

Supporting Information for
Reaction Chemistry of the U³⁺ Metallocene Amidinate (C₅Me₅)₂[ⁱPrNC(Me)NⁱPr]U
Including the Isolation of a Uranium Complex of a Monodentate Acetate

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X-ray Data Collection, Structure Solution and Refinement for **(C₅Me₅)₂[ⁱPrNC(Me)NⁱPr- κ^2 N,N']U(SPh), 2.**

A red crystal of approximate dimensions 0.18 x 0.19 x 0.22 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. The diffraction symmetry was *2/m* and the systematic absences were consistent with the monoclinic space group *P*2₁/*c* that was later determined to be correct.

The structure was solved by direct methods and refined on F² by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. The pentamethylcyclopentadienyl ring defined by atoms C(11)-C(20) was disordered and included using multiple components, partial site-occupancy-factors (0.56:0.44) and isotropic thermal parameters. The thermal parameters of the phenyl ring were set equal via the EADP command⁴.

At convergence, wR2 = 0.0622 and Goof = 1.089 for 324 variables refined against 8900 data (0.72Å), R1 = 0.0295 for those 8011 data with I > 2.0σ(I).

Table 1. Crystal data and structure refinement for **(C₅Me₅)₂[ⁱPrNC(Me)NⁱPr- κ^2 N,N']U(SPh), 2.**

Identification code	jrw27 (Justin Walensky)	
Empirical formula	C ₃₄ H ₅₂ N ₂ S U	
Formula weight	758.87	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	<i>P</i> 2 ₁ / <i>c</i>	
Unit cell dimensions	a = 11.5156(6) Å	α = 90°.
	b = 17.1703(9) Å	β = 90.2320(10)°.
	c = 16.0926(8) Å	γ = 90°.
Volume	3181.9(3) Å ³	
Z	4	
Density (calculated)	1.584 Mg/m ³	
Absorption coefficient	5.191 mm ⁻¹	
F(000)	1512	
Crystal color	red	

Crystal size	0.22 x 0.19 x 0.18 mm ³
Theta range for data collection	4.17 to 29.57°.
Index ranges	-15 ≤ <i>h</i> ≤ 15, -23 ≤ <i>k</i> ≤ 23, -22 ≤ <i>l</i> ≤ 22
Reflections collected	41574
Independent reflections	8900 [R(int) = 0.0231]
Completeness to theta = 29.57°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.4551 and 0.3947
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	8900 / 0 / 324
Goodness-of-fit on F ²	1.089
Final R indices [I>2sigma(I) = 8011 data]	R1 = 0.0295, wR2 = 0.0605
R indices (all data, 0.72Å)	R1 = 0.0344, wR2 = 0.0622
Largest diff. peak and hole	2.836 and -1.795 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrww27. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
U(1)	7980(1)	471(1)	7421(1)	15(1)
S(1)	7314(1)	-1077(1)	7432(1)	29(1)
N(1)	7041(2)	1769(2)	7327(2)	20(1)
N(2)	5946(2)	702(2)	7326(2)	20(1)
C(1)	7692(3)	859(2)	9062(2)	22(1)
C(2)	8853(3)	1075(2)	8873(2)	27(1)
C(3)	9505(3)	375(3)	8784(2)	32(1)
C(4)	8757(4)	-261(2)	8896(2)	30(1)
C(5)	7629(3)	32(2)	9073(2)	26(1)
C(6)	6715(3)	1382(2)	9340(2)	27(1)
C(7)	9351(4)	1887(3)	8868(3)	37(1)
C(8)	10812(4)	306(4)	8790(3)	52(2)
C(9)	9147(5)	-1096(3)	8981(3)	47(1)
C(10)	6604(4)	-431(2)	9355(2)	35(1)
C(11)	8449(5)	855(4)	5798(4)	13(1)
C(12)	8629(6)	41(4)	5836(4)	18(1)
C(13)	9607(6)	-122(4)	6331(4)	22(1)
C(14)	10082(6)	594(5)	6582(4)	23(1)
C(15)	9368(7)	1203(4)	6264(5)	20(2)
C(16)	7530(5)	1225(4)	5277(4)	23(1)
C(17)	8023(6)	-543(4)	5273(4)	29(1)
C(18)	10138(7)	-916(4)	6482(5)	35(2)
C(19)	11276(7)	759(5)	6920(5)	42(2)
C(20)	9713(6)	2052(4)	6226(4)	28(1)
C(11B)	8509(8)	604(6)	5758(5)	23(2)
C(12B)	9049(8)	-84(5)	5977(5)	20(2)
C(13B)	9980(7)	102(5)	6504(5)	17(1)
C(14B)	10059(6)	911(5)	6583(4)	15(1)
C(15B)	9148(9)	1240(6)	6120(6)	22(2)
C(16B)	7478(10)	726(7)	5169(7)	45(3)
C(17B)	8904(9)	-863(6)	5566(6)	39(2)

C(18B)	10852(8)	-508(6)	6787(6)	36(2)
C(19B)	11079(8)	1375(6)	6933(6)	34(2)
C(20B)	9134(10)	2081(7)	5861(7)	46(3)
C(21)	5974(3)	1485(2)	7268(2)	21(1)
C(22)	4903(4)	1980(3)	7150(3)	39(1)
C(23)	7302(4)	2616(2)	7297(2)	28(1)
C(24)	6892(4)	3074(2)	8051(3)	36(1)
C(25)	6910(5)	3035(3)	6495(3)	50(1)
C(26)	4878(3)	231(2)	7284(2)	26(1)
C(27)	4034(4)	356(3)	8006(3)	44(1)
C(28)	4247(3)	274(2)	6450(2)	30(1)
C(29)	6844(4)	-1628(3)	6570(3)	44(1)
C(30)	7347(4)	-2344(3)	6420(3)	44(1)
C(31)	7011(4)	-2805(3)	5752(3)	44(1)
C(32)	6117(4)	-2571(3)	5239(3)	44(1)
C(33)	5596(4)	-1885(3)	5384(3)	44(1)
C(34)	5955(4)	-1411(3)	6040(3)	44(1)

Table 3. Bond lengths [Å] and angles [°] for jr_w27.

U(1)-Cnt1	2.510
U(1)-Cnt2	2.515
U(1)-N(2)	2.380(3)
U(1)-N(1)	2.482(3)
U(1)-C(2)	2.743(3)
U(1)-C(1)	2.746(3)
U(1)-C(11)	2.749(6)
U(1)-C(11B)	2.756(9)
U(1)-C(12)	2.761(6)
U(1)-C(15)	2.761(8)
U(1)-C(13)	2.766(6)
U(1)-S(1)	2.7665(9)
U(1)-C(14)	2.784(7)
U(1)-C(5)	2.794(3)
U(1)-C(12B)	2.801(8)
U(1)-C(3)	2.809(3)
U(1)-C(13B)	2.812(7)
U(1)-C(15B)	2.821(10)
U(1)-C(4)	2.830(3)
U(1)-C(14B)	2.855(7)
U(1)-C(21)	2.902(3)
S(1)-C(29)	1.762(5)
N(1)-C(21)	1.324(4)
N(1)-C(23)	1.486(4)
N(2)-C(21)	1.349(4)
N(2)-C(26)	1.472(4)
C(1)-C(5)	1.421(5)
C(1)-C(2)	1.422(5)
C(1)-C(6)	1.508(5)
C(2)-C(3)	1.425(5)
C(2)-C(7)	1.508(6)
C(3)-C(4)	1.403(6)
C(3)-C(8)	1.510(6)
C(4)-C(5)	1.424(5)

C(4)-C(9)	1.507(5)
C(5)-C(10)	1.495(6)
C(11)-C(12)	1.414(9)
C(11)-C(15)	1.426(10)
C(11)-C(16)	1.491(8)
C(12)-C(13)	1.405(9)
C(12)-C(17)	1.519(9)
C(13)-C(14)	1.403(10)
C(13)-C(18)	1.513(10)
C(14)-C(15)	1.424(10)
C(14)-C(19)	1.504(11)
C(15)-C(20)	1.513(10)
C(11B)-C(12B)	1.380(13)
C(11B)-C(15B)	1.439(14)
C(11B)-C(16B)	1.531(14)
C(12B)-C(13B)	1.401(11)
C(12B)-C(17B)	1.501(13)
C(13B)-C(14B)	1.397(10)
C(13B)-C(18B)	1.520(12)
C(14B)-C(15B)	1.404(13)
C(14B)-C(19B)	1.525(12)
C(15B)-C(20B)	1.502(15)
C(21)-C(22)	1.508(5)
C(23)-C(24)	1.523(5)
C(23)-C(25)	1.543(6)
C(26)-C(28)	1.526(5)
C(26)-C(27)	1.534(5)
C(29)-C(34)	1.380(6)
C(29)-C(30)	1.380(6)
C(30)-C(31)	1.389(6)
C(31)-C(32)	1.377(6)
C(32)-C(33)	1.343(6)
C(33)-C(34)	1.395(6)
Cnt1-U(1)-N(1)	101.1
Cnt1-U(1)-N(2)	107.1

Cnt1-U(1)-S(1)	91.2
Cnt2-U(1)-N(1)	100.1
Cnt2-U(1)-N(2)	122.3
Cnt2-U(1)-S(1)	102.4
Cnt1-U(1)-Cnt2	129.7
N(2)-U(1)-N(1)	54.41(10)
N(2)-U(1)-C(2)	110.40(10)
N(1)-U(1)-C(2)	82.54(10)
N(2)-U(1)-C(1)	84.16(10)
N(1)-U(1)-C(1)	77.65(10)
C(2)-U(1)-C(1)	30.02(11)
N(2)-U(1)-C(11)	95.55(14)
N(1)-U(1)-C(11)	79.32(16)
C(2)-U(1)-C(11)	130.23(16)
C(1)-U(1)-C(11)	151.75(17)
N(2)-U(1)-C(11B)	98.4(2)
N(1)-U(1)-C(11B)	88.0(2)
C(2)-U(1)-C(11B)	135.6(2)
C(1)-U(1)-C(11B)	160.4(2)
C(11)-U(1)-C(11B)	9.2(2)
N(2)-U(1)-C(12)	104.81(17)
N(1)-U(1)-C(12)	107.69(16)
C(2)-U(1)-C(12)	142.02(16)
C(1)-U(1)-C(12)	171.02(17)
C(11)-U(1)-C(12)	29.73(18)
C(11B)-U(1)-C(12)	20.6(2)
N(2)-U(1)-C(15)	116.98(19)
N(1)-U(1)-C(15)	78.69(18)
C(2)-U(1)-C(15)	101.02(19)
C(1)-U(1)-C(15)	127.65(18)
C(11)-U(1)-C(15)	30.0(2)
C(11B)-U(1)-C(15)	34.6(3)
C(12)-U(1)-C(15)	48.7(2)
N(2)-U(1)-C(13)	133.63(17)
N(1)-U(1)-C(13)	126.03(15)
C(2)-U(1)-C(13)	115.62(18)

C(1)-U(1)-C(13)	141.64(17)
C(11)-U(1)-C(13)	49.41(19)
C(11B)-U(1)-C(13)	42.4(2)
C(12)-U(1)-C(13)	29.45(18)
C(15)-U(1)-C(13)	49.0(2)
N(2)-U(1)-S(1)	83.54(7)
N(1)-U(1)-S(1)	137.95(7)
C(2)-U(1)-S(1)	117.25(9)
C(1)-U(1)-S(1)	101.06(8)
C(11)-U(1)-S(1)	106.99(15)
C(11B)-U(1)-S(1)	98.5(2)
C(12)-U(1)-S(1)	79.95(13)
C(15)-U(1)-S(1)	127.09(16)
C(13)-U(1)-S(1)	80.76(15)
N(2)-U(1)-C(14)	144.48(16)
N(1)-U(1)-C(14)	106.40(18)
C(2)-U(1)-C(14)	93.90(16)
C(1)-U(1)-C(14)	123.83(16)
C(11)-U(1)-C(14)	49.21(18)
C(11B)-U(1)-C(14)	47.7(2)
C(12)-U(1)-C(14)	48.19(19)
C(15)-U(1)-C(14)	29.8(2)
C(13)-U(1)-C(14)	29.3(2)
S(1)-U(1)-C(14)	108.52(17)
N(2)-U(1)-C(5)	87.68(10)
N(1)-U(1)-C(5)	103.58(10)
C(2)-U(1)-C(5)	49.10(12)
C(1)-U(1)-C(5)	29.70(10)
C(11)-U(1)-C(5)	176.57(15)
C(11B)-U(1)-C(5)	168.4(2)
C(12)-U(1)-C(5)	147.95(15)
C(15)-U(1)-C(5)	148.26(19)
C(13)-U(1)-C(5)	127.25(15)
S(1)-U(1)-C(5)	72.15(8)
C(14)-U(1)-C(5)	127.66(16)
N(2)-U(1)-C(12B)	116.1(2)

N(1)-U(1)-C(12B)	116.64(19)
C(2)-U(1)-C(12B)	132.4(2)
C(1)-U(1)-C(12B)	159.4(2)
C(11)-U(1)-C(12B)	37.3(2)
C(11B)-U(1)-C(12B)	28.8(3)
C(12)-U(1)-C(12B)	11.84(17)
C(15)-U(1)-C(12B)	48.5(2)
C(13)-U(1)-C(12B)	17.7(2)
S(1)-U(1)-C(12B)	78.55(16)
C(14)-U(1)-C(12B)	40.3(2)
C(5)-U(1)-C(12B)	139.8(2)
N(2)-U(1)-C(3)	132.19(10)
N(1)-U(1)-C(3)	111.77(11)
C(2)-U(1)-C(3)	29.70(11)
C(1)-U(1)-C(3)	48.74(10)
C(11)-U(1)-C(3)	129.14(15)
C(11B)-U(1)-C(3)	128.5(2)
C(12)-U(1)-C(3)	122.34(17)
C(15)-U(1)-C(3)	101.0(2)
C(13)-U(1)-C(3)	92.90(17)
S(1)-U(1)-C(3)	96.36(10)
C(14)-U(1)-C(3)	80.85(16)
C(5)-U(1)-C(3)	48.21(12)
C(12B)-U(1)-C(3)	110.6(2)
N(2)-U(1)-C(13B)	144.28(18)
N(1)-U(1)-C(13B)	121.87(17)
C(2)-U(1)-C(13B)	103.53(19)
C(1)-U(1)-C(13B)	131.43(18)
C(11)-U(1)-C(13B)	52.5(2)
C(11B)-U(1)-C(13B)	47.5(2)
C(12)-U(1)-C(13B)	39.6(2)
C(15)-U(1)-C(13B)	43.2(2)
C(13)-U(1)-C(13B)	13.13(16)
S(1)-U(1)-C(13B)	90.86(17)
C(14)-U(1)-C(13B)	17.7(2)
C(5)-U(1)-C(13B)	124.09(17)

C(12B)-U(1)-C(13B)	28.9(2)
C(3)-U(1)-C(13B)	83.44(18)
N(2)-U(1)-C(15B)	110.3(2)
N(1)-U(1)-C(15B)	75.1(2)
C(2)-U(1)-C(15B)	106.3(2)
C(1)-U(1)-C(15B)	131.3(2)
C(11)-U(1)-C(15B)	24.1(2)
C(11B)-U(1)-C(15B)	29.9(3)
C(12)-U(1)-C(15B)	46.2(2)
C(15)-U(1)-C(15B)	7.1(2)
C(13)-U(1)-C(15B)	51.4(2)
S(1)-U(1)-C(15B)	126.0(2)
C(14)-U(1)-C(15B)	35.6(3)
C(5)-U(1)-C(15B)	154.6(2)
C(12B)-U(1)-C(15B)	48.1(3)
C(3)-U(1)-C(15B)	108.0(2)
C(13B)-U(1)-C(15B)	47.3(3)
N(2)-U(1)-C(4)	115.82(11)
N(1)-U(1)-C(4)	125.88(10)
C(2)-U(1)-C(4)	48.65(12)
C(1)-U(1)-C(4)	48.64(10)
C(11)-U(1)-C(4)	147.26(15)
C(11B)-U(1)-C(4)	141.4(2)
C(12)-U(1)-C(4)	124.79(17)
C(15)-U(1)-C(4)	125.9(2)
C(13)-U(1)-C(4)	98.98(16)
S(1)-U(1)-C(4)	69.77(9)
C(14)-U(1)-C(4)	99.66(17)
C(5)-U(1)-C(4)	29.32(11)
C(12B)-U(1)-C(4)	114.0(2)
C(3)-U(1)-C(4)	28.81(13)
C(13B)-U(1)-C(4)	94.78(17)
C(15B)-U(1)-C(4)	132.9(2)
N(2)-U(1)-C(14B)	138.85(17)
N(1)-U(1)-C(14B)	95.73(19)
C(2)-U(1)-C(14B)	89.84(17)

