Reactivity of $(C_5Me_5)Lu(CH_2SiMe_3)_2(THF)$ with Pyridine Ring Systems: Synthesis and Structural Characterization of a η^2-(N,C)-Pyridyl (Mono)pentamethylcyclopentadienyl Lutetium(III) Complex

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SUPPORTING INFORMATION

General Procedures and Considerations.

Methods and Materials. Reactions and manipulations were performed at 21 °C in a recirculating MBraun 150 B-G nitrogen atmosphere drybox, or using standard Schlenk and high vacuum line techniques. Glassware was dried at 150 °C before use. All NMR spectra were obtained using a Bruker Avance 300 MHz spectrometer. ^{1}H, ^{2}H, ^{13}C{^{1}H}, DEPT-135 and two-dimensional ^{13}C{^{1}H}-^{1}H NMR spectra were collected in either benzene-d_6 or toluene-d_8 as specified below. Chemical shifts were referenced to the protio solvent impurity in benzene-d_6 at δ 7.15 ppm or toluene-d_8 at δ 2.09 ppm (^{1}H NMR) and δ 20.4 ppm (^{13}C{^{1}H} NMR). ^{1}H and ^{13}C NMR assignments were confirmed through the use of DEPT-135 and two-dimensional ^{13}C{^{1}H}-^{1}H NMR experiments. All ^{2}H NMR spectra were referenced to external toluene-d_8 at δ 2.09 (^{1}H).

Unless otherwise noted, reagents were purchased from commercial suppliers and used without further purification. Celite (Aldrich) and alumina (Brockman I, Aldrich) were dried under reduced pressure at 250 °C for 48 h prior to use. Anhydrous toluene (Aldrich), hexanes (Aldrich), tetrahydrofuran (Aldrich), pyridine (Aldrich), pyridine-d_5 (Aldrich), benzene-d_6 (Aldrich) and toluene-d_8 (Cambridge Isotope Laboratories) were passed through a column of activated alumina under nitrogen and stored over 4 Å activated molecular sieves prior to use. Pyridine-d_1 (CDN Isotopes) was stored over 4 Å activated molecular sieves prior to use. Ferrocene (Acros) was purified by recrystallization from toluene at –35 °C. $Lu(CH_2SiMe_3)_3(THF)_2$[1] and $(C_5Me_5)Lu(CH_2SiMe_3)_2(THF)$ (**1**)[2] were prepared according to literature procedures. X-ray data were collected and the structures solved at the Los Alamos National Laboratory X-ray facility.

Synthesis of $(C_5Me_5)Lu(NC_5H_5)_2(CH_2SiMe_3)_2$ (2). A 50 mL side-arm flask equipped with a stir bar was charged with **1** (0.394 g, 0.71 mmol) and hexanes (20 mL). To the clear, colorless solution pyridine (0.12 g, 0.12 mL, 0.98 g/mL, 1.49 mmol) was added drop-wise with stirring. The reaction mixture immediately turned bright yellow in color and was stirred at ambient temperature for 1 min. The volatiles were removed under reduced pressure to give **2** as a pale yellow powder (0.334 g, 0.52mmol, 73 %). Crystals suitable for X-ray diffraction analysis were obtained overnight from a concentrated hexanes solution at –35 °C. ^{1}H NMR (benzene-d_6, 298 K): δ 8.28 (m, 4H, ortho *H*), 6.83 (m, 2H, para *H*), 6.56 (m, 4H, meta *H*), 1.96 (s, 15H, C_5Me_5), 0.25 (s, 18H, CH_2SiMe_3), -0.63 (s, 4H, CH_2SiMe_3). ^{1}H NMR (toluene-d_8, 248 K): δ 8.38 (m, 4H,

ortho *H*), 6.77 (m. 2H, para *H*), 6.51 (m, 4H, meta *H*), 1.92 (s, 15H, C_5Me_5), 0.26 (s, 18H, CH_2SiMe_3), -0.65 (s, 4H, CH_2SiMe_3). $^{13}C\{^1H\}$ NMR (toluene-d_8, 248 K): δ 148.82 (s, ortho *C*), 138.82 (s, para *C*), 124.32 (s, meta *C*), 116.52 (s, C_5Me_5), 38.70 (s, CH_2SiMe_3), 11.46 (s, C_5Me_5), 4.79 (s, CH_2SiMe_3).

Synthesis of $(C_5Me_5)Lu(NC_5H_5)_2(CH_2SiMe_3)_2(THF)$ (2·THF). This compound was not isolable as loss of the bound THF occurred upon removal of the solvent under reduced pressure. Complex **2·THF** was generated by charging a 20 mL scintillation vial with **1** (0.024 g, 0.043 mmol), toluene-d_8 (0.4 mL), and pyridine (7.1 mg, 7.3 μL, 0.98 g/mL, 0.091 mmol). The reaction mixture immediately turned bright yellow in color upon addition of pyridine. After 1 min of standing at ambient temperature, a toluene-d_8 solution (0.4 mL) of ferrocene (0.008 g, 0.043 mmol) was added as an internal standard. The resultant reaction mixture was loaded into a NMR tube. A ^1H NMR spectrum was collected 12 min after addition of pyridine to **1**, and the yield of **2·THF** was determined as >95 % (based on internal standard). The following NMR data are reported without added ferrocene. ^1H NMR (toluene-d_8, 298 K): δ 8.50 (m, 4H, ortho *H*), 7.03 (m, 2H, para *H*), 6.74 (m, 4H, meta *H*), 3.55 (m, 4H, α THF *H*), 1.88 (s, 15H, C_5Me_5), 1.48 (m, 4H, β THF *H*), 0.14 (s, 18H, CH_2SiMe_3), -0.75 (s, 4H, CH_2SiMe_3). ^1H NMR (toluene-d_8, 243 K): δ 8.75 (m, 4H, ortho *H*), 6.88 (m, 2H, para *H*), 6.64 (m, 4H, meta *H*), 3.56 (m, 4H, α THF *H*), 1.81 (s, 15H, C_5Me_5), 1.42 (m, 4H, β THF *H*), 0.21 (s, 18H, CH_2SiMe_3), -0.71 (s, 4H, CH_2SiMe_3). $^{13}C\{^1H\}$ NMR (toluene-d_8, 243 K): δ 150.46 (s, ortho *C*), 137.54 (s, para *C*), 123.70 (s, meta *C*), 115.83 (s, C_5Me_5), 67.73 (s, α THF *C*), 36.57 (s, CH_2SiMe_3), 25.63 (s, β THF *C*), 11.70 (s, C_5Me_5), 5.03 (s, CH_2SiMe_3).

