Table 1. Crystal data and structure refinement for $UO_2Cl_2(THF)_3$.

Empirical formula	$C_{12}H_{24}O_5Cl_2U$
Formula weight	557.2
Temperature	-70°C
Wavelength	0.710 73 Å
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 6.8225(4)$ Å
	$b = 16.791(1)$ Å
	$c = 15.6088(9)$ Å
	$\beta = 92.893(1)$ deg
Volume	1785.9(2) Å^3
Density (calculated)	2.073 g cm^{-3}
Absorption coefficient	9.401 mm^{-1}
F(000)	1048
Crystal size	0.17 mm X 0.12 mm X 0.12 mm
Theta range for data collection	1.78 to 26.48 deg
Limiting indices	$-8 \leq h \leq 8$, $0 \leq k \leq 21$, $0 \leq l \leq 19$
Reflections collected	3592
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3592 / 0 / 181
Goodness-of-fit on F^2	0.799
Final R indices [I> 2σ(I)]	$R_1 = 0.040$, $wR_2 = 0.107$
R indices (all data)	$R_1 = 0.059$, $wR_2 = 0.120$
Largest diff. peak and hole	1.725 and -1.536 e.Å^{-3}

Table 2. Bond lengths [Å] and angles [°] for $UO_2Cl_2(THF)_3$.

U(1)-O(2)	1.765(6)
U(1)-O(1)	1.766(6)
U(1)-O(4)	2.443(6)
U(1)-O(5)	2.464(5)
U(1)-O(3)	2.467(6)
U(1)-Cl(2)	2.687(2)
U(1)-Cl(1)	2.698(2)
O(3)-C(4)	1.428(13)
O(3)-C(1)	1.462(11)
O(4)-C(5)	1.426(11)
O(4)-C(8)	1.428(10)
O(5)-C(9)	1.430(11)
O(5)-C(12)	1.464(10)
C(1)-C(2)	1.43(2)
C(2)-C(3)	1.48(2)
C(3)-C(4)	1.49(2)
C(5)-C(6)	1.45(2)
C(6)-C(7)	1.42(2)
C(7)-C(8)	1.51(2)
C(9)-C(10)	1.48(2)
C(10)-C(11)	1.48(2)
C(11)-C(12)	1.45(2)
O(2)-U(1)-O(1)	176.2(3)
O(2)-U(1)-O(4)	101.6(3)
O(1)-U(1)-O(4)	82.2(3)
O(2)-U(1)-O(5)	89.3(3)
O(1)-U(1)-O(5)	87.4(2)
O(4)-U(1)-O(5)	145.9(2)
O(2)-U(1)-O(3)	90.2(2)
O(1)-U(1)-O(3)	86.8(3)
O(4)-U(1)-O(3)	143.1(2)
O(5)-U(1)-O(3)	67.8(2)
O(2)-U(1)-Cl(2)	86.9(2)
O(1)-U(1)-Cl(2)	94.1(2)
O(4)-U(1)-Cl(2)	73.1(2)
O(5)-U(1)-Cl(2)	75.4(2)

O(3)-U(1)-Cl(2)	143.1(2)
O(2)-U(1)-Cl(1)	87.6(2)
O(1)-U(1)-Cl(1)	93.8(2)
O(4)-U(1)-Cl(1)	72.4(2)
O(5)-U(1)-Cl(1)	141.0(2)
O(3)-U(1)-Cl(1)	73.4(2)
Cl(2)-U(1)-Cl(1)	143.06(8)
C(4)-O(3)-C(1)	110.3(8)
C(4)-O(3)-U(1)	122.8(6)
C(1)-O(3)-U(1)	122.6(6)
C(5)-O(4)-C(8)	107.6(7)
C(5)-O(4)-U(1)	127.2(5)
C(8)-O(4)-U(1)	124.8(5)
C(9)-O(5)-C(12)	107.7(7)
C(9)-O(5)-U(1)	123.9(5)
C(12)-O(5)-U(1)	126.9(5)
C(2)-C(1)-O(3)	105.8(10)
C(1)-C(2)-C(3)	108.7(11)
C(2)-C(3)-C(4)	105.9(10)
O(3)-C(4)-C(3)	106.6(9)
O(4)-C(5)-C(6)	108.4(9)
C(7)-C(6)-C(5)	107.9(10)
C(6)-C(7)-C(8)	106.7(9)
O(4)-C(8)-C(7)	105.9(8)
O(5)-C(9)-C(10)	107.0(9)
C(11)-C(10)-C(9)	105.5(9)
C(12)-C(11)-C(10)	105.0(9)
C(11)-C(12)-O(5)	105.2(8)