C(1)-U(1)-C(14B)	119.68(17)
C(11)-U(1)-C(14B)	47.10(19)
C(11B)-U(1)-C(14B)	48.0(2)
C(12)-U(1)-C(14B)	53.4(2)
C(15)-U(1)-C(14B)	21.9(2)
C(13)-U(1)-C(14B)	39.3(2)
S(1)-U(1)-C(14B)	119.39(18)
C(14)-U(1)-C(14B)	11.01(16)
C(5)-U(1)-C(14B)	130.22(17)
C(12B)-U(1)-C(14B)	47.6(2)
C(3)-U(1)-C(14B)	82.04(17)
C(13B)-U(1)-C(14B)	28.5(2)
C(15B)-U(1)-C(14B)	28.6(3)
C(4)-U(1)-C(14B)	104.54(18)
N(2)-U(1)-C(21)	27.37(10)
N(1)-U(1)-C(21)	27.06(9)
C(2)-U(1)-C(21)	97.69(10)
C(1)-U(1)-C(21)	80.59(9)
C(11)-U(1)-C(21)	86.30(15)
C(11B)-U(1)-C(21)	92.7(2)
C(12)-U(1)-C(21)	107.50(16)
C(15)-U(1)-C(21)	97.63(18)
C(13)-U(1)-C(21)	135.08(15)
S(1)-U(1)-C(21)	110.88(7)
C(14)-U(1)-C(21)	127.36(17)
C(5)-U(1)-C(21)	97.12(10)
C(12B)-U(1)-C(21)	119.1(2)
C(3)-U(1)-C(21)	126.58(10)
C(13B)-U(1)-C(21)	138.06(16)
C(15B)-U(1)-C(21)	92.2(2)
C(4)-U(1)-C(21)	125.91(10)
C(14B)-U(1)-C(21)	118.04(19)
C(29)-S(1)-U(1)	126.46(18)
C(21)-N(1)-C(23)	123.1(3)
C(21)-N(1)-U(1)	94.4(2)
C(23)-N(1)-U(1)	142.4(2)

C(21)-N(2)-C(26)	124.4(3)
C(21)-N(2)-U(1)	98.4(2)
C(26)-N(2)-U(1)	137.1(2)
C(5)-C(1)-C(2)	108.1(3)
C(5)-C(1)-C(6)	123.6(3)
C(2)-C(1)-C(6)	127.7(3)
C(5)-C(1)-U(1)	77.05(19)
C(2)-C(1)-U(1)	74.90(19)
C(6)-C(1)-U(1)	121.5(2)
C(1)-C(2)-C(3)	107.3(3)
C(1)-C(2)-C(7)	126.9(4)
C(3)-C(2)-C(7)	125.4(4)
C(1)-C(2)-U(1)	75.08(19)
C(3)-C(2)-U(1)	77.7(2)
C(7)-C(2)-U(1)	118.9(2)
C(4)-C(3)-C(2)	108.7(3)
C(4)-C(3)-C(8)	123.4(4)
C(2)-C(3)-C(8)	126.2(4)
C(4)-C(3)-U(1)	76.4(2)
C(2)-C(3)-U(1)	72.59(19)
C(8)-C(3)-U(1)	129.0(2)
C(3)-C(4)-C(5)	108.1(3)
C(3)-C(4)-C(9)	124.7(4)
C(5)-C(4)-C(9)	126.2(4)
C(3)-C(4)-U(1)	74.8(2)
C(5)-C(4)-U(1)	73.97(19)
C(9)-C(4)-U(1)	126.2(2)
C(1)-C(5)-C(4)	107.7(4)
C(1)-C(5)-C(10)	125.1(3)
C(4)-C(5)-C(10)	126.4(4)
C(1)-C(5)-U(1)	73.25(19)
C(4)-C(5)-U(1)	76.7(2)
C(10)-C(5)-U(1)	123.3(2)
C(12)-C(11)-C(15)	106.4(6)
C(12)-C(11)-C(16)	123.4(6)
C(15)-C(11)-C(16)	129.8(7)

C(12)-C(11)-U(1)	75.6(3)
C(15)-C(11)-U(1)	75.5(4)
C(16)-C(11)-U(1)	119.6(4)
C(13)-C(12)-C(11)	109.7(5)
C(13)-C(12)-C(17)	124.9(6)
C(11)-C(12)-C(17)	124.0(6)
C(13)-C(12)-U(1)	75.5(3)
C(11)-C(12)-U(1)	74.7(3)
C(17)-C(12)-U(1)	127.0(4)
C(14)-C(13)-C(12)	107.5(6)
C(14)-C(13)-C(18)	125.8(7)
C(12)-C(13)-C(18)	126.3(7)
C(14)-C(13)-U(1)	76.1(4)
C(12)-C(13)-U(1)	75.1(3)
C(18)-C(13)-U(1)	120.2(4)
C(13)-C(14)-C(15)	108.4(6)
C(13)-C(14)-C(19)	128.7(7)
C(15)-C(14)-C(19)	121.1(7)
C(13)-C(14)-U(1)	74.6(4)
C(15)-C(14)-U(1)	74.2(4)
C(19)-C(14)-U(1)	129.4(5)
C(14)-C(15)-C(11)	107.9(6)
C(14)-C(15)-C(20)	124.8(7)
C(11)-C(15)-C(20)	125.2(7)
C(14)-C(15)-U(1)	76.0(4)
C(11)-C(15)-U(1)	74.5(4)
C(20)-C(15)-U(1)	128.2(5)
C(12B)-C(11B)-C(15B)	108.5(8)
C(12B)-C(11B)-C(16B)	128.5(10)
C(15B)-C(11B)-C(16B)	122.7(10)
C(12B)-C(11B)-U(1)	77.4(5)
C(15B)-C(11B)-U(1)	77.6(5)
C(16B)-C(11B)-U(1)	116.0(6)
C(11B)-C(12B)-C(13B)	107.5(7)
C(11B)-C(12B)-C(17B)	127.0(9)
C(13B)-C(12B)-C(17B)	123.6(9)

C(11B)-C(12B)-U(1)	73.8(5)
C(13B)-C(12B)-U(1)	76.0(4)
C(17B)-C(12B)-U(1)	128.3(6)
C(14B)-C(13B)-C(12B)	109.4(7)
C(14B)-C(13B)-C(18B)	128.0(8)
C(12B)-C(13B)-C(18B)	121.8(8)
C(14B)-C(13B)-U(1)	77.4(4)
C(12B)-C(13B)-U(1)	75.1(4)
C(18B)-C(13B)-U(1)	122.6(5)
C(13B)-C(14B)-C(15B)	107.7(7)
C(13B)-C(14B)-C(19B)	127.1(8)
C(15B)-C(14B)-C(19B)	124.0(8)
C(13B)-C(14B)-U(1)	74.0(4)
C(15B)-C(14B)-U(1)	74.3(5)
C(19B)-C(14B)-U(1)	127.6(5)
C(14B)-C(15B)-C(11B)	106.8(8)
C(14B)-C(15B)-C(20B)	122.8(9)
C(11B)-C(15B)-C(20B)	127.8(10)
C(14B)-C(15B)-U(1)	77.0(5)
C(11B)-C(15B)-U(1)	72.5(5)
C(20B)-C(15B)-U(1)	130.6(7)
N(1)-C(21)-N(2)	112.7(3)
N(1)-C(21)-C(22)	124.0(3)
N(2)-C(21)-C(22)	123.4(3)
N(1)-C(21)-U(1)	58.52(17)
N(2)-C(21)-U(1)	54.21(17)
C(22)-C(21)-U(1)	176.6(3)
N(1)-C(23)-C(24)	114.5(3)
N(1)-C(23)-C(25)	115.1(3)
C(24)-C(23)-C(25)	109.6(3)
N(2)-C(26)-C(28)	114.1(3)
N(2)-C(26)-C(27)	114.8(3)
C(28)-C(26)-C(27)	111.0(3)
C(34)-C(29)-C(30)	116.3(4)
C(34)-C(29)-S(1)	124.5(4)
C(30)-C(29)-S(1)	119.2(4)

C(29)-C(30)-C(31)	121.8(5)
C(32)-C(31)-C(30)	120.2(5)
C(33)-C(32)-C(31)	119.0(4)
C(32)-C(33)-C(34)	120.8(5)
C(29)-C(34)-C(33)	121.8(5)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw27. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
U(1)	17(1)	17(1)	11(1)	-1(1)	-1(1)	3(1)
S(1)	46(1)	19(1)	21(1)	-1(1)	2(1)	1(1)
N(1)	25(1)	15(1)	18(1)	-1(1)	0(1)	3(1)
N(2)	16(1)	20(1)	23(1)	0(1)	0(1)	0(1)
C(1)	26(2)	28(2)	13(1)	-1(1)	-2(1)	7(1)
C(2)	28(2)	37(2)	14(1)	-3(1)	-4(1)	3(2)
C(3)	29(2)	52(3)	14(1)	-4(2)	-4(1)	14(2)
C(4)	43(2)	34(2)	14(2)	-1(1)	-4(1)	20(2)
C(5)	36(2)	28(2)	13(1)	3(1)	0(1)	9(2)
C(6)	33(2)	30(2)	18(2)	-3(1)	2(1)	10(2)
C(7)	37(2)	50(3)	26(2)	-2(2)	-9(2)	-9(2)
C(8)	28(2)	104(4)	23(2)	-8(2)	-9(2)	27(2)
C(9)	76(3)	43(2)	23(2)	3(2)	-6(2)	37(2)
C(10)	54(3)	31(2)	20(2)	6(2)	9(2)	2(2)
C(21)	23(2)	22(2)	17(1)	1(1)	2(1)	6(1)
C(22)	27(2)	36(2)	55(3)	14(2)	7(2)	15(2)
C(23)	43(2)	14(2)	27(2)	1(1)	1(2)	3(1)
C(24)	55(3)	22(2)	31(2)	-8(2)	-1(2)	5(2)
C(25)	98(4)	24(2)	29(2)	8(2)	6(2)	7(2)
C(26)	18(2)	29(2)	30(2)	0(1)	1(1)	-3(1)
C(27)	28(2)	69(3)	36(2)	-3(2)	7(2)	-13(2)
C(28)	24(2)	30(2)	35(2)	-9(2)	0(1)	0(1)
C(29)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)
C(30)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)
C(31)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)
C(32)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)
C(33)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)
C(34)	52(1)	45(1)	36(1)	-11(1)	-8(1)	8(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jrw27.

	x	y	z	U(eq)
H(6A)	6327	1149	9820	41
H(6B)	6155	1445	8884	41
H(6C)	7029	1892	9495	41
H(7A)	10092	1890	9170	56
H(7B)	8807	2244	9138	56
H(7C)	9478	2054	8293	56
H(8A)	11079	164	9348	78
H(8B)	11156	806	8631	78
H(8C)	11051	-96	8394	78
H(9A)	9597	-1157	9495	71
H(9B)	9631	-1236	8504	71
H(9C)	8465	-1437	8998	71
H(10A)	6643	-502	9958	53
H(10B)	6610	-941	9082	53
H(10C)	5888	-154	9208	53
H(16A)	7341	884	4807	35
H(16B)	7811	1727	5068	35
H(16C)	6833	1309	5613	35
H(17A)	8295	-475	4701	44
H(17B)	7182	-458	5293	44
H(17C)	8201	-1073	5461	44
H(18A)	10597	-1070	5998	53
H(18B)	9518	-1298	6573	53
H(18C)	10641	-894	6974	53
H(19A)	11792	905	6462	63
H(19B)	11580	293	7196	63
H(19C)	11235	1188	7320	63
H(20A)	10351	2117	5830	42
H(20B)	9967	2225	6778	42
H(20C)	9046	2364	6045	42

H(16D)	7763	822	4606	68
H(16E)	7022	1175	5356	68
H(16F)	6987	260	5170	68
H(17D)	9464	-913	5112	59
H(17E)	8114	-909	5344	59
H(17F)	9041	-1277	5975	59
H(18D)	11139	-795	6303	54
H(18E)	10474	-871	7170	54
H(18F)	11503	-252	7069	54
H(19D)	11549	1577	6475	51
H(19E)	11558	1036	7284	51
H(19F)	10785	1810	7265	51
H(20D)	9722	2167	5433	69
H(20E)	9305	2410	6344	69
H(20F)	8366	2214	5639	69
H(22A)	5073	2517	7317	59
H(22B)	4272	1773	7492	59
H(22C)	4670	1970	6564	59
H(23A)	8168	2655	7305	34
H(24A)	7226	2846	8557	54
H(24B)	6043	3054	8081	54
H(24C)	7144	3617	8002	54
H(25A)	6908	2664	6032	75
H(25B)	7447	3462	6373	75
H(25C)	6126	3244	6571	75
H(26A)	5143	-322	7336	31
H(27A)	4468	370	8531	66
H(27B)	3472	-72	8021	66
H(27C)	3621	850	7929	66
H(28A)	4814	253	5998	44
H(28B)	3811	764	6416	44
H(28C)	3708	-165	6400	44
H(30A)	7939	-2526	6784	53
H(31A)	7399	-3284	5649	53
H(32A)	5873	-2891	4788	53
H(33A)	4975	-1721	5035	53

X-ray Data Collection, Structure Solution and Refinement for $(C_5Me_5)_2[{}^iPrNC(Me)N^iPr-\kappa^2N,N']U(Spy)$, **3**.

A red crystal of approximate dimensions 0.13 x 0.20 x 0.22 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (15 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. The diffraction symmetry was 2/*m* and the systematic absences were consistent with the monoclinic space groups *C2/c* and *Cc*. It was later determined that the centrosymmetric space group *C2/c* was correct.

The structure was solved by direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model. There was one-half molecule of toluene solvent present per formula unit. The toluene molecule was located about an inversion center and was disordered. Hydrogen atoms associated with the toluene molecule were not included in the refinement.

At convergence, $wR2 = 0.0468$ and $Goof = 1.026$ for 379 variables refined against 7609 data ($0.78\text{\AA}$), $R1 = 0.0181$ for those 7118 data with $I > 2.0\sigma(I)$.

Table 1. Crystal data and structure refinement for $(C_5Me_5)_2[{}^iPrNC(Me)N^iPr-\kappa^2N,N']U(Spy)$, **3**.

Identification code	jrw30 (Justin Walensky)	
Empirical formula	$C_{33}H_{51}N_3SU \cdot \frac{1}{2}(C_7H_8)$	
Formula weight	805.93	
Temperature	103(2) K	
Wavelength	0.71073 $\text{\AA}$	
Crystal system	Monoclinic	
Space group	<i>C2/c</i>	
Unit cell dimensions	$a = 34.4356(18) \text{\AA}$	$\alpha = 90^\circ$.
	$b = 12.3473(7) \text{\AA}$	$\beta = 90.6820(10)^\circ$.
	$c = 16.1941(9) \text{\AA}$	$\gamma = 90^\circ$.
Volume	$6885.0(7) \text{\AA}^3$	
Z	8	

Density (calculated)	1.555 Mg/m ³
Absorption coefficient	4.804 mm ⁻¹
F(000)	3224
Crystal color	red
Crystal size	0.22 x 0.20 x 0.13 mm ³
Theta range for data collection	1.75 to 27.10°
Index ranges	-44 ≤ <i>h</i> ≤ 44, -15 ≤ <i>k</i> ≤ 15, -20 ≤ <i>l</i> ≤ 20
Reflections collected	38488
Independent reflections	7609 [R(int) = 0.0209]
Completeness to theta = 27.10°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5740 and 0.4179
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7609 / 8 / 379
Goodness-of-fit on F ²	1.026
Final R indices [I > 2σ(I) = 7118 data]	R1 = 0.0181, wR2 = 0.0458
R indices (all data, 0.78Å)	R1 = 0.0201, wR2 = 0.0468
Largest diff. peak and hole	1.418 and -1.130 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jr30. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
U(1)	6126(1)	7668(1)	5132(1)	12(1)
S(1)	6777(1)	8858(1)	4649(1)	18(1)
N(1)	6610(1)	6545(2)	5926(1)	15(1)
N(2)	5999(1)	6628(2)	6357(1)	17(1)
N(3)	6539(1)	8745(2)	6180(1)	17(1)
C(1)	6465(1)	6190(2)	4006(1)	17(1)
C(2)	6319(1)	7009(2)	3481(1)	18(1)
C(3)	5909(1)	6970(2)	3491(1)	19(1)
C(4)	5799(1)	6147(2)	4058(1)	18(1)
C(5)	6144(1)	5650(2)	4369(1)	17(1)
C(6)	6884(1)	5844(2)	4011(2)	22(1)
C(7)	6553(1)	7651(2)	2874(2)	24(1)
C(8)	5667(1)	7482(2)	2815(2)	25(1)
C(9)	5393(1)	5759(2)	4223(2)	24(1)
C(10)	6161(1)	4628(2)	4871(2)	22(1)
C(11)	5625(1)	9150(2)	5947(1)	18(1)
C(12)	5851(1)	9791(2)	5409(1)	18(1)
C(13)	5728(1)	9562(2)	4588(1)	18(1)
C(14)	5416(1)	8814(2)	4624(1)	19(1)
C(15)	5360(1)	8539(2)	5463(1)	19(1)
C(16)	5604(1)	9284(2)	6870(1)	24(1)
C(17)	6104(1)	10740(2)	5642(2)	24(1)
C(18)	5868(1)	10153(2)	3836(2)	26(1)
C(19)	5099(1)	8657(2)	3985(2)	29(1)
C(20)	5001(1)	7971(2)	5770(2)	27(1)
C(21)	6360(1)	6256(2)	6501(1)	17(1)
C(22)	6469(1)	5596(2)	7257(2)	26(1)
C(23)	7034(1)	6374(2)	5993(1)	18(1)
C(24)	7168(1)	5182(2)	5983(2)	24(1)
C(25)	7234(1)	6961(2)	6716(2)	24(1)
C(26)	5663(1)	6339(2)	6870(2)	23(1)

C(27)	5516(1)	5192(2)	6701(2)	35(1)
C(28)	5702(1)	6531(2)	7806(2)	31(1)
C(29)	6815(1)	9183(2)	5698(1)	18(1)
C(30)	7107(1)	9849(2)	6034(2)	24(1)
C(31)	7111(1)	10050(2)	6871(2)	27(1)
C(32)	6831(1)	9574(2)	7372(2)	26(1)
C(33)	6555(1)	8923(2)	6999(1)	21(1)
C(34)	7692(2)	7408(6)	10231(3)	77(1)
C(35)	7665(1)	7537(3)	9379(3)	77(1)
C(36)	7301(1)	7674(5)	9016(4)	77(1)
C(37)	6940(2)	7765(3)	9383(3)	77(1)
C(38)	6977(2)	7604(6)	10231(4)	77(1)

Table 3. Bond lengths [Å] and angles [°] for jrw30.

