14)	1.387(4)	O(1)-Na(1)-C(1)	104.69(8)
C(14)-C(15)	1.387(4)	O(3)-Na(1)-C(1)	131.95(8)
C(15)-C(16)	1.393(4)	O(2)-Na(1)-C(5)	147.83(8)
C(16)-C(17)	1.382(4)	O(1)-Na(1)-C(5)	115.63(8)
C(18)-C(23)	1.394(4)	O(3)-Na(1)-C(5)	101.89(8)
C(18)-C(19)	1.405(3)	C(1)-Na(1)-C(5)	30.40(7)
C(19)-C(20)	1.388(4)	O(2)-Na(1)-C(2)	103.21(8)
C(20)-C(21)	1.382(4)	O(1)-Na(1)-C(2)	123.15(8)
C(21)-C(22)	1.383(4)	O(3)-Na(1)-C(2)	140.51(8)

C(1)-Na(1)-C(2)	29.69(7)	C(4)-C(3)-C(2)	107.9(2)
C(5)-Na(1)-C(2)	48.78(7)	C(4)-C(3)-C(18)	123.9(2)
O(2)-Na(1)-C(4)	122.60(8)	C(2)-C(3)-C(18)	128.2(2)
O(1)-Na(1)-C(4)	144.38(8)	C(4)-C(3)-Na(1)	74.11(14)
O(3)-Na(1)-C(4)	93.97(7)	C(2)-C(3)-Na(1)	71.31(14)
C(1)-Na(1)-C(4)	48.25(7)	C(18)-C(3)-Na(1)	121.60(16)
C(5)-Na(1)-C(4)	28.98(7)	C(3)-C(4)-C(5)	108.6(2)
C(2)-Na(1)-C(4)	47.07(7)	C(3)-C(4)-C(24)	125.4(2)
O(2)-Na(1)-C(3)	100.32(8)	C(5)-C(4)-C(24)	125.7(2)
O(1)-Na(1)-C(3)	150.91(8)	C(3)-C(4)-Na(1)	77.92(14)
O(3)-Na(1)-C(3)	113.79(7)	C(5)-C(4)-Na(1)	69.19(13)
C(1)-Na(1)-C(3)	47.84(7)	C(24)-C(4)-Na(1)	123.11(16)
C(5)-Na(1)-C(3)	47.56(7)	C(4)-C(5)-C(1)	107.6(2)
C(2)-Na(1)-C(3)	28.32(7)	C(4)-C(5)-C(30)	123.2(2)
C(4)-Na(1)-C(3)	27.97(7)	C(1)-C(5)-C(30)	129.3(2)
C(39)-O(1)-C(36)	107.3(2)	C(4)-C(5)-Na(1)	81.83(14)
C(39)-O(1)-Na(1)	112.27(16)	C(1)-C(5)-Na(1)	73.21(14)
C(36)-O(1)-Na(1)	140.31(17)	C(30)-C(5)-Na(1)	112.83(16)
C(2)-C(1)-C(5)	107.9(2)	C(7)-C(6)-C(11)	116.9(2)
C(2)-C(1)-C(6)	124.6(2)	C(7)-C(6)-C(1)	122.4(2)
C(5)-C(1)-C(6)	127.6(2)	C(11)-C(6)-C(1)	120.7(2)
C(2)-C(1)-Na(1)	80.44(14)	C(8)-C(7)-C(6)	121.5(2)
C(5)-C(1)-Na(1)	76.39(14)	C(7)-C(8)-C(9)	120.4(2)
C(6)-C(1)-Na(1)	108.43(16)	C(10)-C(9)-C(8)	119.1(2)
C(43)-O(2)-C(40)	106.1(2)	C(11)-C(10)-C(9)	120.2(3)
C(43)-O(2)-Na(1)	126.16(17)	C(10)-C(11)-C(6)	121.9(2)
C(40)-O(2)-Na(1)	127.55(17)	C(17)-C(12)-C(13)	117.6(2)
C(3)-C(2)-C(1)	108.1(2)	C(17)-C(12)-C(2)	121.0(2)
C(3)-C(2)-C(12)	126.9(2)	C(13)-C(12)-C(2)	121.3(2)
C(1)-C(2)-C(12)	125.0(2)	C(14)-C(13)-C(12)	121.0(3)
C(3)-C(2)-Na(1)	80.37(14)	C(15)-C(14)-C(13)	120.7(3)
C(1)-C(2)-Na(1)	69.87(14)	C(14)-C(15)-C(16)	118.8(3)
C(12)-C(2)-Na(1)	117.69(16)	C(17)-C(16)-C(15)	120.6(3)
C(44)-O(3)-C(47)	108.9(2)	C(16)-C(17)-C(12)	121.2(2)
C(44)-O(3)-Na(1)	132.05(17)	C(23)-C(18)-C(19)	117.3(2)
C(47)-O(3)-Na(1)	118.77(16)	C(23)-C(18)-C(3)	122.4(2)