Synthesis of $(C_5Me_5)Lu(\eta^2\text{-}(N,C)\text{-}NC_5H_5)(CH_2SiMe_3)(NC_5H_5)$ (3). A 20 mL scintillation vial equipped with a stir bar was charged with **1** (0.214 g, 0.42 mmol), pentane (5 ml) and toluene (3 mL). To the clear, colorless solution pyridine (0.07 g, 0.07 mL, 0.98 g/mL, 0.88 mmol) was added by syringe. The reaction mixture immediately turned bright yellow in color and was stirred at ambient temperature for 5 min and then allowed to stand for 21 hrs. After this time the reaction vial was placed in a –35 °C freezer and orange block-shaped crystals of **3** suitable for X-ray analysis were grown overnight.

Synthesis of $(C_5Me_5)Lu(\eta^2\text{-}(N,C)\text{-}NC_5H_5)(CH_2SiMe_3)(NC_5H_5)(THF)$ (3·THF). This compound was not isolable as decomposition occurred upon removal of the solvent under

reduced pressure. Complex **3·THF** was generated by charging a 20 mL scintillation vial with **1** (0.036 g, 0.065 mmol) and toluene-d_8 (0.4 mL). To the clear, colorless solution pyridine (11 mg, 11 μL, 0.98 g/mL, 0.14 mmol) was added by syringe. The reaction mixture immediately turned bright yellow in color. After 1 min of standing at ambient temperature, a toluene-d_8 solution (0.4 mL) of ferrocene (0.012 g, 0.065 mmol) was added as an internal standard. The resultant reaction mixture was loaded into an NMR tube. Over a period of 21 h, the reaction mixture turned dark orange in color and the yield of **3·THF** was determined as 64 % (based on internal standard. The following NMR data are reported without added ferrocene. ^{1}H NMR (toluene-d_8, 298 K): δ 8.56 (br s, 2H, ortho *H*), 8.47 (dt, 1H, 5.2 Hz, 1.4 Hz, Ar *H*), 7.95 (dt, 1H, 7.4 Hz, 1.4 Hz, Ar *H*), 7.16 (td, 1H, 7.4 Hz, 1.4 Hz, Ar *H*), 6.95 (br m, 1H, para *H*), 6.72 (ddd, 1H, 7.4 Hz, 5.2 Hz, 1.4 Hz, Ar *H*), 6.68 (br m, 2H, meta *H*), 3.56 (m, 4H, α THF *H*), 1.92 (s, 15H, C_5Me_5), 1.45 (m, 4H, β THF *H*), -0.07 (s, 9H, CH_2SiMe_3), -0.69 (s, 2H, CH_2SiMe_3). ^{1}H NMR (toluene-d_8, 248 K): δ 8.56 (m, 2H, ortho *H*), 8.45 (m, 1H, Ar *H*), 8.01 (m, 1H, Ar *H*), 7.16 (m, 1H, Ar *H*), 6.84 (m, 1H, para *H*), 6.69 (m, 1H, Ar *H*), 6.59 (m, 2H, meta *H*), 3.55 (m, 4H, α THF *H*), 1.95 (s, 15H, C_5Me_5), 1.43 (m, 4H, β THF *H*), 0.02 (s, 9H, CH_2SiMe_3), -0.72 (s, 2H, CH_2SiMe_3). ^{13}C{^{1}H} NMR (toluene-d_8, 248 K): δ 149.88 (s, ortho *C*), 145.26 (s, Ar *H*), 137.72 (s, para *C*), 132.96 (s, Ar *C*), 131.62 (s, Ar *C*), 123.81 (s, meta *C*), 121.39 (s, Ar *C*), 115.66 (s, quat Ar *C*), 114.98 (s, C_5Me_5), 67.79 (s, α THF *C*), 36.62 (s, CH_2SiMe_3), 25.60 (s, β THF *C*), 11.22 (s, C_5Me_5), 4.14 (CH_2SiMe_3).

Reaction of Complex 1 with Pyridine-d_5 in Toluene-d_8. An NMR tube was charged with **1** (0.019 g, 0.034 mmol), pyridine-d_5 (6.0 mg, 5.7 μL, 1.1 g/mL, 0.072 mmol), and toluene-d_8 (0.5 mL). The reaction mixture immediately turned bright yellow in color. After 30 min at ambient temperature, the ^{1}H NMR spectrum was recorded and displayed resonances consistent with the formation of the bis(η^1-pyridyl) complex, $(C_5Me_5)Lu(CH_2SiMe_3)_2(NC_5D_5)_2(THF)$ (**2·THF-d_{10}**). ^{1}H NMR (298 K): δ 3.55 (m, 4H, α THF *H*), 1.94 (s, 15H, C_5Me_5), 1.45 (m, 4H, β THF *H*), 0.21 (s, 18H, CH_2SiMe_3), -0.69 (s, 4H, CH_2SiMe_3). Upon standing at ambient temperature, the reaction mixture darkened to a brownish-orange color and resonances consistent with the formation of $SiMe_3CH_2D$ were apparent after 1 d. ^{1}H NMR (298 K): δ 0.00 (s, $SiMe_3CH_2D$), -0.02 (t, 2.0 Hz, $SiMe_3CH_2D$). Complete conversion to the η^2-pyridyl complex, $(C_5Me_5)Lu[\eta^2$-(N,C)-$NC_5D_4](CH_2SiMe_3)(NC_5D_5)(THF)$ (**3·THF-d_9**), was not observed even after 11 d at

ambient temperature, due to the instability of **3·THF-*d*$_9$**. ^{1}H NMR of **3·THF-*d*$_9$** (toluene-d_8, 298 K): δ 3.55 (m, 4H, α THF *H*), 1.90 (s, 15H, C_5Me_5), 1.46 (m, 4H, β THF *H*), -0.07 (s, 9H, CH_2SiMe_3), -0.71 (s, 2H, CH_2SiMe_3).

Reaction of complex 1 with pyridine-*d*$_5$ in toluene. An NMR tube was charged with **1** (0.019 g, 0.034 mmol), pyridine-d_5 (6.0 mg, 5.7 μL, 1.1 g/mL, 0.072 mmol), and toluene (0.5 mL). The reaction mixture immediately turned bright yellow in color. Upon standing at ambient temperature, the reaction mixture darkened to a brownish-orange color and ^{2}H NMR resonances consistent with the formation of $SiMe_3CH_2D$ were apparent after 1 d. ^{2}H NMR (298 K): δ 0.21 (t, 1D, 2.0 Hz, $SiMe_3CH_2D$).