U(1)-Cnt1	2.565
U(1)-Cnt2	2.608
U(1)-N(2)	2.4078(18)
U(1)-N(1)	2.5099(18)
U(1)-N(3)	2.5717(19)
U(1)-C(5)	2.782(2)
U(1)-C(4)	2.788(2)
U(1)-S(1)	2.7997(6)
U(1)-C(12)	2.825(2)
U(1)-C(1)	2.840(2)
U(1)-C(13)	2.846(2)
U(1)-C(11)	2.851(2)
U(1)-C(2)	2.879(2)
U(1)-C(3)	2.884(2)
U(1)-C(15)	2.904(2)
U(1)-C(21)	2.926(2)
U(1)-C(14)	2.935(2)
S(1)-C(29)	1.748(2)
N(1)-C(21)	1.324(3)
N(1)-C(23)	1.480(3)
N(2)-C(21)	1.345(3)
N(2)-C(26)	1.476(3)
N(3)-C(33)	1.344(3)
N(3)-C(29)	1.350(3)
C(1)-C(2)	1.410(3)
C(1)-C(5)	1.423(3)
C(1)-C(6)	1.505(3)
C(2)-C(3)	1.411(3)
C(2)-C(7)	1.506(3)
C(3)-C(4)	1.424(3)
C(3)-C(8)	1.507(3)
C(4)-C(5)	1.424(3)
C(4)-C(9)	1.506(3)
C(5)-C(10)	1.502(3)

C(11)-C(15)	1.412(3)
C(11)-C(12)	1.418(3)
C(11)-C(16)	1.506(3)
C(12)-C(13)	1.421(3)
C(12)-C(17)	1.505(3)
C(13)-C(14)	1.419(3)
C(13)-C(18)	1.503(3)
C(14)-C(15)	1.415(3)
C(14)-C(19)	1.508(3)
C(15)-C(20)	1.510(3)
C(21)-C(22)	1.514(3)
C(23)-C(25)	1.533(3)
C(23)-C(24)	1.543(3)
C(26)-C(27)	1.527(4)
C(26)-C(28)	1.539(3)
C(29)-C(30)	1.404(3)
C(30)-C(31)	1.378(4)
C(31)-C(32)	1.395(4)
C(32)-C(33)	1.379(3)
C(34)-C(36)#1	1.224(10)
C(34)-C(38)#1	1.372(10)
C(34)-C(35)#1	1.3904(10)
C(34)-C(35)	1.3919(10)
C(34)-C(37)#1	1.423(9)
C(34)-C(34)#1	1.527(15)
C(35)-C(36)	1.3889(10)
C(35)-C(38)#1	1.3896(10)
C(35)-C(34)#1	1.3904(10)
C(36)-C(34)#1	1.224(10)
C(36)-C(37)	1.3890(10)
C(37)-C(38)	1.3915(10)
C(37)-C(34)#1	1.423(9)
C(38)-C(34)#1	1.372(10)
C(38)-C(35)#1	1.3896(10)

Cnt1-U(1)-N(1) 93.4

Cnt1-U(1)-N(2)	109.0
Cnt1-U(1)-N(3)	146.4
Cnt1-U(1)-S(1)	95.3
Cnt2-U(1)-N(1)	146.2
Cnt2-U(1)-N(2)	101.9
Cnt2-U(1)-N(3)	89.1
Cnt2-U(1)-S(1)	101.7
Cnt1-U(1)-Cnt2	118.7
N(2)-U(1)-N(1)	53.84(6)
N(2)-U(1)-N(3)	80.60(6)
N(1)-U(1)-N(3)	65.74(6)
N(2)-U(1)-C(5)	83.89(7)
N(1)-U(1)-C(5)	73.42(6)
N(3)-U(1)-C(5)	137.83(6)
N(2)-U(1)-C(4)	94.49(7)
N(1)-U(1)-C(4)	102.02(6)
N(3)-U(1)-C(4)	167.44(6)
C(5)-U(1)-C(4)	29.63(7)
N(2)-U(1)-S(1)	131.65(5)
N(1)-U(1)-S(1)	84.50(4)
N(3)-U(1)-S(1)	58.31(4)
C(5)-U(1)-S(1)	108.90(5)
C(4)-U(1)-S(1)	119.89(5)
N(2)-U(1)-C(12)	107.39(6)
N(1)-U(1)-C(12)	130.76(6)
N(3)-U(1)-C(12)	66.37(6)
C(5)-U(1)-C(12)	155.62(7)
C(4)-U(1)-C(12)	126.18(7)
S(1)-U(1)-C(12)	80.13(5)
N(2)-U(1)-C(1)	105.46(7)
N(1)-U(1)-C(1)	72.47(6)
N(3)-U(1)-C(1)	121.87(6)
C(5)-U(1)-C(1)	29.30(6)
C(4)-U(1)-C(1)	48.14(6)
S(1)-U(1)-C(1)	79.73(5)
C(12)-U(1)-C(1)	147.08(7)

N(2)-U(1)-C(13)	126.96(6)
N(1)-U(1)-C(13)	158.01(6)
N(3)-U(1)-C(13)	92.33(6)
C(5)-U(1)-C(13)	127.69(6)
C(4)-U(1)-C(13)	99.81(7)
S(1)-U(1)-C(13)	82.37(5)
C(12)-U(1)-C(13)	29.01(6)
C(1)-U(1)-C(13)	121.96(6)
N(2)-U(1)-C(11)	80.98(6)
N(1)-U(1)-C(11)	121.31(6)
N(3)-U(1)-C(11)	72.31(6)
C(5)-U(1)-C(11)	142.84(7)
C(4)-U(1)-C(11)	118.57(7)
S(1)-U(1)-C(11)	106.51(5)
C(12)-U(1)-C(11)	28.92(7)
C(1)-U(1)-C(11)	164.85(6)
C(13)-U(1)-C(11)	47.42(6)
N(2)-U(1)-C(2)	131.35(7)
N(1)-U(1)-C(2)	99.25(6)
N(3)-U(1)-C(2)	128.85(6)
C(5)-U(1)-C(2)	47.79(7)
C(4)-U(1)-C(2)	47.65(7)
S(1)-U(1)-C(2)	72.24(5)
C(12)-U(1)-C(2)	119.42(7)
C(1)-U(1)-C(2)	28.54(7)
C(13)-U(1)-C(2)	93.44(7)
C(11)-U(1)-C(2)	139.34(6)
N(2)-U(1)-C(3)	123.50(7)
N(1)-U(1)-C(3)	118.04(6)
N(3)-U(1)-C(3)	153.90(6)
C(5)-U(1)-C(3)	47.93(7)
C(4)-U(1)-C(3)	29.02(7)
S(1)-U(1)-C(3)	95.69(5)
C(12)-U(1)-C(3)	109.88(7)
C(1)-U(1)-C(3)	47.18(6)
C(13)-U(1)-C(3)	80.87(7)

C(11)-U(1)-C(3)	117.80(6)
C(2)-U(1)-C(3)	28.36(6)
N(2)-U(1)-C(15)	82.54(6)
N(1)-U(1)-C(15)	135.12(6)
N(3)-U(1)-C(15)	100.55(6)
C(5)-U(1)-C(15)	116.00(7)
C(4)-U(1)-C(15)	90.18(7)
S(1)-U(1)-C(15)	126.12(5)
C(12)-U(1)-C(15)	47.17(7)
C(1)-U(1)-C(15)	137.48(7)
C(13)-U(1)-C(15)	46.95(6)
C(11)-U(1)-C(15)	28.39(7)
C(2)-U(1)-C(15)	119.71(7)
C(3)-U(1)-C(15)	93.13(7)
N(2)-U(1)-C(21)	27.04(6)
N(1)-U(1)-C(21)	26.82(6)
N(3)-U(1)-C(21)	70.29(6)
C(5)-U(1)-C(21)	78.21(6)
C(4)-U(1)-C(21)	100.19(7)
S(1)-U(1)-C(21)	108.06(5)
C(12)-U(1)-C(21)	121.48(6)
C(1)-U(1)-C(21)	89.55(6)
C(13)-U(1)-C(21)	148.39(6)
C(11)-U(1)-C(21)	101.22(6)
C(2)-U(1)-C(21)	118.09(6)
C(3)-U(1)-C(21)	125.89(6)
C(15)-U(1)-C(21)	108.85(6)
N(2)-U(1)-C(14)	109.14(6)
N(1)-U(1)-C(14)	162.86(6)
N(3)-U(1)-C(14)	112.85(6)
C(5)-U(1)-C(14)	109.26(6)
C(4)-U(1)-C(14)	79.66(7)
S(1)-U(1)-C(14)	109.68(5)
C(12)-U(1)-C(14)	46.96(6)
C(1)-U(1)-C(14)	118.50(6)
C(13)-U(1)-C(14)	28.37(7)

C(11)-U(1)-C(14)	46.57(6)
C(2)-U(1)-C(14)	94.39(6)
C(3)-U(1)-C(14)	71.33(6)
C(15)-U(1)-C(14)	28.03(6)
C(21)-U(1)-C(14)	136.08(6)
C(29)-S(1)-U(1)	84.24(8)
C(21)-N(1)-C(23)	124.02(18)
C(21)-N(1)-U(1)	94.39(13)
C(23)-N(1)-U(1)	139.92(14)
C(21)-N(2)-C(26)	123.34(19)
C(21)-N(2)-U(1)	98.49(14)
C(26)-N(2)-U(1)	138.13(14)
C(33)-N(3)-C(29)	119.0(2)
C(33)-N(3)-U(1)	138.71(16)
C(29)-N(3)-U(1)	102.27(14)
C(2)-C(1)-C(5)	108.2(2)
C(2)-C(1)-C(6)	122.8(2)
C(5)-C(1)-C(6)	127.9(2)
C(2)-C(1)-U(1)	77.29(13)
C(5)-C(1)-U(1)	73.09(12)
C(6)-C(1)-U(1)	125.42(14)
C(1)-C(2)-C(3)	108.5(2)
C(1)-C(2)-C(7)	125.6(2)
C(3)-C(2)-C(7)	124.7(2)
C(1)-C(2)-U(1)	74.17(12)
C(3)-C(2)-U(1)	76.00(12)
C(7)-C(2)-U(1)	126.07(15)
C(2)-C(3)-C(4)	107.8(2)
C(2)-C(3)-C(8)	121.5(2)
C(4)-C(3)-C(8)	128.2(2)
C(2)-C(3)-U(1)	75.65(12)
C(4)-C(3)-U(1)	71.77(12)
C(8)-C(3)-U(1)	132.78(16)
C(3)-C(4)-C(5)	107.9(2)
C(3)-C(4)-C(9)	126.6(2)
C(5)-C(4)-C(9)	125.0(2)

C(3)-C(4)-U(1)	79.22(13)
C(5)-C(4)-U(1)	74.94(12)
C(9)-C(4)-U(1)	118.28(15)
C(1)-C(5)-C(4)	107.5(2)
C(1)-C(5)-C(10)	126.3(2)
C(4)-C(5)-C(10)	125.5(2)
C(1)-C(5)-U(1)	77.61(12)
C(4)-C(5)-U(1)	75.43(12)
C(10)-C(5)-U(1)	120.89(15)
C(15)-C(11)-C(12)	108.28(19)
C(15)-C(11)-C(16)	124.9(2)
C(12)-C(11)-C(16)	125.5(2)
C(15)-C(11)-U(1)	77.90(13)
C(12)-C(11)-U(1)	74.52(12)
C(16)-C(11)-U(1)	124.39(15)
C(11)-C(12)-C(13)	107.6(2)
C(11)-C(12)-C(17)	127.0(2)
C(13)-C(12)-C(17)	123.8(2)
C(11)-C(12)-U(1)	76.56(13)
C(13)-C(12)-U(1)	76.30(13)
C(17)-C(12)-U(1)	124.64(15)
C(14)-C(13)-C(12)	108.0(2)
C(14)-C(13)-C(18)	126.9(2)
C(12)-C(13)-C(18)	124.5(2)
C(14)-C(13)-U(1)	79.32(13)
C(12)-C(13)-U(1)	74.69(12)
C(18)-C(13)-U(1)	119.43(15)
C(15)-C(14)-C(13)	107.9(2)
C(15)-C(14)-C(19)	121.6(2)
C(13)-C(14)-C(19)	126.6(2)
C(15)-C(14)-U(1)	74.77(12)
C(13)-C(14)-U(1)	72.31(12)
C(19)-C(14)-U(1)	136.44(16)
C(11)-C(15)-C(14)	108.1(2)
C(11)-C(15)-C(20)	126.1(2)
C(14)-C(15)-C(20)	123.2(2)

C(11)-C(15)-U(1)	73.71(12)
C(14)-C(15)-U(1)	77.20(13)
C(20)-C(15)-U(1)	129.59(16)
N(1)-C(21)-N(2)	113.16(19)
N(1)-C(21)-C(22)	123.9(2)
N(2)-C(21)-C(22)	122.9(2)
N(1)-C(21)-U(1)	58.78(11)
N(2)-C(21)-U(1)	54.47(11)
C(22)-C(21)-U(1)	175.29(16)
N(1)-C(23)-C(25)	115.00(19)
N(1)-C(23)-C(24)	115.43(19)
C(25)-C(23)-C(24)	109.14(19)
N(2)-C(26)-C(27)	112.5(2)
N(2)-C(26)-C(28)	117.2(2)
C(27)-C(26)-C(28)	110.1(2)
N(3)-C(29)-C(30)	121.0(2)
N(3)-C(29)-S(1)	115.17(17)
C(30)-C(29)-S(1)	123.78(19)
C(31)-C(30)-C(29)	119.0(2)
C(30)-C(31)-C(32)	119.8(2)
C(33)-C(32)-C(31)	117.9(2)
N(3)-C(33)-C(32)	123.2(2)
C(36)#1-C(34)-C(38)#1	122.3(6)
C(36)#1-C(34)-C(35)#1	63.8(2)
C(38)#1-C(34)-C(35)#1	173.7(7)
C(36)#1-C(34)-C(35)	176.8(7)
C(38)#1-C(34)-C(35)	60.4(2)
C(35)#1-C(34)-C(35)	113.4(7)
C(36)#1-C(34)-C(37)#1	62.8(4)
C(38)#1-C(34)-C(37)#1	59.7(3)
C(35)#1-C(34)-C(37)#1	126.5(6)
C(35)-C(34)-C(37)#1	120.0(5)
C(36)#1-C(34)-C(34)#1	120.5(4)
C(38)#1-C(34)-C(34)#1	117.0(4)
C(35)#1-C(34)-C(34)#1	56.8(4)
C(35)-C(34)-C(34)#1	56.7(4)

C(37)#1-C(34)-C(34)#1	176.7(4)
C(36)-C(35)-C(38)#1	177.9(5)
C(36)-C(35)-C(34)#1	52.3(5)
C(38)#1-C(35)-C(34)#1	125.7(7)
C(36)-C(35)-C(34)	118.8(7)
C(38)#1-C(35)-C(34)	59.1(5)
C(34)#1-C(35)-C(34)	66.6(7)
C(34)#1-C(36)-C(35)	63.9(2)
C(34)#1-C(36)-C(37)	65.7(5)
C(35)-C(36)-C(37)	129.6(6)
C(36)-C(37)-C(38)	109.8(6)
C(36)-C(37)-C(34)#1	51.6(5)
C(38)-C(37)-C(34)#1	58.3(5)
C(34)#1-C(38)-C(35)#1	60.5(2)
C(34)#1-C(38)-C(37)	62.0(5)
C(35)#1-C(38)-C(37)	122.5(6)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw30. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
U(1)	13(1)	13(1)	11(1)	0(1)	0(1)	1(1)
S(1)	19(1)	19(1)	17(1)	-2(1)	2(1)	-3(1)
N(1)	15(1)	15(1)	15(1)	0(1)	-2(1)	2(1)
N(2)	17(1)	17(1)	16(1)	3(1)	2(1)	1(1)
N(3)	18(1)	16(1)	16(1)	-2(1)	-2(1)	2(1)
C(1)	17(1)	18(1)	15(1)	-5(1)	0(1)	0(1)
C(2)	22(1)	20(1)	13(1)	-4(1)	2(1)	-1(1)
C(3)	21(1)	19(1)	16(1)	-5(1)	-2(1)	0(1)
C(4)	19(1)	18(1)	17(1)	-5(1)	-1(1)	-3(1)
C(5)	19(1)	15(1)	17(1)	-4(1)	0(1)	0(1)
C(6)	19(1)	28(1)	20(1)	-7(1)	0(1)	2(1)
C(7)	29(1)	26(1)	17(1)	-1(1)	3(1)	-5(1)
C(8)	29(1)	26(1)	19(1)	-2(1)	-5(1)	3(1)
C(9)	19(1)	23(1)	29(1)	-5(1)	1(1)	-2(1)
C(10)	26(1)	17(1)	24(1)	0(1)	0(1)	-1(1)
C(11)	19(1)	20(1)	14(1)	1(1)	0(1)	8(1)
C(12)	21(1)	16(1)	17(1)	0(1)	-1(1)	7(1)
C(13)	21(1)	17(1)	16(1)	1(1)	0(1)	6(1)
C(14)	20(1)	20(1)	16(1)	-1(1)	-2(1)	6(1)
C(15)	17(1)	20(1)	22(1)	2(1)	2(1)	7(1)
C(16)	30(1)	28(1)	14(1)	0(1)	3(1)	10(1)
C(17)	28(1)	18(1)	26(1)	-2(1)	-3(1)	4(1)
C(18)	36(1)	23(1)	17(1)	5(1)	2(1)	6(1)
C(19)	26(1)	32(1)	27(1)	-6(1)	-9(1)	8(1)
C(20)	19(1)	30(1)	33(1)	3(1)	3(1)	4(1)
C(21)	21(1)	15(1)	15(1)	-1(1)	-1(1)	1(1)
C(22)	24(1)	30(1)	24(1)	10(1)	0(1)	5(1)
C(23)	16(1)	20(1)	19(1)	0(1)	-1(1)	2(1)
C(24)	21(1)	22(1)	28(1)	-2(1)	-2(1)	6(1)
C(25)	20(1)	24(1)	27(1)	-2(1)	-7(1)	3(1)
C(26)	19(1)	29(1)	20(1)	8(1)	6(1)	4(1)