C(19)-C(18)-C(3)	120.3(2)	C(33)-C(32)-C(31)	120.6(3)
C(20)-C(19)-C(18)	121.5(2)	C(32)-C(33)-C(34)	118.8(3)
C(21)-C(20)-C(19)	119.9(2)	C(33)-C(34)-C(35)	121.1(3)
C(20)-C(21)-C(22)	119.7(2)	C(34)-C(35)-C(30)	120.9(3)
C(21)-C(22)-C(23)	120.4(2)	O(1)-C(36)-C(37)	107.2(2)
C(22)-C(23)-C(18)	121.2(2)	C(36)-C(37)-C(38)	103.4(2)
C(29)-C(24)-C(25)	117.6(2)	C(39)-C(38)-C(37)	101.2(2)
C(29)-C(24)-C(4)	121.9(2)	O(1)-C(39)-C(38)	104.9(2)
C(25)-C(24)-C(4)	120.5(2)	O(2)-C(40)-C(41)	104.3(2)
C(26)-C(25)-C(24)	121.1(2)	C(40)-C(41)-C(42)	103.4(3)
C(27)-C(26)-C(25)	120.7(2)	C(41)-C(42)-C(43)	105.3(3)
C(26)-C(27)-C(28)	118.9(2)	O(2)-C(43)-C(42)	106.5(2)
C(27)-C(28)-C(29)	120.3(2)	O(3)-C(44)-C(45)	105.6(2)
C(28)-C(29)-C(24)	121.4(2)	C(44)-C(45)-C(46)	101.9(2)
C(35)-C(30)-C(31)	116.8(2)	C(47)-C(46)-C(45)	103.3(3)
C(35)-C(30)-C(5)	123.4(2)	O(3)-C(47)-C(46)	106.9(2)
C(31)-C(30)-C(5)	119.7(2)		
C(32)-C(31)-C(30)	121.7(2)		

X-ray Data Collection, Structure Solution and Refinement for 3.

A purple crystal of approximate dimensions 0.260 x 0.274 x 0.291 mm was mounted in a cryoloop and transferred to a Bruker SMART APEX II diffractometer system. The APEX2[1] program package was used to determine the unit-cell parameters and for data collection (120 sec/frame scan time for 519 frames of data). The raw frame data was processed using SAINT[2] and SADABS[3] to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL[4] program package. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space group $P2_1/n$ that was later determined to be correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors[5] for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. One tetrahydrofuran ligand was disordered and included using multiple components, partial site-occupancy-factors, geometric and displacement constraints.

Least-squares analysis yielded wR2 = 0.2038 and Goof = 1.036 for 550 variables refined against 9041 data (0.83Å), R1 = 0.0701 for those 5780 data with $I > 2.0\sigma(I)$. The low bond precision may have been a result of disorder and the incomplete, low multiplicity data set.

There were high residuals present in the final difference-Fourier map. It was probable that additional tetrahydrofuran solvent was present. The SQUEEZE[7a] routine in the PLATON[7b] program package was used to account for the electrons in the solvent accessible voids.

Table S7. Crystal data and structure refinement for 3.