Reaction of complex 3·THF with pyridine-*d*$_5$ in toluene-*d*$_8$. An NMR tube was charged with **1** (0.020 g, 0.036 mmol), pyridine (5.9 mg, 6 μL, 0.98 g/mL, 0.075 mmol), and toluene-d_8 (0.5 mL). The reaction mixture was allowed to stand at ambient temperature for 21 h to generate complex **3·THF**, then pyridine-d_5 (61 mg, 58 μL, 1.1 g/mL, 0.72 mmol) was added by syringe. Approximately 10 min after the addition of pyridine-d_5, resonances consistent with the formation of pyridine-2-d_1, pyridine and $(C_5Me_5)Lu[\eta^2\text{-}(N,C)\text{-}NC_5D_5](CH_2SiMe_3)(NC_5D_5)(THF)$ (**3·THF-*d*$_9$**) were evident. ^{1}H NMR of **3·THF-*d*$_9$** (toluene-d_8, 298 K): δ 3.55 (m, 4H, α THF *H*), 1.90 (s, 15H, C_5Me_5), 1.46 (m, 4H, β THF *H*), -0.07 (s, 9H, CH_2SiMe_3), -0.71 (s, 2H, CH_2SiMe_3).

Figure S1. ^{1}H NMR spectrum of **2** in benzene-d_6 recorded at 298 K.

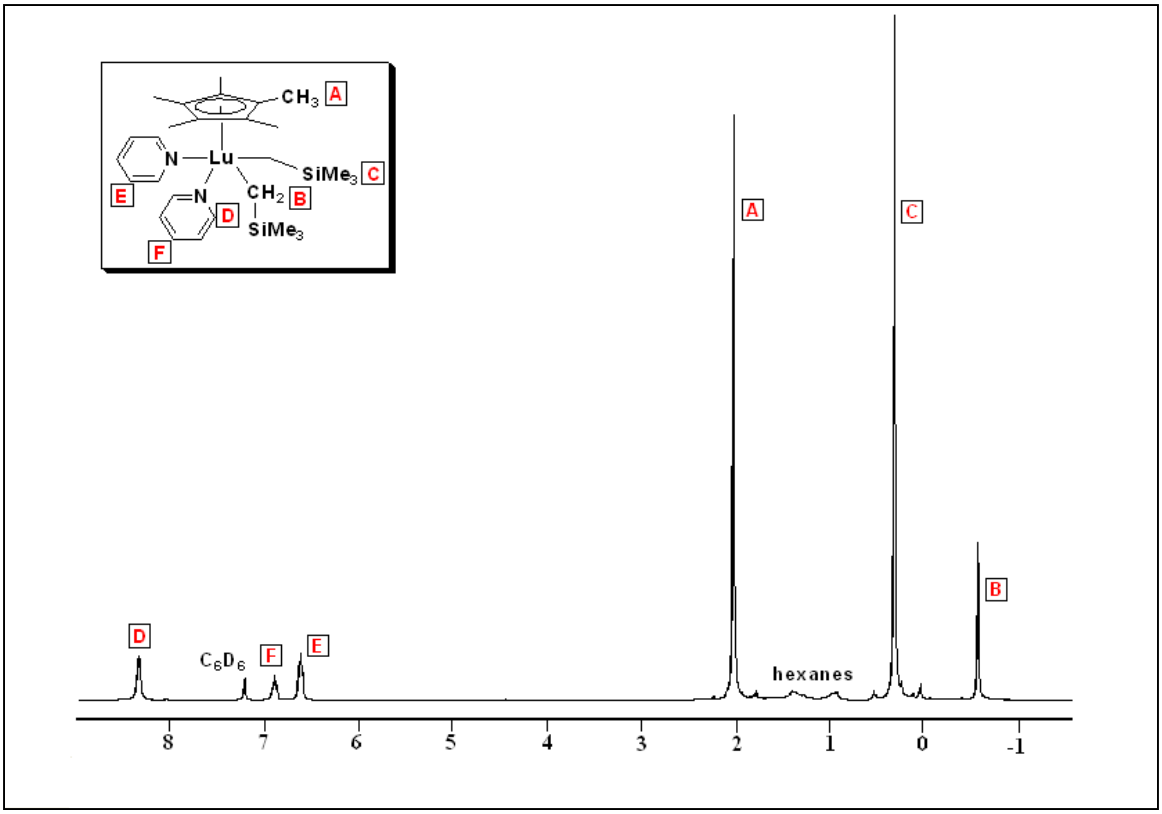


Figure S2. ^{1}H NMR spectrum of **2·THF** in toluene-d_8 recorded at 298 K.

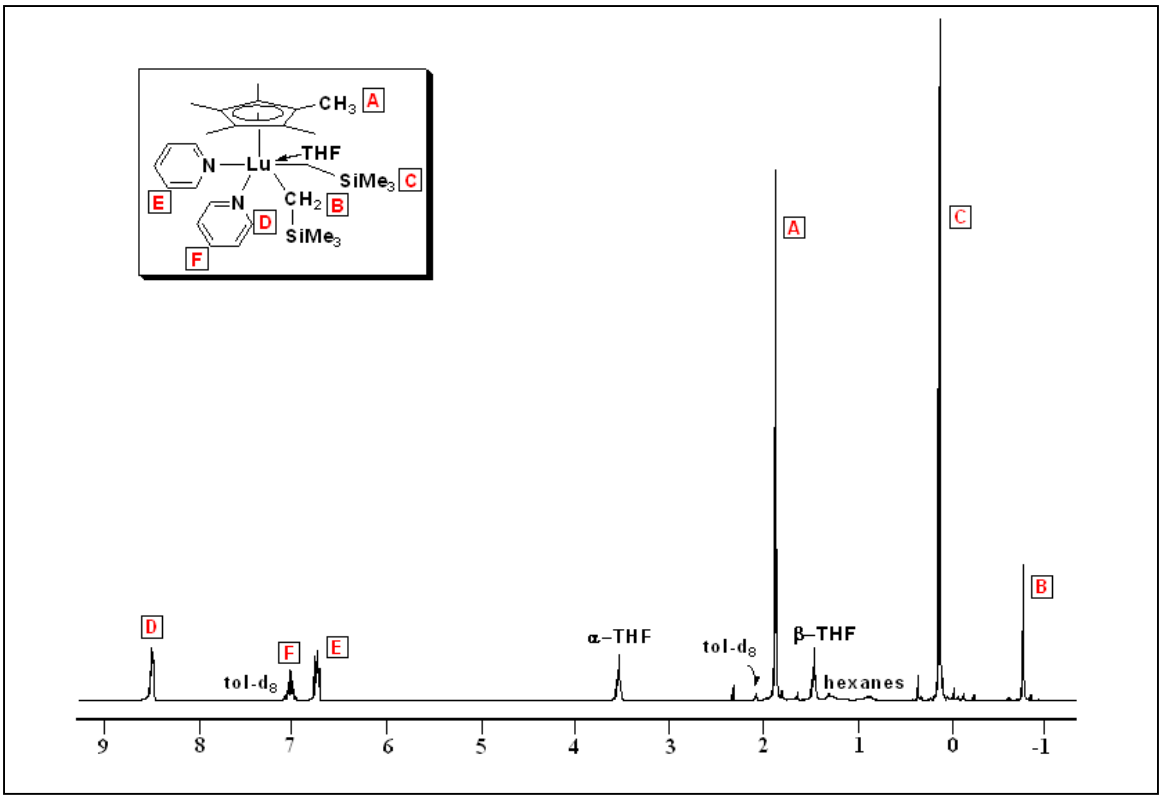


Figure S3. ^{1}H NMR spectrum of **3·THF** in toluene-d_8 recorded at 298 K.