C(27)	29(1)	42(2)	34(2)	7(1)	5(1)	-12(1)
C(28)	39(2)	30(1)	23(1)	7(1)	13(1)	8(1)
C(29)	19(1)	15(1)	20(1)	-2(1)	-3(1)	3(1)
C(30)	19(1)	19(1)	32(1)	-5(1)	-3(1)	1(1)
C(31)	24(1)	23(1)	33(1)	-11(1)	-10(1)	2(1)
C(32)	29(1)	26(1)	22(1)	-8(1)	-7(1)	8(1)
C(33)	25(1)	19(1)	19(1)	-2(1)	-2(1)	7(1)
C(34)	104(2)	21(1)	106(2)	-9(1)	23(2)	-9(1)
C(35)	104(2)	21(1)	106(2)	-9(1)	23(2)	-9(1)
C(36)	104(2)	21(1)	106(2)	-9(1)	23(2)	-9(1)
C(37)	104(2)	21(1)	106(2)	-9(1)	23(2)	-9(1)
C(38)	104(2)	21(1)	106(2)	-9(1)	23(2)	-9(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for jrw30.

	x	y	z	U(eq)
H(6A)	6956	5611	3456	33
H(6B)	6920	5242	4399	33
H(6C)	7048	6455	4183	33
H(7A)	6570	7251	2353	36
H(7B)	6815	7770	3099	36
H(7C)	6427	8352	2773	36
H(8A)	5765	7254	2276	37
H(8B)	5682	8272	2861	37
H(8C)	5396	7251	2869	37
H(9A)	5388	4966	4228	36
H(9B)	5217	6026	3788	36
H(9C)	5308	6034	4759	36
H(10A)	6362	4150	4651	34
H(10B)	5909	4261	4841	34
H(10C)	6223	4806	5447	34
H(16A)	5354	9603	7015	36
H(16B)	5815	9760	7059	36
H(16C)	5631	8574	7136	36
H(17A)	5959	11414	5558	36
H(17B)	6336	10745	5297	36
H(17C)	6182	10680	6224	36
H(18A)	5644	10377	3497	38
H(18B)	6034	9673	3514	38
H(18C)	6016	10794	4007	38
H(19A)	4863	9035	4161	43
H(19B)	5043	7883	3923	43
H(19C)	5183	8953	3455	43
H(20A)	4770	8316	5531	41
H(20B)	4993	8020	6374	41
H(20C)	5008	7208	5605	41

H(22A)	6717	5231	7166	39
H(22B)	6267	5054	7358	39
H(22C)	6492	6076	7737	39
H(23A)	7145	6706	5483	22
H(24A)	6980	4747	5667	36
H(24B)	7185	4909	6550	36
H(24C)	7423	5132	5725	36
H(25A)	7176	7737	6685	35
H(25B)	7516	6851	6687	35
H(25C)	7138	6669	7238	35
H(26A)	5448	6828	6681	27
H(27A)	5460	5109	6110	52
H(27B)	5279	5063	7016	52
H(27C)	5716	4669	6869	52
H(28A)	5859	7180	7908	46
H(28B)	5828	5904	8065	46
H(28C)	5444	6632	8042	46
H(30A)	7299	10157	5690	28
H(31A)	7303	10511	7107	32
H(32A)	6831	9694	7951	31
H(33A)	6367	8583	7337	25

X-ray Data Collection, Structure Solution and Refinement for $(C_5Me_5)_2[{}^iPrNC(Me)N^iPr-\kappa^2N,N']U(O_2CMe)$, 7.

An orange crystal of approximate dimensions 0.09 x 0.17 x 0.23 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ program. 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 factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were included using a riding model.

At convergence, $wR2 = 0.0604$ and $Goof = 1.047$ for 332 variables refined against 6623 data ($0.77\text{\AA}$), $R1 = 0.0240$ for those 5833 data with $I > 2.0\sigma(I)$.

Table 1. Crystal data and structure refinement for $(C_5Me_5)_2[{}^iPrNC(Me)N^iPr-\kappa^2N,N']U(O_2CMe)$, 7.

Identification code	jrw33 (Justin Walensky)
Empirical formula	$C_{30}H_{50}N_2O_2U$
Formula weight	708.75
Temperature	143(2) K
Wavelength	0.71073 $\text{\AA}$
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	$a = 9.5795(6) \text{\AA} \angle = 90^\circ$ $b = 17.4341(11) \text{\AA} \angle = 101.4380(10)^\circ$ $c = 17.8520(11) \text{\AA} \angle = 90^\circ$
Volume	2922.2(3) $\text{\AA}^3$
Z	4
Density (calculated)	1.611 Mg/m^3
Absorption coefficient	5.582 mm^{-1}
$F(000)$	1408
Crystal color	orange
Crystal size	0.23 x 0.17 x 0.09 mm^3
Theta range for data collection	1.65 to 27.48°
Index ranges	$-12 \leq h \leq 12, -22 \leq k \leq 22, -22 \leq l \leq 23$

Reflections collected	32550
Independent reflections	6623 [R(int) = 0.0244]
Completeness to theta = 27.48°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.6335 and 0.3600
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6623 / 0 / 332
Goodness-of-fit on F ²	1.047
Final R indices [I > 2sigma(I) = 5833 data]	R1 = 0.0240, wR2 = 0.0576
R indices (all data, 0.77 Å)	R1 = 0.0299, wR2 = 0.0604
Largest diff. peak and hole	2.155 and -0.633 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrww33. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
U(1)	4264(1)	1919(1)	1630(1)	19(1)
N(1)	4909(3)	3087(1)	957(2)	21(1)
N(2)	2702(3)	2942(2)	1165(2)	30(1)
O(1)	2366(3)	1435(1)	1991(1)	32(1)
O(2)	-5(3)	1420(2)	1698(2)	42(1)
C(1)	4028(4)	1408(2)	151(2)	26(1)
C(2)	5453(4)	1227(2)	509(2)	26(1)
C(3)	5402(4)	628(2)	1037(2)	32(1)
C(4)	3979(5)	450(2)	1021(2)	38(1)
C(5)	3113(4)	928(2)	472(2)	34(1)
C(6)	3556(5)	1934(2)	-519(2)	38(1)
C(7)	6805(4)	1520(2)	307(2)	38(1)
C(8)	6674(6)	152(2)	1402(2)	56(1)
C(9)	3482(7)	-207(2)	1447(3)	68(2)
C(10)	1533(4)	869(3)	197(3)	58(1)
C(11)	5367(3)	2871(2)	2847(2)	23(1)
C(12)	6576(3)	2482(2)	2689(2)	23(1)
C(13)	6481(4)	1707(2)	2895(2)	27(1)
C(14)	5217(4)	1608(2)	3168(2)	27(1)
C(15)	4522(4)	2331(2)	3144(2)	24(1)
C(16)	5099(4)	3721(2)	2807(2)	29(1)
C(17)	7883(4)	2822(2)	2467(2)	30(1)
C(18)	7681(4)	1140(2)	2970(2)	39(1)
C(19)	4780(4)	873(2)	3507(2)	37(1)
C(20)	3195(4)	2514(2)	3443(2)	34(1)
C(21)	3607(3)	3375(2)	861(2)	25(1)
C(22)	3147(5)	4113(2)	442(2)	45(1)
C(23)	6105(3)	3471(2)	702(2)	25(1)
C(24)	5974(4)	3558(2)	-163(2)	35(1)
C(25)	6544(4)	4244(2)	1089(2)	36(1)
C(26)	1191(4)	3108(3)	1152(3)	56(1)

C(27)	902(5)	3691(4)	1656(3)	78(2)
C(28)	227(4)	2996(3)	413(3)	49(1)
C(29)	1122(4)	1196(2)	2081(2)	29(1)
C(30)	1134(4)	611(2)	2707(2)	40(1)

Table 3. Bond lengths [Å] and angles [°] for jrw33.

U(1)-Cnt1	2.495
U(1)-Cnt2	2.504
U(1)-O(1)	2.213(2)
U(1)-N(2)	2.370(3)
U(1)-N(1)	2.503(3)
U(1)-C(5)	2.751(3)
U(1)-C(1)	2.753(3)
U(1)-C(15)	2.759(3)
U(1)-C(2)	2.768(3)
U(1)-C(14)	2.770(3)
U(1)-C(11)	2.770(3)
U(1)-C(4)	2.776(3)
U(1)-C(12)	2.789(3)
U(1)-C(3)	2.798(3)
U(1)-C(13)	2.801(3)
U(1)-C(21)	2.895(3)
N(1)-C(21)	1.324(4)
N(1)-C(23)	1.474(4)
N(2)-C(21)	1.343(5)
N(2)-C(26)	1.472(5)
O(1)-C(29)	1.302(4)
O(2)-C(29)	1.221(4)
C(1)-C(5)	1.413(5)
C(1)-C(2)	1.423(5)
C(1)-C(6)	1.503(5)
C(2)-C(3)	1.414(5)
C(2)-C(7)	1.500(5)
C(3)-C(4)	1.393(6)
C(3)-C(8)	1.512(5)
C(4)-C(5)	1.421(6)
C(4)-C(9)	1.503(5)
C(5)-C(10)	1.500(5)
C(11)-C(15)	1.411(5)
C(11)-C(12)	1.417(4)

C(11)-C(16)	1.504(4)
C(12)-C(13)	1.409(5)
C(12)-C(17)	1.507(5)
C(13)-C(14)	1.404(5)
C(13)-C(18)	1.501(5)
C(14)-C(15)	1.422(5)
C(14)-C(19)	1.511(5)
C(15)-C(20)	1.508(5)
C(21)-C(22)	1.509(5)
C(23)-C(24)	1.532(5)
C(23)-C(25)	1.534(5)
C(26)-C(27)	1.421(6)
C(26)-C(28)	1.465(6)
C(29)-C(30)	1.511(5)

Cnt1-U(1)-O(1)	95.9
Cnt1-U(1)-N(1)	99.8
Cnt1-U(1)-N(2)	112.9
Cnt1-U(1)-C(21)	107.9
Cnt1-U(1)-O(1)	96.2
Cnt1-U(1)-N(1)	99.2
Cnt1-U(1)-N(2)	111.0
Cnt1-U(1)-C(21)	107.4
Cnt1-U(1)-Cnt2	135.4
O(1)-U(1)-N(2)	83.72(10)
O(1)-U(1)-N(1)	138.18(9)
N(2)-U(1)-N(1)	54.46(9)
O(1)-U(1)-C(5)	75.45(10)
N(2)-U(1)-C(5)	94.49(11)
N(1)-U(1)-C(5)	104.52(10)
O(1)-U(1)-C(1)	103.85(9)
N(2)-U(1)-C(1)	88.95(10)
N(1)-U(1)-C(1)	77.55(9)
C(5)-U(1)-C(1)	29.75(10)
O(1)-U(1)-C(15)	74.53(9)
N(2)-U(1)-C(15)	94.30(10)

N(1)-U(1)-C(15)	106.02(9)
C(5)-U(1)-C(15)	147.52(10)
C(1)-U(1)-C(15)	176.16(9)
O(1)-U(1)-C(2)	121.57(10)
N(2)-U(1)-C(2)	113.37(10)
N(1)-U(1)-C(2)	80.31(9)
C(5)-U(1)-C(2)	49.02(10)
C(1)-U(1)-C(2)	29.87(10)
C(15)-U(1)-C(2)	148.39(10)
O(1)-U(1)-C(14)	76.40(9)
N(2)-U(1)-C(14)	123.75(10)
N(1)-U(1)-C(14)	124.83(9)
C(5)-U(1)-C(14)	128.73(11)
C(1)-U(1)-C(14)	146.66(10)
C(15)-U(1)-C(14)	29.80(10)
C(2)-U(1)-C(14)	121.96(10)
O(1)-U(1)-C(11)	101.99(9)
N(2)-U(1)-C(11)	86.56(10)
N(1)-U(1)-C(11)	78.30(9)
C(5)-U(1)-C(11)	177.09(10)
C(1)-U(1)-C(11)	153.10(10)
C(15)-U(1)-C(11)	29.58(10)
C(2)-U(1)-C(11)	132.88(10)
C(14)-U(1)-C(11)	48.76(10)
O(1)-U(1)-C(4)	74.87(11)
N(2)-U(1)-C(4)	123.43(12)
N(1)-U(1)-C(4)	125.26(9)
C(5)-U(1)-C(4)	29.79(12)
C(1)-U(1)-C(4)	48.88(10)
C(15)-U(1)-C(4)	127.34(10)
C(2)-U(1)-C(4)	48.47(10)
C(14)-U(1)-C(4)	101.25(11)
C(11)-U(1)-C(4)	148.50(11)
O(1)-U(1)-C(12)	121.65(9)
N(2)-U(1)-C(12)	109.50(10)
N(1)-U(1)-C(12)	78.49(9)

C(5)-U(1)-C(12)	151.20(11)
C(1)-U(1)-C(12)	131.84(10)
C(15)-U(1)-C(12)	48.70(10)
C(2)-U(1)-C(12)	104.97(10)
C(14)-U(1)-C(12)	48.41(10)
C(11)-U(1)-C(12)	29.54(9)
C(4)-U(1)-C(12)	126.44(11)
O(1)-U(1)-C(3)	101.96(10)
N(2)-U(1)-C(3)	137.65(10)
N(1)-U(1)-C(3)	108.72(10)
C(5)-U(1)-C(3)	48.62(11)
C(1)-U(1)-C(3)	48.77(10)
C(15)-U(1)-C(3)	127.85(10)
C(2)-U(1)-C(3)	29.42(10)
C(14)-U(1)-C(3)	98.10(10)
C(11)-U(1)-C(3)	131.43(10)
C(4)-U(1)-C(3)	28.95(12)
C(12)-U(1)-C(3)	102.89(10)
O(1)-U(1)-C(13)	104.50(10)
N(2)-U(1)-C(13)	135.01(10)
N(1)-U(1)-C(13)	105.94(9)
C(5)-U(1)-C(13)	130.50(11)
C(1)-U(1)-C(13)	129.44(10)
C(15)-U(1)-C(13)	48.59(10)
C(2)-U(1)-C(13)	99.80(10)
C(14)-U(1)-C(13)	29.18(10)
C(11)-U(1)-C(13)	48.47(10)
C(4)-U(1)-C(13)	101.18(11)
C(12)-U(1)-C(13)	29.20(10)
C(3)-U(1)-C(13)	84.75(10)
O(1)-U(1)-C(21)	111.01(9)
N(2)-U(1)-C(21)	27.30(10)
N(1)-U(1)-C(21)	27.17(9)
C(5)-U(1)-C(21)	100.22(10)
C(1)-U(1)-C(21)	81.98(9)
C(15)-U(1)-C(21)	101.84(9)

C(2)-U(1)-C(21)	96.98(9)
C(14)-U(1)-C(21)	129.77(9)
C(11)-U(1)-C(21)	81.95(9)
C(4)-U(1)-C(21)	128.92(10)
C(12)-U(1)-C(21)	94.67(9)
C(3)-U(1)-C(21)	126.17(10)
C(13)-U(1)-C(21)	123.85(10)
C(21)-N(1)-C(23)	123.9(3)
C(21)-N(1)-U(1)	93.2(2)
C(23)-N(1)-U(1)	143.0(2)
C(21)-N(2)-C(26)	126.5(3)
C(21)-N(2)-U(1)	98.7(2)
C(26)-N(2)-U(1)	134.8(3)
C(29)-O(1)-U(1)	169.4(2)
C(5)-C(1)-C(2)	107.7(3)
C(5)-C(1)-C(6)	124.8(3)
C(2)-C(1)-C(6)	127.1(3)
C(5)-C(1)-U(1)	75.04(18)
C(2)-C(1)-U(1)	75.66(17)
C(6)-C(1)-U(1)	121.3(2)
C(3)-C(2)-C(1)	107.8(3)
C(3)-C(2)-C(7)	123.8(3)
C(1)-C(2)-C(7)	127.8(3)
C(3)-C(2)-U(1)	76.46(19)
C(1)-C(2)-U(1)	74.47(18)
C(7)-C(2)-U(1)	121.6(2)
C(4)-C(3)-C(2)	108.3(3)
C(4)-C(3)-C(8)	126.0(4)
C(2)-C(3)-C(8)	124.2(4)
C(4)-C(3)-U(1)	74.6(2)
C(2)-C(3)-U(1)	74.12(18)
C(8)-C(3)-U(1)	128.3(2)
C(3)-C(4)-C(5)	108.5(3)
C(3)-C(4)-C(9)	124.5(4)
C(5)-C(4)-C(9)	126.6(4)
C(3)-C(4)-U(1)	76.43(19)