Identification code	jcw41 (Justin Wedal)	
Empirical formula	$C_{55}\ H_{65}\ K\ O_8$	
Formula weight	893.17	
Temperature	133(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.7325(14) Å	$\alpha = 90°$.
	b = 17.7160(18) Å	$\beta = 105.802(2)°$.
	c = 21.728(2) Å	$\gamma = 90°$.
Volume	5086.4(9) $Å^3$	
Z	4	
Density (calculated)	1.166 Mg/m^3	
Absorption coefficient	0.156 mm^{-1}	
F(000)	1912	
Crystal color	purple	
Crystal size	0.291 x 0.274 x 0.260 mm^3	
Theta range for data collection	1.507 to 25.350°	

Index ranges	$-14 \le h \le 16$, $-21 \le k \le 21$, $-17 \le l \le 26$
Reflections collected	20078
Independent reflections	9041 [R(int) = 0.0501]
Completeness to theta = 25.242°	97.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7454 and 0.6847
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9041 / 0 / 550
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I) = 5780 data]	R1 = 0.0701, wR2 = 0.1764
R indices (all data, 0.83 Å)	R1 = 0.1153, wR2 = 0.2038
Largest diff. peak and hole	1.324 and -0.996 e.$Å^{-3}$

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

	x	y	z	U(eq)
C(1)	8458(2)	3491(2)	6176(2)	19(1)
C(2)	8004(2)	2992(2)	5665(2)	20(1)
C(3)	8018(2)	2258(2)	5926(2)	20(1)
C(4)	8485(2)	2299(2)	6599(2)	20(1)
C(5)	8740(2)	3064(2)	6746(2)	20(1)
C(6)	8611(2)	4309(2)	6130(2)	21(1)
C(7)	9535(3)	4651(2)	6458(2)	27(1)
C(8)	9681(3)	5421(2)	6428(2)	31(1)
C(9)	8922(3)	5877(2)	6079(2)	34(1)
C(10)	8005(3)	5559(2)	5755(2)	34(1)
C(11)	7855(3)	4786(2)	5784(2)	25(1)
C(12)	7590(2)	3193(2)	4985(2)	19(1)
C(13)	8168(3)	3560(2)	4638(2)	25(1)
C(14)	7771(3)	3746(2)	4002(2)	29(1)
C(15)	6772(3)	3577(2)	3688(2)	30(1)
C(16)	6191(3)	3217(2)	4024(2)	27(1)
C(17)	6589(3)	3025(2)	4657(2)	24(1)
C(18)	7586(2)	1580(2)	5555(2)	21(1)
C(19)	7854(3)	1361(2)	5010(2)	27(1)
C(20)	7473(3)	711(2)	4679(2)	34(1)

C(21)	6809(3)	257(2)	4884(2)	32(1)
C(22)	6504(3)	468(2)	5409(2)	35(1)
C(23)	6882(3)	1124(2)	5742(2)	30(1)
C(24)	8629(2)	1653(2)	7048(2)	24(1)
C(25)	8881(3)	932(2)	6874(2)	31(1)
C(26)	8964(3)	323(2)	7281(2)	46(1)
C(27)	8812(3)	410(2)	7874(2)	48(1)
C(28)	8585(3)	1113(2)	8068(2)	40(1)
C(29)	8495(3)	1729(2)	7660(2)	28(1)
C(30)	9115(2)	3407(2)	7391(2)	20(1)
C(31)	10035(3)	3209(2)	7819(2)	26(1)
C(32)	10361(3)	3554(2)	8410(2)	30(1)
C(33)	9778(3)	4099(2)	8595(2)	29(1)
C(34)	8856(3)	4302(2)	8175(2)	26(1)
C(35)	8541(2)	3961(2)	7585(2)	23(1)
K(1)	6543(1)	7386(1)	3603(1)	28(1)
O(1)	8562(2)	6929(1)	3854(1)	33(1)
O(2)	7151(2)	6015(1)	4223(1)	31(1)
O(3)	5085(2)	6297(1)	3707(1)	30(1)
O(4)	4529(2)	7780(1)	3297(1)	31(1)
O(5)	5946(2)	8748(1)	2945(1)	30(1)
O(6)	8003(2)	8424(2)	3486(1)	34(1)
C(36)	8860(3)	6354(2)	4322(2)	33(1)
C(37)	8099(3)	5735(2)	4178(2)	36(1)
C(38)	6403(3)	5437(2)	4129(2)	33(1)
C(39)	5447(3)	5769(2)	4208(2)	34(1)
C(40)	4133(3)	6617(2)	3711(2)	33(1)
C(41)	3825(3)	7162(2)	3170(2)	34(1)
C(42)	4245(3)	8359(2)	2830(2)	35(1)
C(43)	4990(3)	8992(2)	3011(2)	34(1)
C(44)	6694(3)	9319(2)	3129(2)	37(1)
C(45)	7670(3)	9018(2)	3039(2)	39(1)
C(46)	8937(3)	8099(2)	3442(2)	43(1)
C(47)	9285(3)	7529(2)	3958(2)	38(1)
O(7)	6693(2)	8155(2)	4723(2)	53(1)
C(48)	5860(3)	8139(3)	4991(2)	50(1)