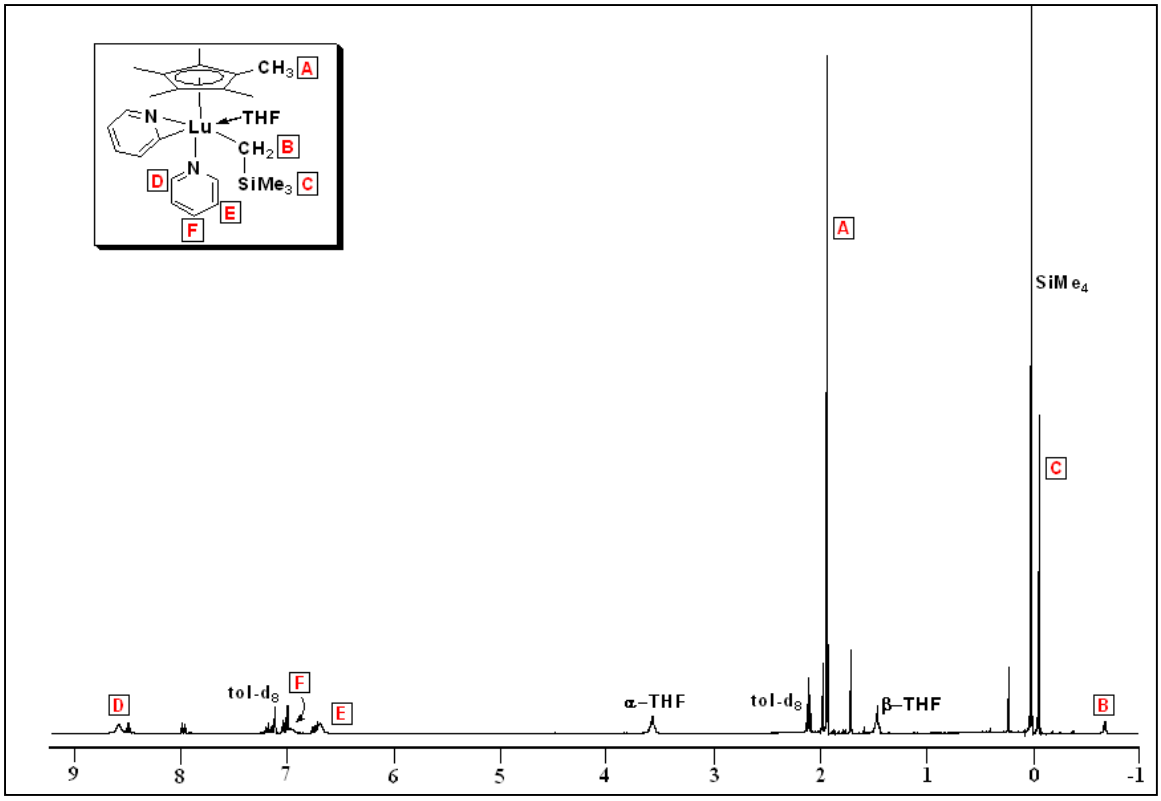
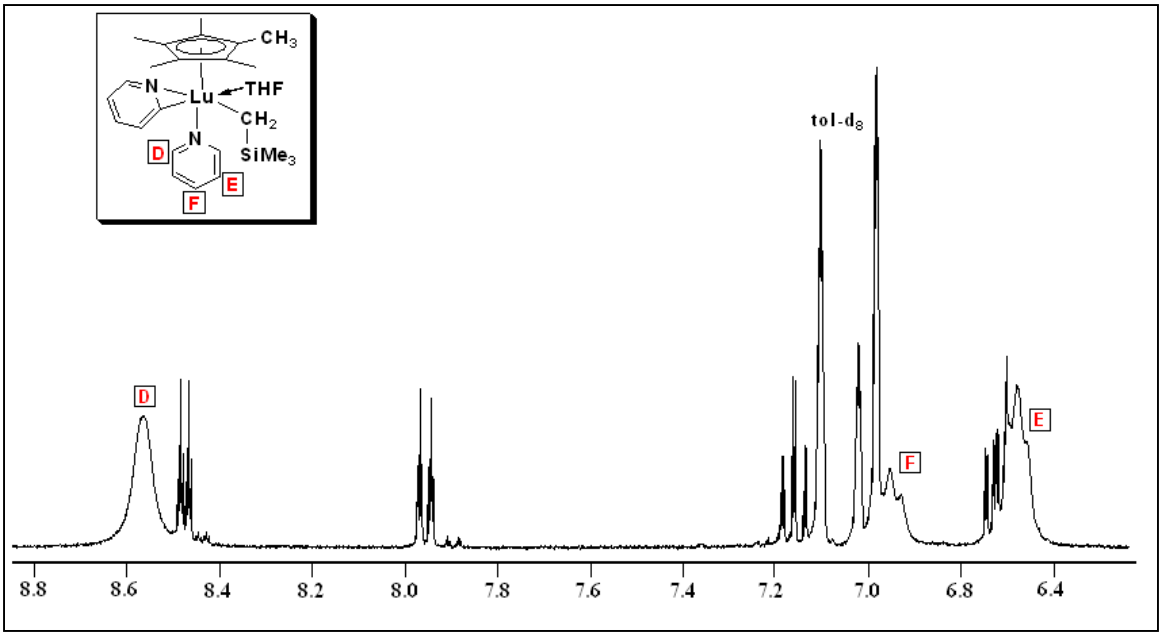


Figure S4. Expanded view of the ^{1}H NMR spectrum of **3·THF** in toluene-d_8 recorded at 298 K.