C(5)-C(4)-U(1)	74.14(19)
C(9)-C(4)-U(1)	121.4(2)
C(1)-C(5)-C(4)	107.6(3)
C(1)-C(5)-C(10)	125.1(4)
C(4)-C(5)-C(10)	126.8(4)
C(1)-C(5)-U(1)	75.21(18)
C(4)-C(5)-U(1)	76.07(19)
C(10)-C(5)-U(1)	121.2(3)
C(15)-C(11)-C(12)	107.9(3)
C(15)-C(11)-C(16)	124.8(3)
C(12)-C(11)-C(16)	126.8(3)
C(15)-C(11)-U(1)	74.78(17)
C(12)-C(11)-U(1)	75.97(17)
C(16)-C(11)-U(1)	121.2(2)
C(13)-C(12)-C(11)	108.0(3)
C(13)-C(12)-C(17)	123.1(3)
C(11)-C(12)-C(17)	128.2(3)
C(13)-C(12)-U(1)	75.86(17)
C(11)-C(12)-U(1)	74.49(17)
C(17)-C(12)-U(1)	123.3(2)
C(14)-C(13)-C(12)	108.2(3)
C(14)-C(13)-C(18)	125.9(3)
C(12)-C(13)-C(18)	124.6(3)
C(14)-C(13)-U(1)	74.18(18)
C(12)-C(13)-U(1)	74.94(17)
C(18)-C(13)-U(1)	127.2(2)
C(13)-C(14)-C(15)	108.1(3)
C(13)-C(14)-C(19)	124.7(3)
C(15)-C(14)-C(19)	126.8(3)
C(13)-C(14)-U(1)	76.63(18)
C(15)-C(14)-U(1)	74.69(17)
C(19)-C(14)-U(1)	120.0(2)
C(11)-C(15)-C(14)	107.7(3)
C(11)-C(15)-C(20)	125.3(3)
C(14)-C(15)-C(20)	126.8(3)
C(11)-C(15)-U(1)	75.64(17)

C(14)-C(15)-U(1)	75.51(17)
C(20)-C(15)-U(1)	119.0(2)
N(1)-C(21)-N(2)	113.6(3)
N(1)-C(21)-C(22)	124.2(3)
N(2)-C(21)-C(22)	122.1(3)
N(1)-C(21)-U(1)	59.67(17)
N(2)-C(21)-U(1)	54.00(17)
C(22)-C(21)-U(1)	175.6(3)
N(1)-C(23)-C(24)	116.3(3)
N(1)-C(23)-C(25)	114.8(3)
C(24)-C(23)-C(25)	109.1(3)
C(27)-C(26)-C(28)	119.8(4)
C(27)-C(26)-N(2)	116.4(4)
C(28)-C(26)-N(2)	115.5(4)
O(2)-C(29)-O(1)	123.9(3)
O(2)-C(29)-C(30)	120.3(3)
O(1)-C(29)-C(30)	115.8(3)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw33. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23
U(1)	20(1)	23(1)	14(1)	-2(1)
N(1)	23(1)	21(1)	19(1)	0(1)
N(2)	19(1)	43(2)	27(2)	-3(1)
O(1)	29(1)	40(1)	27(1)	0(1)
O(2)	27(1)	52(2)	48(2)	13(1)
C(1)	34(2)	30(2)	13(1)	-6(1)
C(2)	34(2)	28(2)	17(2)	-7(1)
C(3)	54(2)	21(2)	22(2)	-6(1)
C(4)	69(3)	26(2)	24(2)	-9(1)
C(5)	36(2)	42(2)	25(2)	-18(2)
C(6)	49(2)	41(2)	19(2)	-3(1)
C(7)	34(2)	41(2)	43(2)	-12(2)
C(8)	89(4)	37(2)	35(2)	-8(2)
C(9)	129(5)	34(2)	49(3)	-11(2)
C(10)	37(2)	89(4)	48(3)	-31(2)
C(11)	25(2)	27(2)	15(1)	-6(1)
C(12)	23(2)	29(2)	15(1)	-5(1)
C(13)	29(2)	32(2)	16(1)	-2(1)
C(14)	32(2)	29(2)	17(2)	1(1)
C(15)	29(2)	30(2)	12(1)	-2(1)
C(16)	33(2)	28(2)	25(2)	-6(1)
C(17)	24(2)	41(2)	24(2)	-1(1)
C(18)	38(2)	43(2)	32(2)	-3(2)
C(19)	45(2)	33(2)	28(2)	7(2)
C(20)	37(2)	39(2)	30(2)	-1(2)
C(21)	26(2)	28(2)	19(2)	-3(1)
C(22)	46(2)	46(2)	42(2)	12(2)
C(23)	24(2)	26(2)	24(2)	3(1)
C(24)	41(2)	36(2)	28(2)	6(2)
C(25)	39(2)	32(2)	36(2)	0(2)
C(26)	24(2)	97(4)	46(3)	-15(2)

C(27)	29(2)	119(5)	87(4)	-53(4)
C(28)	26(2)	68(3)	49(3)	-5(2)
C(29)	25(2)	32(2)	33(2)	-4(1)
C(30)	32(2)	41(2)	50(2)	14(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw33.

	x	y	z	U(eq)
H(6A)	2730	1710	-862	56
H(6B)	4335	2000	-795	56
H(6C)	3295	2433	-336	56
H(7A)	7401	1752	760	58
H(7B)	6576	1905	-98	58
H(7C)	7319	1093	129	58
H(8A)	6510	-65	1883	85
H(8B)	7527	476	1503	85
H(8C)	6811	-265	1055	85
H(9A)	3752	-693	1239	102
H(9B)	2444	-184	1390	102
H(9C)	3927	-171	1990	102
H(10A)	1177	1340	-74	86
H(10B)	1071	797	635	86
H(10C)	1317	430	-150	86
H(16A)	4525	3852	2306	43
H(16B)	6011	3994	2880	43
H(16C)	4588	3871	3208	43
H(17A)	8721	2704	2862	45
H(17B)	7772	3380	2417	45
H(17C)	8005	2605	1978	45
H(18A)	8349	1225	3455	58
H(18B)	8179	1206	2545	58
H(18C)	7299	618	2960	58
H(19A)	4608	474	3112	55
H(19B)	3907	961	3702	55
H(19C)	5542	707	3926	55
H(20A)	3423	2887	3860	52
H(20B)	2826	2044	3633	52
H(20C)	2474	2730	3030	52

H(22A)	3917	4303	203	68
H(22B)	2931	4496	804	68
H(22C)	2296	4019	48	68
H(23A)	6943	3126	870	29
H(24A)	5683	3067	-414	52
H(24B)	6896	3712	-274	52
H(24C)	5259	3949	-355	52
H(25A)	5846	4637	875	54
H(25B)	7485	4390	1000	54
H(25C)	6581	4199	1640	54
H(26A)	938	2645	1429	67
H(27A)	1046	4195	1440	117
H(27B)	1546	3634	2152	117
H(27C)	-87	3646	1722	117
H(28A)	-755	2955	491	73
H(28B)	486	2525	175	73
H(28C)	304	3434	80	73
H(30A)	1222	874	3199	60
H(30B)	1943	262	2725	60
H(30C)	245	317	2602	60

Table 6. Torsion angles [°] for jrw33.

O(1)-U(1)-N(1)-C(21)	-0.2(2)
N(2)-U(1)-N(1)-C(21)	-1.01(18)
C(5)-U(1)-N(1)-C(21)	84.1(2)
C(1)-U(1)-N(1)-C(21)	96.74(19)
C(15)-U(1)-N(1)-C(21)	-84.74(19)
C(2)-U(1)-N(1)-C(21)	127.1(2)
C(14)-U(1)-N(1)-C(21)	-110.6(2)
C(11)-U(1)-N(1)-C(21)	-95.18(19)
C(4)-U(1)-N(1)-C(21)	107.9(2)
C(12)-U(1)-N(1)-C(21)	-125.35(19)
C(3)-U(1)-N(1)-C(21)	134.79(19)
C(13)-U(1)-N(1)-C(21)	-135.42(19)
O(1)-U(1)-N(1)-C(23)	178.5(3)
N(2)-U(1)-N(1)-C(23)	177.7(4)
C(5)-U(1)-N(1)-C(23)	-97.2(3)
C(1)-U(1)-N(1)-C(23)	-84.5(3)
C(15)-U(1)-N(1)-C(23)	94.0(3)
C(2)-U(1)-N(1)-C(23)	-54.2(3)
C(14)-U(1)-N(1)-C(23)	68.1(3)
C(11)-U(1)-N(1)-C(23)	83.5(3)
C(4)-U(1)-N(1)-C(23)	-73.4(4)
C(12)-U(1)-N(1)-C(23)	53.4(3)
C(3)-U(1)-N(1)-C(23)	-46.5(3)
C(13)-U(1)-N(1)-C(23)	43.3(3)
C(21)-U(1)-N(1)-C(23)	178.7(4)
O(1)-U(1)-N(2)-C(21)	-178.5(2)
N(1)-U(1)-N(2)-C(21)	1.00(18)
C(5)-U(1)-N(2)-C(21)	-103.7(2)
C(1)-U(1)-N(2)-C(21)	-74.4(2)
C(15)-U(1)-N(2)-C(21)	107.6(2)
C(2)-U(1)-N(2)-C(21)	-56.7(2)
C(14)-U(1)-N(2)-C(21)	112.5(2)
C(11)-U(1)-N(2)-C(21)	79.1(2)
C(4)-U(1)-N(2)-C(21)	-111.3(2)

C(12)-U(1)-N(2)-C(21)	60.1(2)
C(3)-U(1)-N(2)-C(21)	-77.6(3)
C(13)-U(1)-N(2)-C(21)	77.3(2)
O(1)-U(1)-N(2)-C(26)	-0.4(3)
N(1)-U(1)-N(2)-C(26)	179.0(4)
C(5)-U(1)-N(2)-C(26)	74.4(4)
C(1)-U(1)-N(2)-C(26)	103.6(4)
C(15)-U(1)-N(2)-C(26)	-74.3(4)
C(2)-U(1)-N(2)-C(26)	121.3(3)
C(14)-U(1)-N(2)-C(26)	-69.5(4)
C(11)-U(1)-N(2)-C(26)	-102.9(4)
C(4)-U(1)-N(2)-C(26)	66.8(4)
C(12)-U(1)-N(2)-C(26)	-121.8(3)
C(3)-U(1)-N(2)-C(26)	100.4(4)
C(13)-U(1)-N(2)-C(26)	-104.7(4)
C(21)-U(1)-N(2)-C(26)	178.0(5)
N(2)-U(1)-O(1)-C(29)	41.1(13)
N(1)-U(1)-O(1)-C(29)	40.4(13)
C(5)-U(1)-O(1)-C(29)	-55.2(13)
C(1)-U(1)-O(1)-C(29)	-46.3(13)
C(15)-U(1)-O(1)-C(29)	137.3(13)
C(2)-U(1)-O(1)-C(29)	-72.5(13)
C(14)-U(1)-O(1)-C(29)	168.1(13)
C(11)-U(1)-O(1)-C(29)	126.2(13)
C(4)-U(1)-O(1)-C(29)	-86.1(13)
C(12)-U(1)-O(1)-C(29)	150.2(12)
C(3)-U(1)-O(1)-C(29)	-96.4(13)
C(13)-U(1)-O(1)-C(29)	176.0(13)
C(21)-U(1)-O(1)-C(29)	40.3(13)
O(1)-U(1)-C(1)-C(5)	-17.7(2)
N(2)-U(1)-C(1)-C(5)	-100.9(2)
N(1)-U(1)-C(1)-C(5)	-154.7(2)
C(15)-U(1)-C(1)-C(5)	47.1(15)
C(2)-U(1)-C(1)-C(5)	113.1(3)
C(14)-U(1)-C(1)-C(5)	68.6(3)
C(11)-U(1)-C(1)-C(5)	178.8(2)

C(4)-U(1)-C(1)-C(5)	37.4(2)
C(12)-U(1)-C(1)-C(5)	143.5(2)
C(3)-U(1)-C(1)-C(5)	76.2(2)
C(13)-U(1)-C(1)-C(5)	104.8(2)
C(21)-U(1)-C(1)-C(5)	-127.4(2)
O(1)-U(1)-C(1)-C(2)	-130.79(19)
N(2)-U(1)-C(1)-C(2)	145.9(2)
N(1)-U(1)-C(1)-C(2)	92.2(2)
C(5)-U(1)-C(1)-C(2)	-113.1(3)
C(15)-U(1)-C(1)-C(2)	-66.0(15)
C(14)-U(1)-C(1)-C(2)	-44.6(3)
C(11)-U(1)-C(1)-C(2)	65.6(3)
C(4)-U(1)-C(1)-C(2)	-75.7(2)
C(12)-U(1)-C(1)-C(2)	30.4(2)
C(3)-U(1)-C(1)-C(2)	-36.90(19)
C(13)-U(1)-C(1)-C(2)	-8.3(2)
C(21)-U(1)-C(1)-C(2)	119.4(2)
O(1)-U(1)-C(1)-C(6)	104.3(3)
N(2)-U(1)-C(1)-C(6)	21.0(3)
N(1)-U(1)-C(1)-C(6)	-32.7(3)
C(5)-U(1)-C(1)-C(6)	121.9(4)
C(15)-U(1)-C(1)-C(6)	169.0(13)
C(2)-U(1)-C(1)-C(6)	-124.9(4)
C(14)-U(1)-C(1)-C(6)	-169.5(3)
C(11)-U(1)-C(1)-C(6)	-59.3(4)
C(4)-U(1)-C(1)-C(6)	159.4(3)
C(12)-U(1)-C(1)-C(6)	-94.6(3)
C(3)-U(1)-C(1)-C(6)	-161.8(3)
C(13)-U(1)-C(1)-C(6)	-133.3(3)
C(21)-U(1)-C(1)-C(6)	-5.5(3)
C(5)-C(1)-C(2)-C(3)	1.0(4)
C(6)-C(1)-C(2)-C(3)	-171.5(3)
U(1)-C(1)-C(2)-C(3)	69.8(2)
C(5)-C(1)-C(2)-C(7)	173.0(3)
C(6)-C(1)-C(2)-C(7)	0.5(5)
U(1)-C(1)-C(2)-C(7)	-118.2(3)

C(5)-C(1)-C(2)-U(1)	-68.8(2)
C(6)-C(1)-C(2)-U(1)	118.7(3)
O(1)-U(1)-C(2)-C(3)	-53.5(2)
N(2)-U(1)-C(2)-C(3)	-150.8(2)
N(1)-U(1)-C(2)-C(3)	165.0(2)
C(5)-U(1)-C(2)-C(3)	-76.0(2)
C(1)-U(1)-C(2)-C(3)	-113.2(3)
C(15)-U(1)-C(2)-C(3)	60.1(3)
C(14)-U(1)-C(2)-C(3)	39.8(2)
C(11)-U(1)-C(2)-C(3)	101.1(2)
C(4)-U(1)-C(2)-C(3)	-36.0(2)
C(12)-U(1)-C(2)-C(3)	89.8(2)
C(13)-U(1)-C(2)-C(3)	60.3(2)
C(21)-U(1)-C(2)-C(3)	-173.5(2)
O(1)-U(1)-C(2)-C(1)	59.6(2)
N(2)-U(1)-C(2)-C(1)	-37.6(2)
N(1)-U(1)-C(2)-C(1)	-81.8(2)
C(5)-U(1)-C(2)-C(1)	37.2(2)
C(15)-U(1)-C(2)-C(1)	173.29(19)
C(14)-U(1)-C(2)-C(1)	152.96(19)
C(11)-U(1)-C(2)-C(1)	-145.78(19)
C(4)-U(1)-C(2)-C(1)	77.2(2)
C(12)-U(1)-C(2)-C(1)	-157.06(19)
C(3)-U(1)-C(2)-C(1)	113.2(3)
C(13)-U(1)-C(2)-C(1)	173.48(19)
C(21)-U(1)-C(2)-C(1)	-60.3(2)
O(1)-U(1)-C(2)-C(7)	-175.2(3)
N(2)-U(1)-C(2)-C(7)	87.6(3)
N(1)-U(1)-C(2)-C(7)	43.4(3)
C(5)-U(1)-C(2)-C(7)	162.4(3)
C(1)-U(1)-C(2)-C(7)	125.2(4)
C(15)-U(1)-C(2)-C(7)	-61.5(4)
C(14)-U(1)-C(2)-C(7)	-81.8(3)
C(11)-U(1)-C(2)-C(7)	-20.6(3)
C(4)-U(1)-C(2)-C(7)	-157.6(3)
C(12)-U(1)-C(2)-C(7)	-31.8(3)