Table 3. Anisotropic displacement parameters [Å^2 x 10^3] for $UO_2Cl_2(THF)_3$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12}]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
U(1)	25(1)	38(1)	44(1)	3(1)	5(1)	-1(1)
Cl(1)	69(2)	40(1)	81(2)	-5(1)	-11(1)	10(1)
Cl(2)	61(1)	59(2)	59(2)	-13(1)	-8(1)	-1(1)
O(1)	31(3)	56(4)	71(5)	15(3)	13(3)	-2(3)
O(2)	32(3)	54(3)	59(4)	-6(3)	10(3)	-9(3)
O(3)	36(3)	47(3)	49(4)	-2(3)	4(3)	0(2)
O(4)	34(3)	56(4)	63(4)	21(3)	3(3)	-8(3)
O(5)	38(3)	34(3)	58(4)	8(3)	-2(3)	2(2)
C(1)	44(5)	71(7)	83(8)	-7(6)	1(5)	-14(5)
C(2)	183(18)	213(21)	74(10)	20(12)	-38(11)	-158(17)
C(3)	68(8)	152(14)	64(8)	-29(9)	-17(6)	5(8)
C(4)	63(7)	88(8)	41(6)	11(5)	0(5)	-17(5)
C(5)	51(6)	147(12)	75(8)	74(9)	7(5)	-9(7)
C(6)	74(8)	149(14)	104(11)	80(11)	-9(8)	-24(9)
C(7)	54(6)	95(9)	96(10)	27(8)	-20(6)	7(6)
C(8)	30(4)	99(9)	83(8)	35(7)	10(5)	9(5)
C(9)	43(5)	59(6)	90(8)	11(6)	1(5)	5(5)
C(10)	82(8)	69(8)	107(11)	-13(7)	4(7)	30(7)
C(11)	89(9)	39(6)	131(12)	-12(6)	0(8)	6(6)
C(12)	60(6)	43(5)	79(8)	22(5)	4(5)	-4(4)

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $UO_2Cl_2(THF)_3$.

	x	y	z	U(eq)
U(1)	710(1)	7166(1)	8985(1)	36(1)
Cl(1)	1282(4)	5662(1)	8445(2)	64(1)
Cl(2)	2106(4)	8278(2)	10093(2)	60(1)
O(1)	-1267(8)	6902(4)	9616(5)	52(2)
O(2)	2572(8)	7464(4)	8308(4)	48(1)
O(3)	-1561(8)	6959(4)	7724(4)	44(1)
O(4)	2602(8)	6467(4)	10123(4)	51(2)
O(5)	-1136(8)	8383(3)	8584(4)	43(1)
C(1)	-3310(14)	6459(7)	7750(8)	66(3)
C(2)	-4035(30)	6376(13)	6880(10)	158(10)
C(3)	-2463(18)	6604(11)	6310(8)	96(5)
C(4)	-968(17)	7033(7)	6863(7)	64(3)
C(5)	1862(15)	5960(10)	10764(8)	91(5)
C(6)	3452(18)	5781(11)	11388(10)	110(6)
C(7)	5204(17)	6104(8)	11081(9)	82(4)
C(8)	4694(13)	6423(8)	10194(8)	70(3)
C(9)	-3182(14)	8489(6)	8710(8)	64(3)
C(10)	-3545(19)	9359(7)	8744(10)	86(4)
C(11)	-1577(18)	9734(6)	8784(10)	86(4)
C(12)	-316(15)	9164(6)	8389(7)	61(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters [$Å^2$ x 10^3] for $UO_2Cl_2(THF)_3$.

	x	y	z	U(eq)
H(1A)	-2979(14)	5942(7)	7996(8)	79
H(1B)	-4286(14)	6708(7)	8093(8)	79
H(2A)	-5170(30)	6716(13)	6773(10)	190
H(2B)	-4430(30)	5829(13)	6769(10)	190
H(3A)	-2977(18)	6947(11)	5852(8)	115
H(3B)	-1894(18)	6135(11)	6058(8)	115
H(4A)	319(17)	6799(7)	6808(7)	77
H(4B)	-912(17)	7590(7)	6699(7)	77
H(5A)	1357(15)	5472(10)	10505(8)	109
H(5B)	801(15)	6223(10)	11044(8)	109
H(6A)	3187(18)	6014(11)	11939(10)	132
H(6B)	3582(18)	5210(11)	11460(10)	132
H(7A)	6205(17)	5695(8)	11058(9)	99
H(7B)	5696(17)	6528(8)	11455(9)	99
H(8A)	5266(13)	6946(8)	10122(8)	84
H(8B)	5177(13)	6070(8)	9760(8)	84
H(9A)	-3530(14)	8239(6)	9242(8)	77
H(9B)	-3962(14)	8250(6)	8241(8)	77
H(10A)	-4306(19)	9534(7)	8237(10)	103
H(10B)	-4252(19)	9496(7)	9247(10)	103
H(11A)	-1600(18)	10234(6)	8472(10)	104
H(11B)	-1130(18)	9834(6)	9374(10)	104
H(12A)	1021(15)	9210(6)	8626(7)	73
H(12B)	-322(15)	9248(6)	7774(7)	73