

[U{(SiMe₂NPh)₃-tacn}(OPPh₃)]

The compound was obtained as a dark red solid in quantitative yield by adding one equiv of OPPh₃ to a solution of [U{(SiMe₂NPh)₃-tacn}] in toluene.

¹H-NMR (C₆D₆, 20 °C) 7.40 (6H, *d*, H-o, OPPh₃); 6.97 (6H, *t*, H-m, OPPh₃), 6.58 (6H, H-m); 6.41 (3H, H-p); 6.07 (6H, CH₂); 5.44 (3H, *t*, H-p,OPPh₃); 3.27 (6H, *b*, H-o); -1.82 (6H, CH₂); -3.18 (18H, SiMe₂)

Dark red crystals of [U{(SiMe₂NPh)₃-tacn}(OPPh₃)]·2C₇H₈ were obtained from a concentrated solution of [U{(SiMe₂NPh)₃-tacn}(OPPh₃)] in toluene. The molecular structure is shown in Figure S1 and selected bond distances and angles are given in Table S1.

Data were collected at 110K on a Bruker APEX CCD area-detector diffractometer with graphite-monochromatized MoK_α radiation (λ=0.71069 Å) in the φ and ω scan mode.

The structure was solved by direct methods using SIR97²⁵ and refined by full-matrix least squares refinements on F² using SHELXL-97²⁴ and the winGX software package.²⁶

All non-hydrogen atoms were refined with anisotropic thermal motion parameters, and the hydrogen atoms were assigned idealized positions based on the geometries of their attached carbon atoms. The drawing was made with ORTEP 3.²⁷ A summary of the crystallographic data is given in Table S2.

CCDC reference 299439.

Table S1. Selected bond lengths [\AA] and angles (deg.) for

$[\text{U}\{(\text{SiMe}_2\text{NPh})_3\text{-tacn}\}(\text{OPPh}_3)]\cdot 2\text{C}_7\text{H}_8$

U-N(1)	2.454(3)
U-N(2)	2.468(3)
U-N(3)	2.436(2)
U-N(4)	2.762(3)
U-N(5)	2.785(3)
U-N(6)	2.750(3)
U-O	2.483(2)
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N(1)-U-N(2)	120.56(9)
N(1)-U-N(3)	117.35(9)
N(2)-U-N(3)	118.43(9)
O-U-N(1)	84.36(8)
O-U-N(2)	83.79(8)
O-U-N(3)	82.69(8)

Table S2. Crystallographic Data

	[U{(SiMe ₂ NPh) ₃ -tacn}(OPPh ₃)]·2C ₇ H ₈
Formula	C ₆₂ H ₇₆ N ₆ Si ₃ OPU
fw	1274.56
crystal syst	orthorhombic
space group	P212121
<i>a</i> , Å	12.2797(4)
<i>b</i> , Å	17.8483(6)
<i>c</i> , Å	27.1851(8)
<i>V</i> , Å ³	5958.2(3)
<i>Z</i>	4
ρ _{calc} , gcm ⁻³	1.421
Crystal size, mm ³	0.28x0.18x0.14
μ(MoKα), mm ⁻¹	2.857
Theta range, °	1.82 to 34.41
Measured reflections	70126
Independent reflections [R(int)]	24465 (0.0590)
Observed reflections	18480
[I>2σ(I)]	
R ₁	0.0481
wR ₂	0.0628

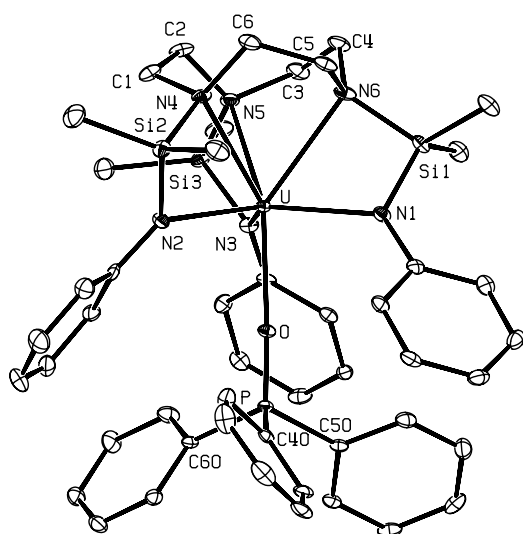


Fig S1 - ORTEP diagram of [U{(SiMe₂NPh)₃-tacn}(OPPh₃)] using 40 % probability ellipsoids