C(3)-U(1)-C(2)-C(7)	-121.6(4)
C(13)-U(1)-C(2)-C(7)	-61.3(3)
C(21)-U(1)-C(2)-C(7)	64.9(3)
C(1)-C(2)-C(3)-C(4)	-1.1(4)
C(7)-C(2)-C(3)-C(4)	-173.5(3)
U(1)-C(2)-C(3)-C(4)	67.4(2)
C(1)-C(2)-C(3)-C(8)	165.6(3)
C(7)-C(2)-C(3)-C(8)	-6.8(5)
U(1)-C(2)-C(3)-C(8)	-125.9(3)
C(1)-C(2)-C(3)-U(1)	-68.5(2)
C(7)-C(2)-C(3)-U(1)	119.1(3)
O(1)-U(1)-C(3)-C(4)	20.9(2)
N(2)-U(1)-C(3)-C(4)	-72.9(3)
N(1)-U(1)-C(3)-C(4)	-130.3(2)
C(5)-U(1)-C(3)-C(4)	-37.2(2)
C(1)-U(1)-C(3)-C(4)	-77.1(2)
C(15)-U(1)-C(3)-C(4)	100.5(2)
C(2)-U(1)-C(3)-C(4)	-114.7(3)
C(14)-U(1)-C(3)-C(4)	98.6(2)
C(11)-U(1)-C(3)-C(4)	138.9(2)
C(12)-U(1)-C(3)-C(4)	147.7(2)
C(13)-U(1)-C(3)-C(4)	124.6(2)
C(21)-U(1)-C(3)-C(4)	-106.6(2)
O(1)-U(1)-C(3)-C(2)	135.5(2)
N(2)-U(1)-C(3)-C(2)	41.7(3)
N(1)-U(1)-C(3)-C(2)	-15.6(2)
C(5)-U(1)-C(3)-C(2)	77.5(2)
C(1)-U(1)-C(3)-C(2)	37.50(19)
C(15)-U(1)-C(3)-C(2)	-144.86(19)
C(14)-U(1)-C(3)-C(2)	-146.7(2)
C(11)-U(1)-C(3)-C(2)	-106.4(2)
C(4)-U(1)-C(3)-C(2)	114.7(3)
C(12)-U(1)-C(3)-C(2)	-97.7(2)
C(13)-U(1)-C(3)-C(2)	-120.7(2)
C(21)-U(1)-C(3)-C(2)	8.0(3)
O(1)-U(1)-C(3)-C(8)	-103.2(4)

N(2)-U(1)-C(3)-C(8)	163.0(3)
N(1)-U(1)-C(3)-C(8)	105.6(4)
C(5)-U(1)-C(3)-C(8)	-161.2(4)
C(1)-U(1)-C(3)-C(8)	158.8(4)
C(15)-U(1)-C(3)-C(8)	-23.6(4)
C(2)-U(1)-C(3)-C(8)	121.3(5)
C(14)-U(1)-C(3)-C(8)	-25.5(4)
C(11)-U(1)-C(3)-C(8)	14.9(4)
C(4)-U(1)-C(3)-C(8)	-124.1(5)
C(12)-U(1)-C(3)-C(8)	23.6(4)
C(13)-U(1)-C(3)-C(8)	0.6(4)
C(21)-U(1)-C(3)-C(8)	129.3(4)
C(2)-C(3)-C(4)-C(5)	0.8(4)
C(8)-C(3)-C(4)-C(5)	-165.6(3)
U(1)-C(3)-C(4)-C(5)	67.8(2)
C(2)-C(3)-C(4)-C(9)	174.0(3)
C(8)-C(3)-C(4)-C(9)	7.6(6)
U(1)-C(3)-C(4)-C(9)	-119.0(3)
C(2)-C(3)-C(4)-U(1)	-67.0(2)
C(8)-C(3)-C(4)-U(1)	126.6(3)
O(1)-U(1)-C(4)-C(3)	-158.8(2)
N(2)-U(1)-C(4)-C(3)	129.5(2)
N(1)-U(1)-C(4)-C(3)	62.2(2)
C(5)-U(1)-C(4)-C(3)	114.1(3)
C(1)-U(1)-C(4)-C(3)	76.8(2)
C(15)-U(1)-C(4)-C(3)	-102.4(2)
C(2)-U(1)-C(4)-C(3)	36.61(19)
C(14)-U(1)-C(4)-C(3)	-86.4(2)
C(11)-U(1)-C(4)-C(3)	-70.5(3)
C(12)-U(1)-C(4)-C(3)	-40.4(2)
C(13)-U(1)-C(4)-C(3)	-56.6(2)
C(21)-U(1)-C(4)-C(3)	96.2(3)
O(1)-U(1)-C(4)-C(5)	87.1(2)
N(2)-U(1)-C(4)-C(5)	15.4(3)
N(1)-U(1)-C(4)-C(5)	-51.9(3)
C(1)-U(1)-C(4)-C(5)	-37.4(2)

C(15)-U(1)-C(4)-C(5)	143.4(2)
C(2)-U(1)-C(4)-C(5)	-77.5(2)
C(14)-U(1)-C(4)-C(5)	159.5(2)
C(11)-U(1)-C(4)-C(5)	175.37(19)
C(12)-U(1)-C(4)-C(5)	-154.5(2)
C(3)-U(1)-C(4)-C(5)	-114.1(3)
C(13)-U(1)-C(4)-C(5)	-170.8(2)
C(21)-U(1)-C(4)-C(5)	-18.0(3)
O(1)-U(1)-C(4)-C(9)	-36.5(4)
N(2)-U(1)-C(4)-C(9)	-108.2(4)
N(1)-U(1)-C(4)-C(9)	-175.4(4)
C(5)-U(1)-C(4)-C(9)	-123.5(5)
C(1)-U(1)-C(4)-C(9)	-160.9(5)
C(15)-U(1)-C(4)-C(9)	19.9(5)
C(2)-U(1)-C(4)-C(9)	159.0(5)
C(14)-U(1)-C(4)-C(9)	35.9(4)
C(11)-U(1)-C(4)-C(9)	51.8(5)
C(12)-U(1)-C(4)-C(9)	82.0(4)
C(3)-U(1)-C(4)-C(9)	122.3(5)
C(13)-U(1)-C(4)-C(9)	65.7(4)
C(21)-U(1)-C(4)-C(9)	-141.5(4)
C(2)-C(1)-C(5)-C(4)	-0.5(4)
C(6)-C(1)-C(5)-C(4)	172.2(3)
U(1)-C(1)-C(5)-C(4)	-69.8(2)
C(2)-C(1)-C(5)-C(10)	-172.8(3)
C(6)-C(1)-C(5)-C(10)	0.0(5)
U(1)-C(1)-C(5)-C(10)	118.0(4)
C(2)-C(1)-C(5)-U(1)	69.3(2)
C(6)-C(1)-C(5)-U(1)	-118.0(3)
C(3)-C(4)-C(5)-C(1)	-0.1(4)
C(9)-C(4)-C(5)-C(1)	-173.2(3)
U(1)-C(4)-C(5)-C(1)	69.2(2)
C(3)-C(4)-C(5)-C(10)	171.9(3)
C(9)-C(4)-C(5)-C(10)	-1.1(6)
U(1)-C(4)-C(5)-C(10)	-118.7(4)
C(3)-C(4)-C(5)-U(1)	-69.4(2)

C(9)-C(4)-C(5)-U(1)	117.6(4)
O(1)-U(1)-C(5)-C(1)	162.3(2)
N(2)-U(1)-C(5)-C(1)	80.0(2)
N(1)-U(1)-C(5)-C(1)	25.6(2)
C(15)-U(1)-C(5)-C(1)	-174.76(19)
C(2)-U(1)-C(5)-C(1)	-37.35(19)
C(14)-U(1)-C(5)-C(1)	-139.0(2)
C(11)-U(1)-C(5)-C(1)	-169(2)
C(4)-U(1)-C(5)-C(1)	-112.8(3)
C(12)-U(1)-C(5)-C(1)	-66.9(3)
C(3)-U(1)-C(5)-C(1)	-76.8(2)
C(13)-U(1)-C(5)-C(1)	-100.9(2)
C(21)-U(1)-C(5)-C(1)	53.0(2)
O(1)-U(1)-C(5)-C(4)	-84.9(2)
N(2)-U(1)-C(5)-C(4)	-167.2(2)
N(1)-U(1)-C(5)-C(4)	138.4(2)
C(1)-U(1)-C(5)-C(4)	112.8(3)
C(15)-U(1)-C(5)-C(4)	-61.9(3)
C(2)-U(1)-C(5)-C(4)	75.5(2)
C(14)-U(1)-C(5)-C(4)	-26.2(3)
C(11)-U(1)-C(5)-C(4)	-56(2)
C(12)-U(1)-C(5)-C(4)	45.9(3)
C(3)-U(1)-C(5)-C(4)	36.1(2)
C(13)-U(1)-C(5)-C(4)	11.9(3)
C(21)-U(1)-C(5)-C(4)	165.9(2)
O(1)-U(1)-C(5)-C(10)	39.9(3)
N(2)-U(1)-C(5)-C(10)	-42.4(3)
N(1)-U(1)-C(5)-C(10)	-96.8(3)
C(1)-U(1)-C(5)-C(10)	-122.4(4)
C(15)-U(1)-C(5)-C(10)	62.9(4)
C(2)-U(1)-C(5)-C(10)	-159.7(4)
C(14)-U(1)-C(5)-C(10)	98.6(4)
C(11)-U(1)-C(5)-C(10)	69(2)
C(4)-U(1)-C(5)-C(10)	124.8(4)
C(12)-U(1)-C(5)-C(10)	170.7(3)
C(3)-U(1)-C(5)-C(10)	160.9(4)

C(13)-U(1)-C(5)-C(10)	136.7(3)
C(21)-U(1)-C(5)-C(10)	-69.3(3)
O(1)-U(1)-C(11)-C(15)	22.1(2)
N(2)-U(1)-C(11)-C(15)	105.0(2)
N(1)-U(1)-C(11)-C(15)	159.3(2)
C(5)-U(1)-C(11)-C(15)	-6(2)
C(1)-U(1)-C(11)-C(15)	-174.2(2)
C(2)-U(1)-C(11)-C(15)	-135.93(19)
C(14)-U(1)-C(11)-C(15)	-37.49(19)
C(4)-U(1)-C(11)-C(15)	-58.4(3)
C(12)-U(1)-C(11)-C(15)	-113.4(3)
C(3)-U(1)-C(11)-C(15)	-95.9(2)
C(13)-U(1)-C(11)-C(15)	-76.7(2)
C(21)-U(1)-C(11)-C(15)	132.0(2)
O(1)-U(1)-C(11)-C(12)	135.51(19)
N(2)-U(1)-C(11)-C(12)	-141.7(2)
N(1)-U(1)-C(11)-C(12)	-87.27(19)
C(5)-U(1)-C(11)-C(12)	107(2)
C(1)-U(1)-C(11)-C(12)	-60.8(3)
C(15)-U(1)-C(11)-C(12)	113.4(3)
C(2)-U(1)-C(11)-C(12)	-22.5(2)
C(14)-U(1)-C(11)-C(12)	75.9(2)
C(4)-U(1)-C(11)-C(12)	55.0(3)
C(3)-U(1)-C(11)-C(12)	17.5(2)
C(13)-U(1)-C(11)-C(12)	36.66(19)
C(21)-U(1)-C(11)-C(12)	-114.6(2)
O(1)-U(1)-C(11)-C(16)	-99.7(3)
N(2)-U(1)-C(11)-C(16)	-16.8(3)
N(1)-U(1)-C(11)-C(16)	37.6(2)
C(5)-U(1)-C(11)-C(16)	-128(2)
C(1)-U(1)-C(11)-C(16)	64.0(4)
C(15)-U(1)-C(11)-C(16)	-121.8(3)
C(2)-U(1)-C(11)-C(16)	102.3(3)
C(14)-U(1)-C(11)-C(16)	-159.3(3)
C(4)-U(1)-C(11)-C(16)	179.8(2)
C(12)-U(1)-C(11)-C(16)	124.8(3)

C(3)-U(1)-C(11)-C(16)	142.3(2)
C(13)-U(1)-C(11)-C(16)	161.5(3)
C(21)-U(1)-C(11)-C(16)	10.2(2)
C(15)-C(11)-C(12)-C(13)	-0.5(3)
C(16)-C(11)-C(12)-C(13)	172.2(3)
U(1)-C(11)-C(12)-C(13)	-69.1(2)
C(15)-C(11)-C(12)-C(17)	-170.9(3)
C(16)-C(11)-C(12)-C(17)	1.8(5)
U(1)-C(11)-C(12)-C(17)	120.5(3)
C(15)-C(11)-C(12)-U(1)	68.6(2)
C(16)-C(11)-C(12)-U(1)	-118.7(3)
O(1)-U(1)-C(12)-C(13)	60.0(2)
N(2)-U(1)-C(12)-C(13)	154.70(19)
N(1)-U(1)-C(12)-C(13)	-159.8(2)
C(5)-U(1)-C(12)-C(13)	-60.6(3)
C(1)-U(1)-C(12)-C(13)	-98.4(2)
C(15)-U(1)-C(12)-C(13)	76.5(2)
C(2)-U(1)-C(12)-C(13)	-83.3(2)
C(14)-U(1)-C(12)-C(13)	36.42(19)
C(11)-U(1)-C(12)-C(13)	113.6(3)
C(4)-U(1)-C(12)-C(13)	-34.2(2)
C(3)-U(1)-C(12)-C(13)	-53.0(2)
C(21)-U(1)-C(12)-C(13)	178.22(19)
O(1)-U(1)-C(12)-C(11)	-53.6(2)
N(2)-U(1)-C(12)-C(11)	41.1(2)
N(1)-U(1)-C(12)-C(11)	86.53(19)
C(5)-U(1)-C(12)-C(11)	-174.2(2)
C(1)-U(1)-C(12)-C(11)	147.99(18)
C(15)-U(1)-C(12)-C(11)	-37.09(18)
C(2)-U(1)-C(12)-C(11)	163.09(19)
C(14)-U(1)-C(12)-C(11)	-77.2(2)
C(4)-U(1)-C(12)-C(11)	-147.88(19)
C(3)-U(1)-C(12)-C(11)	-166.65(19)
C(13)-U(1)-C(12)-C(11)	-113.6(3)
C(21)-U(1)-C(12)-C(11)	64.6(2)
O(1)-U(1)-C(12)-C(17)	-179.5(2)

N(2)-U(1)-C(12)-C(17)	-84.8(3)
N(1)-U(1)-C(12)-C(17)	-39.3(3)
C(5)-U(1)-C(12)-C(17)	59.9(4)
C(1)-U(1)-C(12)-C(17)	22.1(3)
C(15)-U(1)-C(12)-C(17)	-163.0(3)
C(2)-U(1)-C(12)-C(17)	37.2(3)
C(14)-U(1)-C(12)-C(17)	156.9(3)
C(11)-U(1)-C(12)-C(17)	-125.9(4)
C(4)-U(1)-C(12)-C(17)	86.3(3)
C(3)-U(1)-C(12)-C(17)	67.5(3)
C(13)-U(1)-C(12)-C(17)	120.5(3)
C(21)-U(1)-C(12)-C(17)	-61.3(3)
C(11)-C(12)-C(13)-C(14)	0.9(3)
C(17)-C(12)-C(13)-C(14)	171.9(3)
U(1)-C(12)-C(13)-C(14)	-67.3(2)
C(11)-C(12)-C(13)-C(18)	-166.8(3)
C(17)-C(12)-C(13)-C(18)	4.2(5)
U(1)-C(12)-C(13)-C(18)	125.1(3)
C(11)-C(12)-C(13)-U(1)	68.2(2)
C(17)-C(12)-C(13)-U(1)	-120.8(3)
O(1)-U(1)-C(13)-C(14)	-16.0(2)
N(2)-U(1)-C(13)-C(14)	79.7(2)
N(1)-U(1)-C(13)-C(14)	134.96(19)
C(5)-U(1)-C(13)-C(14)	-99.1(2)
C(1)-U(1)-C(13)-C(14)	-138.2(2)
C(15)-U(1)-C(13)-C(14)	37.46(19)
C(2)-U(1)-C(13)-C(14)	-142.4(2)
C(11)-U(1)-C(13)-C(14)	77.3(2)
C(4)-U(1)-C(13)-C(14)	-93.1(2)
C(12)-U(1)-C(13)-C(14)	114.4(3)
C(3)-U(1)-C(13)-C(14)	-117.0(2)
C(21)-U(1)-C(13)-C(14)	112.3(2)
O(1)-U(1)-C(13)-C(12)	-130.41(19)
N(2)-U(1)-C(13)-C(12)	-34.7(3)
N(1)-U(1)-C(13)-C(12)	20.6(2)
C(5)-U(1)-C(13)-C(12)	146.50(19)

C(1)-U(1)-C(13)-C(12)	107.4(2)
C(15)-U(1)-C(13)-C(12)	-76.9(2)
C(2)-U(1)-C(13)-C(12)	103.2(2)
C(14)-U(1)-C(13)-C(12)	-114.4(3)
C(11)-U(1)-C(13)-C(12)	-37.11(18)
C(4)-U(1)-C(13)-C(12)	152.52(19)
C(3)-U(1)-C(13)-C(12)	128.6(2)
C(21)-U(1)-C(13)-C(12)	-2.1(2)
O(1)-U(1)-C(13)-C(18)	107.3(3)
N(2)-U(1)-C(13)-C(18)	-157.0(3)
N(1)-U(1)-C(13)-C(18)	-101.7(3)
C(5)-U(1)-C(13)-C(18)	24.2(4)
C(1)-U(1)-C(13)-C(18)	-14.9(4)
C(15)-U(1)-C(13)-C(18)	160.8(4)
C(2)-U(1)-C(13)-C(18)	-19.1(3)
C(14)-U(1)-C(13)-C(18)	123.3(4)
C(11)-U(1)-C(13)-C(18)	-159.4(4)
C(4)-U(1)-C(13)-C(18)	30.2(3)
C(12)-U(1)-C(13)-C(18)	-122.3(4)
C(3)-U(1)-C(13)-C(18)	6.3(3)
C(21)-U(1)-C(13)-C(18)	-124.4(3)
C(12)-C(13)-C(14)-C(15)	-0.9(3)
C(18)-C(13)-C(14)-C(15)	166.6(3)
U(1)-C(13)-C(14)-C(15)	-68.7(2)
C(12)-C(13)-C(14)-C(19)	-174.7(3)
C(18)-C(13)-C(14)-C(19)	-7.3(5)
U(1)-C(13)-C(14)-C(19)	117.5(3)
C(12)-C(13)-C(14)-U(1)	67.8(2)
C(18)-C(13)-C(14)-U(1)	-124.8(3)
O(1)-U(1)-C(14)-C(13)	164.1(2)
N(2)-U(1)-C(14)-C(13)	-123.2(2)
N(1)-U(1)-C(14)-C(13)	-56.0(2)
C(5)-U(1)-C(14)-C(13)	105.7(2)
C(1)-U(1)-C(14)-C(13)	69.4(3)
C(15)-U(1)-C(14)-C(13)	-113.4(3)
C(2)-U(1)-C(14)-C(13)	45.1(2)