C(49)	6185(4)	7652(3)	5563(3)	58(1)
C(50)	7278(4)	7852(4)	5820(3)	76(2)
C(51)	7596(4)	8076(4)	5226(3)	84(2)
O(8)	5969(7)	6884(5)	2405(4)	102(2)
C(52)	6185(9)	6124(4)	2291(5)	102(2)
C(53)	7014(9)	6160(6)	1947(6)	102(2)
C(54)	6749(10)	6876(7)	1556(5)	102(2)
C(55)	5966(9)	7253(5)	1829(4)	102(2)
O(8B)	6498(7)	6384(4)	2539(4)	102(2)
C(52B)	7197(7)	6360(6)	2167(5)	102(2)
C(53B)	7059(8)	7059(7)	1845(5)	102(2)
C(54B)	5951(9)	7273(6)	1703(5)	102(2)
C(55B)	5536(6)	6726(6)	2104(5)	102(2)

Table S9. Bond lengths [Å] and angles [°] for **3.**

C(1)-C(5)	1.414(5)	C(16)-C(17)	1.378(5)
C(1)-C(2)	1.424(4)	C(18)-C(19)	1.387(5)
C(1)-C(6)	1.471(5)	C(18)-C(23)	1.402(5)
C(2)-C(3)	1.416(5)	C(19)-C(20)	1.383(5)
C(2)-C(12)	1.475(4)	C(20)-C(21)	1.375(5)
C(3)-C(4)	1.430(5)	C(21)-C(22)	1.371(6)
C(3)-C(18)	1.478(5)	C(22)-C(23)	1.393(5)
C(4)-C(5)	1.414(5)	C(24)-C(29)	1.396(5)
C(4)-C(24)	1.481(5)	C(24)-C(25)	1.403(5)
C(5)-C(30)	1.485(5)	C(25)-C(26)	1.380(5)
C(6)-C(11)	1.390(5)	C(26)-C(27)	1.371(7)
C(6)-C(7)	1.413(5)	C(27)-C(28)	1.376(6)
C(7)-C(8)	1.382(5)	C(28)-C(29)	1.388(5)
C(8)-C(9)	1.374(5)	C(30)-C(31)	1.394(5)
C(9)-C(10)	1.384(5)	C(30)-C(35)	1.395(5)
C(10)-C(11)	1.389(5)	C(31)-C(32)	1.382(5)
C(12)-C(13)	1.396(5)	C(32)-C(33)	1.382(5)
C(12)-C(17)	1.397(5)	C(33)-C(34)	1.391(5)
C(13)-C(14)	1.380(5)	C(34)-C(35)	1.376(5)
C(14)-C(15)	1.388(5)	K(1)-O(8)	2.659(8)
C(15)-C(16)	1.376(5)	K(1)-O(7)	2.748(3)