Crystallographic Details for $(C_5Me_5)Lu(NC_5H_5)_2(CH_2SiMe_3)_2$ (2). A yellow crystal grown from concentrated hexanes solution of **2** at –35 °C was mounted from Paratone N oil (Hampton Research) onto a glass fiber under argon gas flow and placed on a Bruker P4/CCD diffractometer, equipped with a Bruker LT-2 temperature device. A hemisphere of data was collected using φ scans, with 30 s frame exposures, and 0.3° frame widths. Data collection and initial indexing and cell refinement were handled using SMART[3] software. Frame integration and final cell parameter calculations were carried out using SAINT[4] software. The data were corrected for absorption using the SADABS program.[5] Decay of reflection data was monitored by analysis of redundant frames. The structure was solved using direct methods, completed by subsequent difference Fourier techniques, and refined by full-matrix least-squares procedures. One of the C_5Me_5 ligands, C29 to C38, was disordered and subsequently refined as two one-half occupancy C_5Me_5 groups (C29 to C38 and C29' to C38'). Each C_5Me_5 was constrained to be rigid with fixed C-C bond distances. In addition, several methyl groups and one pyridine carbon atom were disordered and refined anisotropically as two one-half occupancy positions (C24/C24', C26/C26', C27/C27', C46/C46', and C54/C54'). The anisotropic temperature factors were constrained to be equivalent on corresponding disordered atoms. Hydrogen atom positions were not included on any of the disordered positions. Structure solution, refinement, and creation of publication materials were performed using SHELXTL.[6] The figure was made using ORTEP-3.[7]

Table S1. Crystal data and Structure Refinement for Complex 2.

Identification code	kj2101c1	
Empirical formula	$C_{28}H_{47}N_2LuSi_2$	
Formula weight	642.82 g/mol	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 16.225(3) Å	
	b = 11.999(3) Å	β = 97.654(4) °
	c = 32.866(6)Å	
Volume	6342(2) $Å^3$	
Z	8	
Density (calculated)	1.491 g cm^{-3}	
Absorption coefficient	3.214 mm^{-1}	
F(000)	2888	
Crystal size	0.1 × 0.4 × 0.5 mm^3	
Theta range for data collection	1.34 to 28.31°	
Index ranges	$-21 \le h \le 20$, $-15 \le k \le 15$, $-35 \le l \le 43$	
Reflections collected	62084	
Independent reflections	13658 (R_{int} = 0.0914)	
Max. and min. transmission	0.7393 and 0.2964	
Refinement method	full-matrix least-squares on F^2	
Data/restraints/parameters	13658/24/582	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2σ(I)]	R1 = 0.0705, wR2 = 0.1598	
R indices (all data)	R1 = 0.1176 , wR2 = 0.1799	
Largest diff. peak and hole	2.062 and -1.857 e.$Å^{-3}$	

Table S2. Bond lengths (Å) for 2.

Lu(1)-C(25)	2.398(9)	C(29)-C(29')	0.8537
Lu(1)-C(21)	2.406(11)	C(29)-C(30)	1.4200
Lu(1)-N(2)	2.505(9)	C(29)-C(33)	1.4200
Lu(1)-N(1)	2.506(8)	C(29)-C(34)	1.5095
Lu(1)-C(2)	2.676(6)	C(29)-C(38')	1.7093
Lu(1)-C(3)	2.677(6)	C(29)-C(32')	1.8117
Lu(1)-C(1)	2.686(5)	C(29)-C(30')	1.8848
Lu(1)-C(4)	2.687(6)	C(30)-C(30')	0.6514
Lu(1)-C(5)	2.693(5)	C(30)-C(29')	0.7138
Lu(2)-C(53)	2.375(10)	C(30)-C(31)	1.4200
Lu(2)-C(49)	2.408(11)	C(30)-C(35)	1.5095
Lu(2)-N(4)	2.479(9)	C(30)-C(31')	1.7978
Lu(2)-N(3)	2.534(9)	C(30)-C(33')	1.8744
Lu(2)-C(32')	2.595(6)	C(30)-C(34')	1.9106
Lu(2)-C(33')	2.626(7)	C(30)-C(35')	1.9719
Lu(2)-C(31')	2.631(7)	C(31)-C(31')	0.6481
Lu(2)-C(30')	2.663(6)	C(31)-C(30')	0.8377
Lu(2)-C(29)	2.664(6)	C(31)-C(32)	1.4200
Lu(2)-C(29')	2.666(6)	C(31)-C(36)	1.5095
Lu(2)-C(33)	2.671(7)	C(31)-C(36')	1.5654
Lu(2)-C(30)	2.707(6)	C(31)-C(32')	1.7801
N(1)-C(20)	1.299(13)	C(31)-C(35')	1.8913
N(1)-C(16)	1.332(12)	C(31)-C(29')	1.9884
N(2)-C(15)	1.302(12)	C(32)-C(32')	0.6862
N(2)-C(11)	1.321(14)	C(32)-C(31')	0.7857
N(3)-C(43)	1.303(16)	C(32)-C(33)	1.4200
N(3)-C(39)	1.342(14)	C(32)-C(37)	1.5095
N(4)-C(48)	1.315(14)	C(32)-C(30')	2.0003
N(4)-C(44)	1.339(13)	C(32)-C(33')	2.0135
Si(1)-C(24')	1.70(7)	C(33)-C(32')	0.7355
Si(1)-C(21)	1.826(12)	C(33)-C(33')	0.8556
Si(1)-C(22)	1.865(16)	C(33)-C(37')	1.4806
Si(1)-C(23)	1.911(19)	C(33)-C(38)	1.5095
Si(1)-C(24)	1.96(5)	C(33)-C(31')	1.8845
Si(2)-C(26)	1.78(7)	C(34)-C(38')	0.9115
Si(2)-C(25)	1.823(10)	C(34)-C(33')	1.7898
Si(2)-C(27')	1.90(6)	C(34)-C(29')	1.9014
Si(2)-C(27)	1.90(8)	C(35)-C(34')	1.1968
Si(2)-C(28)	1.908(18)	C(35)-C(29')	1.7669
Si(2)-C(26')	1.95(4)	C(35)-C(35')	1.8002
Si(3)-C(53)	1.843(10)	C(35)-C(30')	1.8083
Si(3)-C(56)	1.847(17)	C(36)-C(36')	0.8169
Si(3)-C(54')	1.86(5)	C(36)-C(35')	1.5939