C(11)-U(1)-C(14)-C(13)	-76.2(2)
C(4)-U(1)-C(14)-C(13)	92.8(2)
C(12)-U(1)-C(14)-C(13)	-36.45(19)
C(3)-U(1)-C(14)-C(13)	63.6(2)
C(21)-U(1)-C(14)-C(13)	-89.8(2)
O(1)-U(1)-C(14)-C(15)	-82.6(2)
N(2)-U(1)-C(14)-C(15)	-9.8(2)
N(1)-U(1)-C(14)-C(15)	57.4(2)
C(5)-U(1)-C(14)-C(15)	-140.9(2)
C(1)-U(1)-C(14)-C(15)	-177.17(18)
C(2)-U(1)-C(14)-C(15)	158.50(18)
C(11)-U(1)-C(14)-C(15)	37.20(19)
C(4)-U(1)-C(14)-C(15)	-153.8(2)
C(12)-U(1)-C(14)-C(15)	76.9(2)
C(3)-U(1)-C(14)-C(15)	177.0(2)
C(13)-U(1)-C(14)-C(15)	113.4(3)
C(21)-U(1)-C(14)-C(15)	23.6(2)
O(1)-U(1)-C(14)-C(19)	41.4(3)
N(2)-U(1)-C(14)-C(19)	114.2(3)
N(1)-U(1)-C(14)-C(19)	-178.6(2)
C(5)-U(1)-C(14)-C(19)	-16.9(3)
C(1)-U(1)-C(14)-C(19)	-53.2(4)
C(15)-U(1)-C(14)-C(19)	124.0(4)
C(2)-U(1)-C(14)-C(19)	-77.5(3)
C(11)-U(1)-C(14)-C(19)	161.2(3)
C(4)-U(1)-C(14)-C(19)	-29.8(3)
C(12)-U(1)-C(14)-C(19)	-159.1(3)
C(3)-U(1)-C(14)-C(19)	-59.0(3)
C(13)-U(1)-C(14)-C(19)	-122.6(4)
C(21)-U(1)-C(14)-C(19)	147.6(2)
C(12)-C(11)-C(15)-C(14)	0.0(3)
C(16)-C(11)-C(15)-C(14)	-172.9(3)
U(1)-C(11)-C(15)-C(14)	69.4(2)
C(12)-C(11)-C(15)-C(20)	175.1(3)
C(16)-C(11)-C(15)-C(20)	2.2(5)
U(1)-C(11)-C(15)-C(20)	-115.5(3)

C(12)-C(11)-C(15)-U(1)	-69.4(2)
C(16)-C(11)-C(15)-U(1)	117.7(3)
C(13)-C(14)-C(15)-C(11)	0.6(3)
C(19)-C(14)-C(15)-C(11)	174.2(3)
U(1)-C(14)-C(15)-C(11)	-69.5(2)
C(13)-C(14)-C(15)-C(20)	-174.4(3)
C(19)-C(14)-C(15)-C(20)	-0.8(5)
U(1)-C(14)-C(15)-C(20)	115.6(3)
C(13)-C(14)-C(15)-U(1)	70.0(2)
C(19)-C(14)-C(15)-U(1)	-116.3(3)
O(1)-U(1)-C(15)-C(11)	-157.5(2)
N(2)-U(1)-C(15)-C(11)	-75.3(2)
N(1)-U(1)-C(15)-C(11)	-21.1(2)
C(5)-U(1)-C(15)-C(11)	179.4(2)
C(1)-U(1)-C(15)-C(11)	136.8(14)
C(2)-U(1)-C(15)-C(11)	76.5(3)
C(14)-U(1)-C(15)-C(11)	112.9(3)
C(4)-U(1)-C(15)-C(11)	146.0(2)
C(12)-U(1)-C(15)-C(11)	37.04(18)
C(3)-U(1)-C(15)-C(11)	109.2(2)
C(13)-U(1)-C(15)-C(11)	76.3(2)
C(21)-U(1)-C(15)-C(11)	-48.7(2)
O(1)-U(1)-C(15)-C(14)	89.5(2)
N(2)-U(1)-C(15)-C(14)	171.8(2)
N(1)-U(1)-C(15)-C(14)	-133.98(19)
C(5)-U(1)-C(15)-C(14)	66.5(3)
C(1)-U(1)-C(15)-C(14)	23.9(15)
C(2)-U(1)-C(15)-C(14)	-36.4(3)
C(11)-U(1)-C(15)-C(14)	-112.9(3)
C(4)-U(1)-C(15)-C(14)	33.0(3)
C(12)-U(1)-C(15)-C(14)	-75.9(2)
C(3)-U(1)-C(15)-C(14)	-3.7(3)
C(13)-U(1)-C(15)-C(14)	-36.63(19)
C(21)-U(1)-C(15)-C(14)	-161.66(19)
O(1)-U(1)-C(15)-C(20)	-34.8(2)
N(2)-U(1)-C(15)-C(20)	47.4(3)

N(1)-U(1)-C(15)-C(20)	101.6(3)
C(5)-U(1)-C(15)-C(20)	-57.9(3)
C(1)-U(1)-C(15)-C(20)	-100.5(14)
C(2)-U(1)-C(15)-C(20)	-160.8(2)
C(14)-U(1)-C(15)-C(20)	-124.4(3)
C(11)-U(1)-C(15)-C(20)	122.7(3)
C(4)-U(1)-C(15)-C(20)	-91.3(3)
C(12)-U(1)-C(15)-C(20)	159.7(3)
C(3)-U(1)-C(15)-C(20)	-128.1(2)
C(13)-U(1)-C(15)-C(20)	-161.0(3)
C(21)-U(1)-C(15)-C(20)	74.0(3)
C(23)-N(1)-C(21)-N(2)	-177.5(3)
U(1)-N(1)-C(21)-N(2)	1.6(3)
C(23)-N(1)-C(21)-C(22)	3.4(5)
U(1)-N(1)-C(21)-C(22)	-177.5(3)
C(23)-N(1)-C(21)-U(1)	-179.1(3)
C(26)-N(2)-C(21)-N(1)	-179.9(3)
U(1)-N(2)-C(21)-N(1)	-1.7(3)
C(26)-N(2)-C(21)-C(22)	-0.8(5)
U(1)-N(2)-C(21)-C(22)	177.4(3)
C(26)-N(2)-C(21)-U(1)	-178.3(4)
O(1)-U(1)-C(21)-N(1)	179.85(17)
N(2)-U(1)-C(21)-N(1)	178.2(3)
C(5)-U(1)-C(21)-N(1)	-101.93(19)
C(1)-U(1)-C(21)-N(1)	-78.32(19)
C(15)-U(1)-C(21)-N(1)	102.05(19)
C(2)-U(1)-C(21)-N(1)	-52.41(19)
C(14)-U(1)-C(21)-N(1)	90.3(2)
C(11)-U(1)-C(21)-N(1)	80.04(19)
C(4)-U(1)-C(21)-N(1)	-93.0(2)
C(12)-U(1)-C(21)-N(1)	53.32(19)
C(3)-U(1)-C(21)-N(1)	-56.4(2)
C(13)-U(1)-C(21)-N(1)	54.4(2)
O(1)-U(1)-C(21)-N(2)	1.6(2)
N(1)-U(1)-C(21)-N(2)	-178.2(3)
C(5)-U(1)-C(21)-N(2)	79.9(2)

C(1)-U(1)-C(21)-N(2)	103.5(2)
C(15)-U(1)-C(21)-N(2)	-76.2(2)
C(2)-U(1)-C(21)-N(2)	129.4(2)
C(14)-U(1)-C(21)-N(2)	-87.9(2)
C(11)-U(1)-C(21)-N(2)	-98.2(2)
C(4)-U(1)-C(21)-N(2)	88.8(2)
C(12)-U(1)-C(21)-N(2)	-124.9(2)
C(3)-U(1)-C(21)-N(2)	125.4(2)
C(13)-U(1)-C(21)-N(2)	-123.9(2)
O(1)-U(1)-C(21)-C(22)	-28(3)
N(2)-U(1)-C(21)-C(22)	-29(3)
N(1)-U(1)-C(21)-C(22)	153(3)
C(5)-U(1)-C(21)-C(22)	51(3)
C(1)-U(1)-C(21)-C(22)	74(3)
C(15)-U(1)-C(21)-C(22)	-105(3)
C(2)-U(1)-C(21)-C(22)	100(3)
C(14)-U(1)-C(21)-C(22)	-117(3)
C(11)-U(1)-C(21)-C(22)	-127(3)
C(4)-U(1)-C(21)-C(22)	60(3)
C(12)-U(1)-C(21)-C(22)	-154(3)
C(3)-U(1)-C(21)-C(22)	96(3)
C(13)-U(1)-C(21)-C(22)	-153(3)
C(21)-N(1)-C(23)-C(24)	-66.1(4)
U(1)-N(1)-C(23)-C(24)	115.4(3)
C(21)-N(1)-C(23)-C(25)	63.0(4)
U(1)-N(1)-C(23)-C(25)	-115.4(3)
C(21)-N(2)-C(26)-C(27)	-74.8(6)
U(1)-N(2)-C(26)-C(27)	107.6(5)
C(21)-N(2)-C(26)-C(28)	73.7(6)
U(1)-N(2)-C(26)-C(28)	-103.8(5)
U(1)-O(1)-C(29)-O(2)	-16.8(15)
U(1)-O(1)-C(29)-C(30)	163.6(11)

X-ray Data Collection, Structure Solution and Refinement for $(C_5Me_5)(C_5H_5)_2[PrNC(Me)N^iPr-\kappa^2N,N]U$, **8**.

A purple crystal of approximate dimensions 0.16 x 0.24 x 0.26 mm was mounted on a glass fiber and transferred to a Bruker SMART APEX II diffractometer. The APEX2¹ program package was used to determine the unit-cell parameters and for data collection (20 sec/frame scan time for a sphere of diffraction data). The raw frame data was processed using SAINT² and SADABS³ to yield the reflection data file. Subsequent calculations were carried out using the SHELXTL⁴ 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 direct methods and refined on F^2 by full-matrix least-squares techniques. The analytical scattering factors⁵ for neutral atoms were used throughout the analysis. Hydrogen atoms were located from a difference-Fourier map and refined (x,y,z and U_{iso}). At convergence, $wR2 = 0.0427$ and $Goof = 1.065$ for 448 variables refined against 5883 data ($0.75\text{\AA}$), $R1 = 0.0166$ for those 5747 data with $I > 2.0\sigma(I)$.

Table 1. Crystal data and structure refinement for $(C_5Me_5)(C_5H_5)_2[PrNC(Me)N^iPr-\kappa^2N,N]U$, **8**.

Identification code	jr49 (Justin Walensky)
Empirical formula	$C_{28}H_{42}N_2U$
Formula weight	644.67
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	$a = 8.2845(4) \text{ Å}$ $\alpha = 81.9930(5)^\circ$. $b = 11.1001(6) \text{ Å}$ $\beta = 76.1897(5)^\circ$. $c = 14.2310(7) \text{ Å}$ $\gamma = 81.9746(6)^\circ$.
Volume	1250.72(11) Å ³
Z	2
Density (calculated)	1.712 Mg/m ³
Absorption coefficient	6.506 mm ⁻¹
F(000)	632
Crystal color	purple
Crystal size	0.26 x 0.24 x 0.16 mm ³
Theta range for data collection	1.86 to 28.28°

Index ranges	$-10 \leq h \leq 11, -14 \leq k \leq 14, -18 \leq l \leq 18$	
Reflections collected	14751	
Independent reflections	5883 [R(int) = 0.0140]	
Completeness to $\theta = 28.28^\circ$	95.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4225 and 0.2825	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5883 / 0 / 448	
Goodness-of-fit on F ²	1.065	
Final R indices [I > 2 σ (I) = 5747 data]	R1 = 0.0166, wR2 = 0.0425	
R indices (all data; 0.75 Å)	R1 = 0.0171, wR2 = 0.0427	
Largest diff. peak and hole	1.794 and -0.673 e.Å ⁻³	

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jr49. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
U(1)	6482(1)	7970(1)	7677(1)	11(1)
N(1)	6992(2)	7157(2)	6083(1)	14(1)
N(2)	6710(2)	5771(2)	7396(1)	14(1)
C(1)	9940(3)	7171(2)	7306(2)	14(1)
C(2)	9393(3)	6772(2)	8308(2)	15(1)
C(3)	8941(3)	7818(2)	8820(2)	15(1)
C(4)	9187(3)	8873(2)	8139(2)	14(1)
C(5)	9816(3)	8473(2)	7193(2)	14(1)
C(6)	10790(3)	6357(2)	6528(2)	18(1)
C(7)	9666(3)	5490(2)	8782(2)	21(1)
C(8)	8727(3)	7788(2)	9904(2)	19(1)
C(9)	9180(3)	10126(2)	8433(2)	18(1)
C(10)	10567(3)	9219(2)	6269(2)	18(1)
C(11)	4087(3)	6618(2)	9035(2)	19(1)
C(12)	3140(3)	7723(2)	8802(2)	20(1)
C(13)	3662(3)	8642(2)	9213(2)	19(1)
C(14)	4967(3)	8121(2)	9662(2)	19(1)
C(15)	5242(3)	6855(2)	9547(2)	19(1)
C(16)	5001(3)	9590(2)	6337(2)	16(1)
C(17)	6642(3)	9928(2)	6177(2)	16(1)
C(18)	6727(3)	10520(2)	6974(2)	18(1)
C(19)	5167(3)	10523(2)	7637(2)	19(1)
C(20)	4090(3)	9966(2)	7236(2)	18(1)
C(21)	6916(3)	5980(2)	6434(2)	14(1)
C(22)	7053(4)	4963(2)	5797(2)	21(1)
C(23)	7105(3)	7576(2)	5037(2)	16(1)
C(24)	8841(3)	7314(2)	4382(2)	22(1)
C(25)	5741(3)	7201(2)	4605(2)	22(1)
C(26)	6427(3)	4552(2)	7938(2)	17(1)
C(27)	4847(4)	4060(2)	7822(2)	23(1)
C(28)	7917(4)	3537(2)	7781(2)	24(1)

Table 3. Bond lengths [Å] and angles [°] for jrw49.