K(1)-O(4)	2.752(3)	O(8B)-C(55B)	1.5242
K(1)-O(6)	2.783(3)	C(52B)-C(53B)	1.4100
K(1)-O(2)	2.793(3)	C(53B)-C(54B)	1.5170
K(1)-O(1)	2.796(3)	C(54B)-C(55B)	1.5148
K(1)-O(5)	2.811(3)		
K(1)-O(3)	2.834(3)	C(5)-C(1)-C(2)	107.9(3)
K(1)-O(8B)	2.901(8)	C(5)-C(1)-C(6)	125.3(3)
O(1)-C(36)	1.419(4)	C(2)-C(1)-C(6)	126.8(3)
O(1)-C(47)	1.429(4)	C(3)-C(2)-C(1)	107.6(3)
O(2)-C(37)	1.421(4)	C(3)-C(2)-C(12)	125.6(3)
O(2)-C(38)	1.425(4)	C(1)-C(2)-C(12)	126.8(3)
O(3)-C(39)	1.419(4)	C(2)-C(3)-C(4)	108.5(3)
O(3)-C(40)	1.427(4)	C(2)-C(3)-C(18)	124.7(3)
O(4)-C(42)	1.422(4)	C(4)-C(3)-C(18)	126.8(3)
O(4)-C(41)	1.437(4)	C(5)-C(4)-C(3)	107.1(3)
O(5)-C(44)	1.419(4)	C(5)-C(4)-C(24)	127.6(3)
O(5)-C(43)	1.426(5)	C(3)-C(4)-C(24)	125.3(3)
O(6)-C(45)	1.420(5)	C(1)-C(5)-C(4)	108.9(3)
O(6)-C(46)	1.433(5)	C(1)-C(5)-C(30)	123.3(3)
C(36)-C(37)	1.489(5)	C(4)-C(5)-C(30)	127.4(3)
C(38)-C(39)	1.490(6)	C(11)-C(6)-C(7)	116.6(3)
C(40)-C(41)	1.491(6)	C(11)-C(6)-C(1)	122.5(3)
C(42)-C(43)	1.496(6)	C(7)-C(6)-C(1)	120.9(3)
C(44)-C(45)	1.503(6)	C(8)-C(7)-C(6)	121.4(3)
C(46)-C(47)	1.488(6)	C(9)-C(8)-C(7)	120.6(3)
O(7)-C(48)	1.418(5)	C(8)-C(9)-C(10)	119.4(3)
O(7)-C(51)	1.419(6)	C(9)-C(10)-C(11)	120.2(4)
C(48)-C(49)	1.478(7)	C(10)-C(11)-C(6)	121.8(3)
C(49)-C(50)	1.494(8)	C(13)-C(12)-C(17)	116.7(3)
C(50)-C(51)	1.523(8)	C(13)-C(12)-C(2)	122.2(3)
O(8)-C(55)	1.4100	C(17)-C(12)-C(2)	121.1(3)
O(8)-C(52)	1.4152	C(14)-C(13)-C(12)	121.6(3)
C(52)-C(53)	1.5245	C(13)-C(14)-C(15)	120.6(3)
C(53)-C(54)	1.5149	C(16)-C(15)-C(14)	118.6(3)
C(54)-C(55)	1.5169	C(15)-C(16)-C(17)	120.9(3)
O(8B)-C(52B)	1.4152	C(16)-C(17)-C(12)	121.7(3)

C(19)-C(18)-C(23)	116.8(3)	O(4)-K(1)-O(1)	176.74(8)
C(19)-C(18)-C(3)	122.1(3)	O(6)-K(1)-O(1)	60.54(8)
C(23)-C(18)-C(3)	121.1(3)	O(2)-K(1)-O(1)	60.23(7)
C(20)-C(19)-C(18)	121.7(4)	O(8)-K(1)-O(5)	79.71(17)
C(21)-C(20)-C(19)	120.6(4)	O(7)-K(1)-O(5)	88.08(9)
C(22)-C(21)-C(20)	119.3(3)	O(4)-K(1)-O(5)	61.62(7)
C(21)-C(22)-C(23)	120.3(4)	O(6)-K(1)-O(5)	60.27(8)
C(22)-C(23)-C(18)	121.3(4)	O(2)-K(1)-O(5)	178.20(8)
C(29)-C(24)-C(25)	116.8(3)	O(1)-K(1)-O(5)	118.98(8)
C(29)-C(24)-C(4)	121.7(3)	O(8)-K(1)-O(3)	79.81(19)
C(25)-C(24)-C(4)	121.6(3)	O(7)-K(1)-O(3)	98.67(9)
C(26)-C(25)-C(24)	121.5(4)	O(4)-K(1)-O(3)	60.44(7)
C(27)-C(26)-C(25)	120.5(4)	O(6)-K(1)-O(3)	178.35(8)
C(26)-C(27)-C(28)	119.6(4)	O(2)-K(1)-O(3)	59.61(7)
C(27)-C(28)-C(29)	120.3(4)	O(1)-K(1)-O(3)	118.15(8)
C(28)-C(29)-C(24)	121.3(4)	O(5)-K(1)-O(3)	120.70(7)
C(31)-C(30)-C(35)	117.4(3)	O(7)-K(1)-O(8B)	171.54(15)
C(31)-C(30)-C(5)	123.0(3)	O(4)-K(1)-O(8B)	99.24(19)
C(35)-C(30)-C(5)	119.6(3)	O(6)-K(1)-O(8B)	101.00(18)
C(32)-C(31)-C(30)	120.9(3)	O(2)-K(1)-O(8B)	77.93(14)
C(33)-C(32)-C(31)	120.9(3)	O(1)-K(1)-O(8B)	77.50(19)
C(32)-C(33)-C(34)	119.1(3)	O(5)-K(1)-O(8B)	100.36(14)
C(35)-C(34)-C(33)	119.8(3)	O(3)-K(1)-O(8B)	77.58(18)
C(34)-C(35)-C(30)	122.0(3)	C(36)-O(1)-C(47)	111.6(3)
O(8)-K(1)-O(7)	164.54(18)	C(36)-O(1)-K(1)	115.2(2)
O(8)-K(1)-O(4)	80.68(18)	C(47)-O(1)-K(1)	115.2(2)
O(7)-K(1)-O(4)	85.20(9)	C(37)-O(2)-C(38)	112.2(3)
O(8)-K(1)-O(6)	99.22(19)	C(37)-O(2)-K(1)	115.4(2)
O(7)-K(1)-O(6)	82.63(9)	C(38)-O(2)-K(1)	116.52(19)
O(4)-K(1)-O(6)	120.81(8)	C(39)-O(3)-C(40)	112.8(3)
O(8)-K(1)-O(2)	98.70(18)	C(39)-O(3)-K(1)	113.7(2)
O(7)-K(1)-O(2)	93.63(9)	C(40)-O(3)-K(1)	113.5(2)
O(4)-K(1)-O(2)	119.06(8)	C(42)-O(4)-C(41)	111.9(3)
O(6)-K(1)-O(2)	119.37(8)	C(42)-O(4)-K(1)	114.7(2)
O(8)-K(1)-O(1)	96.22(18)	C(41)-O(4)-K(1)	115.6(2)
O(7)-K(1)-O(1)	97.99(9)	C(44)-O(5)-C(43)	111.8(3)