Si(3)-C(55)	1.880(15)	C(36)-C(31')	1.9036
Si(3)-C(54)	1.99(7)	C(36)-C(30')	1.9734
Si(4)-C(49)	1.831(11)	C(37)-C(32')	1.9730
Si(4)-C(50)	1.856(19)	C(37)-C(31')	2.0169
Si(4)-C(51)	1.890(16)	C(38)-C(37')	0.8055
Si(4)-C(52)	1.93(2)	C(38)-C(33')	1.9888
C(1)-C(2)	1.4200	C(38)-C(32')	2.0126
C(1)-C(5)	1.4200	C(29')-C(30')	1.3244
C(1)-C(6)	1.5095	C(29')-C(33')	1.4328
C(2)-C(3)	1.4200	C(29')-C(34')	1.6768
C(2)-C(7)	1.5095	C(30')-C(31')	1.3475
C(3)-C(4)	1.4200	C(30')-C(35')	1.5956
C(3)-C(8)	1.5095	C(31')-C(32')	1.2537
C(4)-C(5)	1.4200	C(31')-C(36')	1.6743
C(4)-C(9)	1.5095	C(32')-C(33')	1.4108
C(5)-C(10)	1.5095	C(32')-C(37')	1.7035
C(11)-C(12)	1.40(2)	C(33')-C(38')	1.6584
C(12)-C(13)	1.30(2)	C(39)-C(40)	1.34(2)
C(13)-C(14)	1.34(2)	C(40)-C(41)	1.41(3)
C(14)-C(15)	1.370(18)	C(41)-C(42)	1.35(2)
C(16)-C(17)	1.339(17)	C(42)-C(43)	1.40(2)
C(17)-C(18)	1.342(19)	C(44)-C(45)	1.39(2)
C(18)-C(19)	1.32(2)	C(45)-C(46)	1.23(8)
C(19)-C(20)	1.37(2)	C(45)-C(46')	1.69(10)
C(24)-C(24')	0.52(16)	C(46)-C(47)	1.43(10)
C(26)-C(26')	0.62(9)	C(47)-C(46')	1.17(11)
C(27)-C(27')	0.77(9)	C(47)-C(48)	1.39(2)
C(29)-C(33')	0.6307	C(54)-C(54')	0.53(11)

Table S3. Bond Angles (°) for 2.

C(25)-Lu(1)-C(21)	137.1(4)	C(31)-C(32)-C(30')	20.7
C(25)-Lu(1)-N(2)	84.2(3)	C(33)-C(32)-C(30')	87.4
C(21)-Lu(1)-N(2)	86.8(3)	C(37)-C(32)-C(30')	146.5
C(25)-Lu(1)-N(1)	81.1(3)	C(32')-C(32)-C(33')	23.5
C(25)-Lu(1)-N(1)	81.1(3)	C(31')-C(32)-C(33')	93.3
C(21)-Lu(1)-N(1)	84.1(3)	C(31)-C(32)-C(33')	87.0
N(2)-Lu(1)-N(1)	146.9(3)	C(33)-C(32)-C(33')	21.0
C(25)-Lu(1)-C(2)	93.4(3)	C(37)-C(32)-C(33')	147.0
C(21)-Lu(1)-C(2)	127.5(3)	C(30')-C(32)-C(33')	66.4
N(2)-Lu(1)-C(2)	85.13(13)	C(32')-C(32)-Lu(2)	72.4(2)
N(1)-Lu(1)-C(2)	125.10(14)	C(31')-C(32)-Lu(2)	75.2(2)
C(25)-Lu(1)-C(3)	123.0(3)	C(31)-C(32)-Lu(2)	75.8(2)
C(21)-Lu(1)-C(3)	96.7(3)	C(33)-C(32)-Lu(2)	72.9(2)
N(2)-Lu(1)-C(3)	81.16(12)	C(37)-C(32)-Lu(2)	117.4(2)
N(1)-Lu(1)-C(3)	131.45(12)	C(30')-C(32)-Lu(2)	66.7(2)
C(2)-Lu(1)-C(3)	30.77(6)	C(33')-C(32)-Lu(2)	65.4(2)
C(25)-Lu(1)-C(1)	88.5(3)	C(32')-C(33)-C(33')	124.7
C(21)-Lu(1)-C(1)	132.8(3)	C(32')-C(33)-C(29)	110.3
N(2)-Lu(1)-C(1)	114.76(14)	C(33')-C(33)-C(29)	14.7
N(1)-Lu(1)-C(1)	94.39(14)	C(32')-C(33)-C(32)	2.7
C(2)-Lu(1)-C(1)	30.71(6)	C(33')-C(33)-C(32)	122.5
C(3)-Lu(1)-C(1)	50.73(8)	C(29)-C(33)-C(32)	108.0
C(25)-Lu(1)-C(4)	139.0(3)	C(32')-C(33)-C(37')	94.4
C(21)-Lu(1)-C(4)	83.5(3)	C(33')-C(33)-C(37')	140.2
N(2)-Lu(1)-C(4)	107.94(14)	C(29)-C(33)-C(37')	153.2
N(1)-Lu(1)-C(4)	102.52(14)	C(32)-C(33)-C(37')	96.4
C(2)-Lu(1)-C(4)	50.73(8)	C(32')-C(33)-C(38)	123.7
C(3)-Lu(1)-C(4)	30.70(6)	C(33')-C(33)-C(38)	111.5
C(1)-Lu(1)-C(4)	50.63(8)	C(29)-C(33)-C(38)	126.0
C(25)-Lu(1)-C(5)	113.8(3)	C(32)-C(33)-C(38)	126.0
C(21)-Lu(1)-C(5)	103.5(3)	C(37')-C(33)-C(38)	31.2
N(2)-Lu(1)-C(5)	131.30(12)	C(32')-C(33)-C(31')	24.6
N(1)-Lu(1)-C(5)	81.77(12)	C(33')-C(33)-C(31')	100.2
C(2)-Lu(1)-C(5)	50.67(8)	C(29)-C(33)-C(31')	85.7
C(3)-Lu(1)-C(5)	50.67(8)	C(32)-C(33)-C(31')	22.3
C(1)-Lu(1)-C(5)	30.61(6)	C(37')-C(33)-C(31')	118.6
C(4)-Lu(1)-C(5)	30.61(6)	C(38)-C(33)-C(31')	148.3
C(53)-Lu(2)-C(49)	112.7(4)	C(32')-C(33)-Lu(2)	76.2(2)
C(53)-Lu(2)-N(4)	85.0(3)	C(33')-C(33)-Lu(2)	77.8(2)
C(49)-Lu(2)-N(4)	84.9(3)	C(29)-C(33)-Lu(2)	74.3(2)
C(53)-Lu(2)-N(3)	84.1(3)	C(32)-C(33)-Lu(2)	76.6(2)
C(49)-Lu(2)-N(3)	82.0(3)	C(37')-C(33)-Lu(2)	123.3(2)
N(4)-Lu(2)-N(3)	158.0(3)	C(38)-C(33)-Lu(2)	115.3(2)
C(53)-Lu(2)-C(32')	115.2(3)	C(31')-C(33)-Lu(2)	68.0(2)