U(1)-Cnt1	2.565
U(1)-Cnt2	2.581
U(1)-Cnt3	2.591
U(1)-N(1)	2.4802(18)
U(1)-N(2)	2.5024(19)
U(1)-C(15)	2.792(2)
U(1)-C(5)	2.798(2)
U(1)-C(16)	2.815(2)
U(1)-C(17)	2.820(2)
U(1)-C(14)	2.821(2)
U(1)-C(4)	2.823(2)
U(1)-C(1)	2.823(2)
U(1)-C(11)	2.849(2)
U(1)-C(2)	2.863(2)
U(1)-C(20)	2.866(2)
U(1)-C(3)	2.869(2)
U(1)-C(12)	2.877(2)
U(1)-C(13)	2.885(2)
U(1)-C(18)	2.886(2)
U(1)-C(19)	2.888(2)
U(1)-C(21)	2.950(2)
N(1)-C(21)	1.336(3)
N(1)-C(23)	1.480(3)
N(2)-C(21)	1.331(3)
N(2)-C(26)	1.481(3)
C(1)-C(2)	1.416(3)
C(1)-C(5)	1.423(3)
C(1)-C(6)	1.505(3)
C(2)-C(3)	1.415(3)
C(2)-C(7)	1.499(3)
C(3)-C(4)	1.416(3)
C(3)-C(8)	1.506(3)
C(4)-C(5)	1.431(3)
C(4)-C(9)	1.507(3)

C(5)-C(10)	1.501(3)
C(11)-C(15)	1.404(3)
C(11)-C(12)	1.404(3)
C(12)-C(13)	1.408(4)
C(13)-C(14)	1.401(4)
C(14)-C(15)	1.418(4)
C(16)-C(20)	1.407(3)
C(16)-C(17)	1.419(3)
C(17)-C(18)	1.408(3)
C(18)-C(19)	1.406(3)
C(19)-C(20)	1.414(3)
C(21)-C(22)	1.519(3)
C(23)-C(24)	1.530(3)
C(23)-C(25)	1.537(3)
C(26)-C(27)	1.538(3)
C(26)-C(28)	1.546(4)

Cnt1-U(1)-N(1)	101.9
Cnt1-U(1)-N(2)	94.2
Cnt1-U(1)-C(21)	99.9
Cnt2-U(1)-N(1)	130.9
Cnt2-U(1)-N(2)	90.5
Cnt2-U(1)-C(21)	111.2
Cnt3-U(1)-N(1)	89.3
Cnt3-U(1)-N(2)	138.6
Cnt3-U(1)-C(21)	114.1
Cnt1-U(1)-Cnt2	114.1
Cnt1-U(1)-Cnt3	112.6
Cnt2-U(1)-Cnt3	105.2
N(1)-U(1)-N(2)	53.37(6)
N(1)-U(1)-C(15)	129.63(7)
N(2)-U(1)-C(15)	77.91(7)
N(1)-U(1)-C(5)	87.88(6)
N(2)-U(1)-C(5)	103.07(7)
C(15)-U(1)-C(5)	118.02(7)
N(1)-U(1)-C(16)	68.21(6)

N(2)-U(1)-C(16)	113.54(6)
C(15)-U(1)-C(16)	133.40(7)
C(5)-U(1)-C(16)	103.59(7)
N(1)-U(1)-C(17)	70.40(6)
N(2)-U(1)-C(17)	123.72(6)
C(15)-U(1)-C(17)	153.70(7)
C(5)-U(1)-C(17)	74.61(7)
C(16)-U(1)-C(17)	29.16(7)
N(1)-U(1)-C(14)	155.49(7)
N(2)-U(1)-C(14)	107.01(7)
C(15)-U(1)-C(14)	29.25(7)
C(5)-U(1)-C(14)	112.97(7)
C(16)-U(1)-C(14)	116.00(7)
C(17)-U(1)-C(14)	125.99(7)
N(1)-U(1)-C(4)	117.37(6)
N(2)-U(1)-C(4)	119.58(7)
C(15)-U(1)-C(4)	95.87(7)
C(5)-U(1)-C(4)	29.49(6)
C(16)-U(1)-C(4)	113.15(7)
C(17)-U(1)-C(4)	86.04(7)
C(14)-U(1)-C(4)	84.16(7)
N(1)-U(1)-C(1)	77.31(6)
N(2)-U(1)-C(1)	74.84(6)
C(15)-U(1)-C(1)	104.00(7)
C(5)-U(1)-C(1)	29.32(6)
C(16)-U(1)-C(1)	122.57(7)
C(17)-U(1)-C(1)	96.78(7)
C(14)-U(1)-C(1)	114.36(7)
C(4)-U(1)-C(1)	48.14(6)
N(1)-U(1)-C(11)	108.19(7)
N(2)-U(1)-C(11)	66.37(7)
C(15)-U(1)-C(11)	28.80(7)
C(5)-U(1)-C(11)	144.48(7)
C(16)-U(1)-C(11)	111.74(7)
C(17)-U(1)-C(11)	140.25(7)
C(14)-U(1)-C(11)	47.31(7)

C(4)-U(1)-C(11)	124.66(7)
C(1)-U(1)-C(11)	122.19(7)
N(1)-U(1)-C(2)	98.99(6)
N(2)-U(1)-C(2)	73.26(6)
C(15)-U(1)-C(2)	75.56(7)
C(5)-U(1)-C(2)	47.92(6)
C(16)-U(1)-C(2)	150.48(7)
C(17)-U(1)-C(2)	122.29(7)
C(14)-U(1)-C(2)	86.95(7)
C(4)-U(1)-C(2)	47.64(6)
C(1)-U(1)-C(2)	28.84(6)
C(11)-U(1)-C(2)	97.40(7)
N(1)-U(1)-C(20)	95.18(6)
N(2)-U(1)-C(20)	129.34(7)
C(15)-U(1)-C(20)	108.42(7)
C(5)-U(1)-C(20)	115.52(7)
C(16)-U(1)-C(20)	28.66(6)
C(17)-U(1)-C(20)	47.35(7)
C(14)-U(1)-C(20)	87.46(7)
C(4)-U(1)-C(20)	109.87(7)
C(1)-U(1)-C(20)	142.79(7)
C(11)-U(1)-C(20)	94.88(7)
C(2)-U(1)-C(20)	157.31(7)
N(1)-U(1)-C(3)	124.55(6)
N(2)-U(1)-C(3)	99.78(6)
C(15)-U(1)-C(3)	70.57(7)
C(5)-U(1)-C(3)	47.87(6)
C(16)-U(1)-C(3)	141.44(7)
C(17)-U(1)-C(3)	114.83(7)
C(14)-U(1)-C(3)	68.68(7)
C(4)-U(1)-C(3)	28.81(6)
C(1)-U(1)-C(3)	47.49(6)
C(11)-U(1)-C(3)	98.75(7)
C(2)-U(1)-C(3)	28.59(6)
C(20)-U(1)-C(3)	130.26(7)
N(1)-U(1)-C(12)	112.02(7)

N(2)-U(1)-C(12)	88.00(7)
C(15)-U(1)-C(12)	47.46(7)
C(5)-U(1)-C(12)	159.98(7)
C(16)-U(1)-C(12)	86.68(7)
C(17)-U(1)-C(12)	113.21(7)
C(14)-U(1)-C(12)	47.19(7)
C(4)-U(1)-C(12)	130.56(7)
C(1)-U(1)-C(12)	150.01(7)
C(11)-U(1)-C(12)	28.39(7)
C(2)-U(1)-C(12)	122.76(7)
C(20)-U(1)-C(12)	66.64(7)
C(3)-U(1)-C(12)	114.33(7)
N(1)-U(1)-C(13)	137.89(7)
N(2)-U(1)-C(13)	112.69(7)
C(15)-U(1)-C(13)	47.25(7)
C(5)-U(1)-C(13)	133.08(7)
C(16)-U(1)-C(13)	89.30(7)
C(17)-U(1)-C(13)	106.79(7)
C(14)-U(1)-C(13)	28.41(7)
C(4)-U(1)-C(13)	103.99(7)
C(1)-U(1)-C(13)	142.45(7)
C(11)-U(1)-C(13)	46.55(7)
C(2)-U(1)-C(13)	115.34(7)
C(20)-U(1)-C(13)	61.80(7)
C(3)-U(1)-C(13)	95.48(7)
C(12)-U(1)-C(13)	28.28(7)
N(1)-U(1)-C(18)	98.32(6)
N(2)-U(1)-C(18)	151.51(6)
C(15)-U(1)-C(18)	130.36(7)
C(5)-U(1)-C(18)	69.01(7)
C(16)-U(1)-C(18)	47.25(7)
C(17)-U(1)-C(18)	28.54(6)
C(14)-U(1)-C(18)	101.13(7)
C(4)-U(1)-C(18)	67.16(7)
C(1)-U(1)-C(18)	97.68(7)
C(11)-U(1)-C(18)	135.58(7)

C(2)-U(1)-C(18)	113.17(7)
C(20)-U(1)-C(18)	46.77(7)
C(3)-U(1)-C(18)	94.39(7)
C(12)-U(1)-C(18)	108.49(7)
C(13)-U(1)-C(18)	90.20(7)
N(1)-U(1)-C(19)	113.76(6)
N(2)-U(1)-C(19)	157.77(7)
C(15)-U(1)-C(19)	107.15(7)
C(5)-U(1)-C(19)	93.66(7)
C(16)-U(1)-C(19)	47.14(7)
C(17)-U(1)-C(19)	47.02(7)
C(14)-U(1)-C(19)	79.02(7)
C(4)-U(1)-C(19)	81.94(7)
C(1)-U(1)-C(19)	122.98(7)
C(11)-U(1)-C(19)	107.40(7)
C(2)-U(1)-C(19)	128.90(7)
C(20)-U(1)-C(19)	28.45(7)
C(3)-U(1)-C(19)	102.31(7)
C(12)-U(1)-C(19)	80.66(7)
C(13)-U(1)-C(19)	62.74(7)
C(18)-U(1)-C(19)	28.18(7)
N(1)-U(1)-C(21)	26.74(6)
N(2)-U(1)-C(21)	26.66(6)
C(15)-U(1)-C(21)	103.62(7)
C(5)-U(1)-C(21)	96.93(6)
C(16)-U(1)-C(21)	90.48(6)
C(17)-U(1)-C(21)	97.06(6)
C(14)-U(1)-C(21)	131.93(7)
C(4)-U(1)-C(21)	123.13(6)
C(1)-U(1)-C(21)	75.26(6)
C(11)-U(1)-C(21)	86.59(7)
C(2)-U(1)-C(21)	86.52(6)
C(20)-U(1)-C(21)	113.26(6)
C(3)-U(1)-C(21)	115.11(6)
C(12)-U(1)-C(21)	100.17(7)
C(13)-U(1)-C(21)	128.34(7)

C(18)-U(1)-C(21)	125.05(6)
C(19)-U(1)-C(21)	137.62(6)
C(21)-N(1)-C(23)	121.76(19)
C(21)-N(1)-U(1)	96.64(13)
C(23)-N(1)-U(1)	140.96(14)
C(21)-N(2)-C(26)	122.53(19)
C(21)-N(2)-U(1)	95.78(13)
C(26)-N(2)-U(1)	140.66(14)
C(2)-C(1)-C(5)	108.15(19)
C(2)-C(1)-C(6)	125.4(2)
C(5)-C(1)-C(6)	125.6(2)
C(2)-C(1)-U(1)	77.12(13)
C(5)-C(1)-U(1)	74.33(13)
C(6)-C(1)-U(1)	122.93(15)
C(3)-C(2)-C(1)	108.1(2)
C(3)-C(2)-C(7)	124.2(2)
C(1)-C(2)-C(7)	125.9(2)
C(3)-C(2)-U(1)	75.94(13)
C(1)-C(2)-U(1)	74.04(12)
C(7)-C(2)-U(1)	128.22(16)
C(2)-C(3)-C(4)	108.40(19)
C(2)-C(3)-C(8)	124.3(2)
C(4)-C(3)-C(8)	125.1(2)
C(2)-C(3)-U(1)	75.47(13)
C(4)-C(3)-U(1)	73.80(12)
C(8)-C(3)-U(1)	130.14(15)
C(3)-C(4)-C(5)	107.75(19)
C(3)-C(4)-C(9)	123.0(2)
C(5)-C(4)-C(9)	127.6(2)
C(3)-C(4)-U(1)	77.40(13)
C(5)-C(4)-U(1)	74.28(12)
C(9)-C(4)-U(1)	125.99(15)
C(1)-C(5)-C(4)	107.58(19)
C(1)-C(5)-C(10)	123.7(2)
C(4)-C(5)-C(10)	127.6(2)
C(1)-C(5)-U(1)	76.34(13)

C(4)-C(5)-U(1)	76.22(13)
C(10)-C(5)-U(1)	123.29(15)
C(15)-C(11)-C(12)	108.8(2)
C(15)-C(11)-U(1)	73.37(13)
C(12)-C(11)-U(1)	76.92(14)
C(11)-C(12)-C(13)	107.4(2)
C(11)-C(12)-U(1)	74.69(14)
C(13)-C(12)-U(1)	76.16(14)
C(14)-C(13)-C(12)	108.6(2)
C(14)-C(13)-U(1)	73.29(13)
C(12)-C(13)-U(1)	75.56(13)
C(13)-C(14)-C(15)	107.7(2)
C(13)-C(14)-U(1)	78.30(13)
C(15)-C(14)-U(1)	74.24(13)
C(11)-C(15)-C(14)	107.5(2)
C(11)-C(15)-U(1)	77.83(13)
C(14)-C(15)-U(1)	76.51(13)
C(20)-C(16)-C(17)	107.9(2)
C(20)-C(16)-U(1)	77.69(13)
C(17)-C(16)-U(1)	75.65(13)
C(18)-C(17)-C(16)	107.9(2)
C(18)-C(17)-U(1)	78.32(13)
C(16)-C(17)-U(1)	75.19(13)
C(19)-C(18)-C(17)	108.1(2)
C(19)-C(18)-U(1)	75.98(13)
C(17)-C(18)-U(1)	73.14(13)
C(18)-C(19)-C(20)	108.1(2)
C(18)-C(19)-U(1)	75.84(13)
C(20)-C(19)-U(1)	74.90(13)
C(16)-C(20)-C(19)	108.0(2)
C(16)-C(20)-U(1)	73.66(13)
C(19)-C(20)-U(1)	76.65(13)
N(2)-C(21)-N(1)	114.10(19)
N(2)-C(21)-C(22)	122.5(2)
N(1)-C(21)-C(22)	123.4(2)
N(2)-C(21)-U(1)	57.56(11)

N(1)-C(21)-U(1)	56.63(11)
C(22)-C(21)-U(1)	177.39(17)
N(1)-C(23)-C(24)	114.6(2)
N(1)-C(23)-C(25)	115.28(19)
C(24)-C(23)-C(25)	111.2(2)
N(2)-C(26)-C(27)	113.9(2)
N(2)-C(26)-C(28)	116.6(2)
C(27)-C(26)-C(28)	109.4(2)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw49. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23
U(1)	12(1)	12(1)	8(1)	-2(1)
N(1)	19(1)	14(1)	9(1)	-2(1)
N(2)	20(1)	12(1)	10(1)	0(1)
C(1)	14(1)	15(1)	13(1)	-2(1)
C(2)	15(1)	17(1)	13(1)	-3(1)
C(3)	15(1)	19(1)	12(1)	-2(1)
C(4)	14(1)	17(1)	13(1)	-4(1)
C(5)	13(1)	17(1)	13(1)	-2(1)
C(6)	19(1)	21(1)	12(1)	-4(1)
C(7)	25(1)	19(1)	17(1)	1(1)
C(8)	20(1)	26(1)	12(1)	-3(1)
C(9)	21(1)	19(1)	16(1)	-5(1)
C(10)	18(1)	23(1)	14(1)	-1(1)
C(11)	18(1)	20(1)	16(1)	-3(1)
C(12)	14(1)	27(1)	16(1)	-3(1)
C(13)	18(1)	22(1)	14(1)	-3(1)
C(14)	21(1)	26(1)	10(1)	-5(1)
C(15)	19(1)	23(1)	10(1)	2(1)
C(16)	18(1)	16(1)	13(1)	-2(1)
C(17)	19(1)	14(1)	13(1)	0(1)
C(18)	24(1)	13(1)	17(1)	0(1)
C(19)	27(1)	15(1)	16(1)	-4(1)
C(20)	18(1)	19(1)	15(1)	-2(1)
C(21)	15(1)	16(1)	11(1)	-2(1)
C(22)	35(1)	15(1)	14(1)	-3(1)
C(23)	23(1)	15(1)	9(1)	-1(1)
C(24)	26(1)	22(1)	14(1)	-2(1)
C(25)	29(1)	23(1)	17(1)	-2(1)
C(26)	24(1)	13(1)	12(1)	0(1)
C(27)	31(1)	22(1)	17(1)	-1(1)
C(28)	33(1)	16(1)	22(1)	-2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for jrw49.

	x	y	z	U(eq)
H(6A)	11780(50)	6050(30)	6590(30)	38(10)
H(6B)	11060(40)	6800(30)	5920(30)	32(9)
H(6C)	10180(40)	5700(30)	6480(20)	27(8)
H(7A)	8640(40)	5190(30)	9160(20)	26(8)
H(7B)	10430(50)	5470(30)	9200(30)	35(9)
H(7C)	10140(40)	4950(30)	8320(30)	30(9)
H(8A)	9790(40)	7620(30)	10070(20)	29(8)
H(8B)	8230(40)	8550(30)	10110(20)	22(8)
H(8C)	8050(50)	7190(30)	10270(30)	33(9)
H(9A)	9620(40)	10630(30)	7920(30)	25(8)
H(9B)	8080(40)	10510(30)	8700(20)	24(8)
H(9C)	9820(40)	10100(30)	8920(30)	31(9)
H(10A)	11750(40)	9100(30)	6140(20)	30(9)
H(10B)	10240(40)	9010(30)	5690(20)	24(8)
H(10C)	10150(50)	10050(40)	6250(30)	47(11)
H(11)	3960(40)	5860(30)	8880(20)	24(8)
H(12)	2280(40)	7840(30)	8490(30)	31(9)
H(13)	3220(40)	9450(30)	9190(20)	27(8)
H(14)	5460(40)	8540(30)	9960(20)	22(8)
H(15)	6020(40)	6250(30)	9810(20)	23(8)
H(16)	4560(40)	9180(30)	5900(20)	17(7)
H(17)	7490(40)	9830(30)	5610(20)	15(7)
H(18)	7680(30)	10880(20)	7035(19)	9(6)
H(19)	4870(40)	10900(30)	8240(20)	27(8)
H(20)	2930(40)	9880(30)	7530(20)	21(7)
H(22A)	7460(40)	4230(30)	6070(20)	23(8)
H(22B)	7750(40)	5150(30)	5200(30)	31(9)
H(22C)	5930(50)	4860(30)	5700(30)	41(10)
H(23)	6890(40)	8470(30)	5010(20)	18(7)
H(24A)	9740(40)	7650(30)	4610(20)	30(8)

H(24B)	9200(40)	6450(30)	4370(20)	24(8)
H(24C)	8870(40)	7700(30)	3720(20)	22(7)
H(25A)	4730(40)	7210(30)	5060(20)	23(8)
H(25B)	5960(40)	6400(30)	4390(20)	24(8)
H(25C)	5570(40)	7810(30)	4050(20)	28(8)
H(26)	6250(30)	4650(30)	8630(20)	10(6)
H(27A)	3930(40)	4650(30)	7810(20)	23(8)
H(27B)	4580(40)	3450(30)	8340(30)	33(9)
H(27C)	5070(50)	3660(40)	7230(30)	41(10)
H(28A)	8950(50)	3870(40)	7580(30)	45(11)
H(28B)	7920(40)	3070(30)	8380(30)	29(8)
H(28C)	7840(50)	3030(40)	7300(30)	39(10)