C(44)-O(5)-K(1)	112.3(2)	C(48)-C(49)-C(50)	102.6(4)
C(43)-O(5)-K(1)	111.0(2)	C(49)-C(50)-C(51)	103.7(4)
C(45)-O(6)-C(46)	112.4(3)	O(7)-C(51)-C(50)	106.6(4)
C(45)-O(6)-K(1)	116.5(2)	C(55)-O(8)-C(52)	103.7
C(46)-O(6)-K(1)	114.9(2)	C(55)-O(8)-K(1)	129.9(5)
O(1)-C(36)-C(37)	109.2(3)	C(52)-O(8)-K(1)	117.9(5)
O(2)-C(37)-C(36)	109.4(3)	O(8)-C(52)-C(53)	105.4
O(2)-C(38)-C(39)	108.8(3)	C(54)-C(53)-C(52)	102.3
O(3)-C(39)-C(38)	107.9(3)	C(53)-C(54)-C(55)	103.7
O(3)-C(40)-C(41)	108.4(3)	O(8)-C(55)-C(54)	108.2
O(4)-C(41)-C(40)	108.1(3)	C(52B)-O(8B)-C(55B)	105.4
O(4)-C(42)-C(43)	108.5(3)	C(52B)-O(8B)-K(1)	127.1(5)
O(5)-C(43)-C(42)	109.2(3)	C(55B)-O(8B)-K(1)	94.5(5)
O(5)-C(44)-C(45)	108.3(3)	C(53B)-C(52B)-O(8B)	103.7
O(6)-C(45)-C(44)	107.9(3)	C(52B)-C(53B)-C(54B)	108.2
O(6)-C(46)-C(47)	109.4(3)	C(55B)-C(54B)-C(53B)	103.7
O(1)-C(47)-C(46)	108.6(3)	C(54B)-C(55B)-O(8B)	102.3
C(48)-O(7)-C(51)	108.3(4)	C(54B)-C(55B)-K(1)	102.3(4)
C(48)-O(7)-K(1)	118.7(3)	O(8B)-C(55B)-K(1)	58.8(4)
C(51)-O(7)-K(1)	118.2(3)		
O(7)-C(48)-C(49)	105.3(4)		

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

$R1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$

$Goof = S = [\Sigma[w(F_o^2-F_c^2)^2] / (n-p)]^{1/2}$ where n is the number of reflections and p is the total number of parameters refined.