C(49)-Lu(2)-C(32')	124.3(4)	C(38')-C(34)-C(29)	86.1
N(4)-Lu(2)-C(32')	125.32(16)	C(38')-C(34)-C(33')	66.8
N(3)-Lu(2)-C(32')	76.53(16)	C(29)-C(34)-C(33')	19.8
C(53)-Lu(2)-C(33')	90.9(3)	C(38')-C(34)-C(29')	111.9
C(49)-Lu(2)-C(33')	154.9(3)	C(29)-C(34)-C(29')	25.9
N(4)-Lu(2)-C(33')	106.4(2)	C(33')-C(34)-C(29')	45.6
N(3)-Lu(2)-C(33')	92.6(2)	C(34')-C(35)-C(30)	89.0
C(32')-Lu(2)-C(33')	31.34(7)	C(34')-C(35)-C(29')	65.7
C(53)-Lu(2)-C(31')	140.2(3)	C(30)-C(35)-C(29')	23.5
C(49)-Lu(2)-C(31')	106.0(3)	C(34')-C(35)-C(35')	161.6
N(4)-Lu(2)-C(31')	107.4(2)	C(30)-C(35)-C(35')	72.5
N(3)-Lu(2)-C(31')	93.0(2)	C(29')-C(35)-C(35')	95.9
C(32')-Lu(2)-C(31')	27.75(6)	C(34')-C(35)-C(30')	109.1
C(33')-Lu(2)-C(31')	49.55(9)	C(30)-C(35)-C(30')	20.2
C(53)-Lu(2)-C(30')	129.0(4)	C(29')-C(35)-C(30')	43.5
C(49)-Lu(2)-C(30')	113.9(3)	C(35')-C(35)-C(30')	52.5
N(4)-Lu(2)-C(30')	79.74(18)	C(36')-C(36)-C(31)	78.4
N(3)-Lu(2)-C(30')	121.65(18)	C(36')-C(36)-C(35')	152.4
C(32')-Lu(2)-C(30')	47.37(8)	C(31)-C(36)-C(35')	75.0
C(33')-Lu(2)-C(30')	49.12(8)	C(36')-C(36)-C(31')	61.4
C(31')-Lu(2)-C(30')	29.48(6)	C(31)-C(36)-C(31')	17.5
C(53)-Lu(2)-C(29)	91.9(3)	C(35')-C(36)-C(31')	92.4
C(49)-Lu(2)-C(29)	154.9(3)	C(36')-C(36)-C(30')	101.7
N(4)-Lu(2)-C(29)	92.9(2)	C(31)-C(36)-C(30')	23.3
N(3)-Lu(2)-C(29)	106.3(2)	C(35')-C(36)-C(30')	51.8
C(32')-Lu(2)-C(29)	40.28(8)	C(31')-C(36)-C(30')	40.6
C(33')-Lu(2)-C(29)	13.7	C(32)-C(37)-C(32')	16.9
C(31')-Lu(2)-C(29)	50.85(8)	C(32)-C(37)-C(31')	19.8
C(30')-Lu(2)-C(29)	41.44(8)	C(32')-C(37)-C(31')	36.6
C(53)-Lu(2)-C(29')	100.4(3)	C(37')-C(38)-C(33)	72.4
C(49)-Lu(2)-C(29')	140.8(4)	C(37')-C(38)-C(33')	94.8
N(4)-Lu(2)-C(29')	77.50(17)	C(33)-C(38)-C(33')	23.6
N(3)-Lu(2)-C(29')	123.13(19)	C(37')-C(38)-C(32')	56.3
C(32')-Lu(2)-C(29')	50.06(9)	C(33)-C(38)-C(32')	17.7
C(33')-Lu(2)-C(29')	31.41(7)	C(33')-C(38)-C(32')	41.3
C(31')-Lu(2)-C(29')	49.18(8)	C(30)-C(29')-C(29)	129.7
C(30')-Lu(2)-C(29')	28.78(6)	C(30)-C(29')-C(30')	13.4
C(29)-Lu(2)-C(29')	18.4	C(29)-C(29')-C(30')	118.2
C(53)-Lu(2)-C(33)	99.7(3)	C(30)-C(29')-C(33')	117.7
C(49)-Lu(2)-C(33)	139.3(4)	C(29)-C(29')-C(33')	13.0
N(4)-Lu(2)-C(33)	123.15(19)	C(30')-C(29')-C(33')	105.7
N(3)-Lu(2)-C(33)	77.43(18)	C(30)-C(29')-C(34')	97.9
C(32')-Lu(2)-C(33)	16.0	C(29)-C(29')-C(34')	130.6
C(33')-Lu(2)-C(33)	18.6	C(30')-C(29')-C(34')	110.5
C(31')-Lu(2)-C(33)	41.63(9)	C(33')-C(29')-C(34')	143.5
C(30')-Lu(2)-C(33)	53.49(9)	C(30)-C(29')-C(35)	57.6

C(29)-Lu(2)-C(33)	30.87(7)	C(29)-C(29')-C(35)	169.2
C(29')-Lu(2)-C(33)	45.78(9)	C(30')-C(29')-C(35)	69.9
C(53)-Lu(2)-C(30)	115.1(4)	C(33')-C(29')-C(35)	174.2
C(49)-Lu(2)-C(30)	126.1(3)	C(34')-C(29')-C(35)	40.6
N(4)-Lu(2)-C(30)	75.99(15)	C(30)-C(29')-C(34)	172.3
N(3)-Lu(2)-C(30)	125.85(15)	C(29)-C(29')-C(34)	50.5
C(32')-Lu(2)-C(30)	49.33(8)	C(30')-C(29')-C(34)	168.6
C(33')-Lu(2)-C(30)	41.12(8)	C(33')-C(29')-C(34)	63.1
C(31')-Lu(2)-C(30)	39.33(8)	C(34')-C(29')-C(34)	80.5
C(30')-Lu(2)-C(30)	13.9	C(35)-C(29')-C(34)	121.1
C(29)-Lu(2)-C(30)	30.65(6)	C(30)-C(29')-C(31)	30.5
C(29')-Lu(2)-C(30)	15.2	C(29)-C(29')-C(31)	100.1
C(33)-Lu(2)-C(30)	50.58(8)	C(30')-C(29')-C(31)	18.1
C(20)-N(1)-C(16)	114.9(8)	C(33')-C(29')-C(31)	87.7
C(20)-N(1)-Lu(1)	121.1(6)	C(34')-C(29')-C(31)	128.3
C(16)-N(1)-Lu(1)	123.6(6)	C(35)-C(29')-C(31)	87.9
C(15)-N(2)-C(11)	115.0(9)	C(34)-C(29')-C(31)	150.6
C(15)-N(2)-Lu(1)	122.3(5)	C(30)-C(29')-Lu(2)	85.7(2)
C(11)-N(2)-Lu(1)	122.5(7)	C(29)-C(29')-Lu(2)	80.6(2)
C(43)-N(3)-C(39)	119.1(9)	C(30')-C(29')-Lu(2)	75.5(2)
C(43)-N(3)-Lu(2)	118.1(6)	C(33')-C(29')-Lu(2)	72.8(2)
C(39)-N(3)-Lu(2)	122.5(7)	C(34')-C(29')-Lu(2)	120.5(2)
C(48)-N(4)-C(44)	116.9(10)	C(35)-C(29')-Lu(2)	109.0(2)
C(48)-N(4)-Lu(2)	125.2(7)	C(34)-C(29')-Lu(2)	101.7(2)
C(44)-N(4)-Lu(2)	117.6(7)	C(31)-C(29')-Lu(2)	70.5(2)
C(24')-Si(1)-C(21)	121(4)	C(30)-C(30')-C(31)	144.6
C(24')-Si(1)-C(22)	111(3)	C(30)-C(30')-C(29')	14.7
C(21)-Si(1)-C(22)	110.2(7)	C(31)-C(30')-C(29')	132.5
C(24')-Si(1)-C(23)	97(3)	C(30)-C(30')-C(31')	124.4
C(21)-Si(1)-C(23)	108.4(8)	C(31)-C(30')-C(31')	21.7
C(22)-Si(1)-C(23)	108.4(9)	C(29')-C(30')-C(31')	111.2
C(24')-Si(1)-C(24)	14(5)	C(30)-C(30')-C(35')	116.2
C(21)-Si(1)-C(24)	110.9(17)	C(31)-C(30')-C(35')	97.1
C(22)-Si(1)-C(24)	108.0(18)	C(29')-C(30')-C(35')	130.1
C(23)-Si(1)-C(24)	111(3)	C(31')-C(30')-C(35')	118.6
C(26)-Si(2)-C(25)	113.5(19)	C(30)-C(30')-C(35)	53.1
C(26)-Si(2)-C(27')	103(2)	C(31)-C(30')-C(35)	159.8
C(25)-Si(2)-C(27')	113.7(18)	C(29')-C(30')-C(35)	66.6
C(26)-Si(2)-C(27)	84(3)	C(31')-C(30')-C(35)	176.4
C(25)-Si(2)-C(27)	110.5(18)	C(35')-C(30')-C(35)	63.5
C(27')-Si(2)-C(27)	23(3)	C(30)-C(30')-C(29)	37.0
C(26)-Si(2)-C(28)	116(3)	C(31)-C(30')-C(29)	108.9
C(25)-Si(2)-C(28)	111.6(7)	C(29')-C(30')-C(29)	23.5
C(27')-Si(2)-C(28)	98.1(14)	C(31')-C(30')-C(29)	87.7
C(27)-Si(2)-C(28)	119(2)	C(35')-C(30')-C(29)	153.2
C(26)-Si(2)-C(26')	19(3)	C(35)-C(30')-C(29)	89.9

C(25)-Si(2)-C(26')	107.8(11)	C(30)-C(30')-C(36)	166.1
C(27')-Si(2)-C(26')	120(2)	C(31)-C(30')-C(36)	45.5
C(27)-Si(2)-C(26')	102(3)	C(29')-C(30')-C(36)	177.4
C(28)-Si(2)-C(26')	104(2)	C(31')-C(30')-C(36)	66.9
C(53)-Si(3)-C(56)	112.7(6)	C(35')-C(30')-C(36)	51.7
C(53)-Si(3)-C(54')	111.0(19)	C(35)-C(30')-C(36)	115.2
C(56)-Si(3)-C(54')	111.6(18)	C(29)-C(30')-C(36)	154.4
C(53)-Si(3)-C(55)	110.9(6)	C(30)-C(30')-C(32)	109.1
C(56)-Si(3)-C(55)	109.1(8)	C(31)-C(30')-C(32)	36.7
C(54')-Si(3)-C(55)	100.8(15)	C(29')-C(30')-C(32)	95.9
C(53)-Si(3)-C(54)	113(3)	C(31')-C(30')-C(32)	15.3
C(56)-Si(3)-C(54)	98(3)	C(35')-C(30')-C(32)	133.8
C(54')-Si(3)-C(54)	15(4)	C(35)-C(30')-C(32)	162.1
C(55)-Si(3)-C(54)	112(2)	C(29)-C(30')-C(32)	72.4
C(49)-Si(4)-C(50)	115.8(7)	C(36)-C(30')-C(32)	82.1
C(49)-Si(4)-C(51)	114.8(7)	C(30)-C(30')-Lu(2)	86.9(3)
C(50)-Si(4)-C(51)	105.3(9)	C(31)-C(30')-Lu(2)	86.4(3)
C(49)-Si(4)-C(52)	111.1(8)	C(29')-C(30')-Lu(2)	75.7(2)
C(50)-Si(4)-C(52)	99.1(10)	C(31')-C(30')-Lu(2)	73.9(2)
C(51)-Si(4)-C(52)	109.5(9)	C(35')-C(30')-Lu(2)	120.0(2)
C(2)-C(1)-C(5)	108.0	C(35)-C(30')-Lu(2)	107.8(2)
C(2)-C(1)-C(6)	126.0	C(29)-C(30')-Lu(2)	69.3(2)
C(5)-C(1)-C(6)	126.0	C(36)-C(30')-Lu(2)	105.0(3)
C(2)-C(1)-Lu(1)	74.25(19)	C(32)-C(30')-Lu(2)	69.7(2)
C(5)-C(1)-Lu(1)	74.9(2)	C(31)-C(31')-C(32)	164.0
C(6)-C(1)-Lu(1)	116.86(18)	C(31)-C(31')-C(32')	136.4
C(3)-C(2)-C(1)	108.0	C(32)-C(31')-C(32')	29.3
C(3)-C(2)-C(7)	126.0	C(31)-C(31')-C(30')	28.6
C(1)-C(2)-C(7)	126.0	C(32)-C(31')-C(30')	137.8
C(3)-C(2)-Lu(1)	74.6(2)	C(32')-C(31')-C(30')	108.6
C(1)-C(2)-Lu(1)	75.04(19)	C(31)-C(31')-C(36')	69.1
C(7)-C(2)-Lu(1)	116.43(19)	C(32)-C(31')-C(36')	124.0
C(2)-C(3)-C(4)	108.0	C(32')-C(31')-C(36')	153.0
C(2)-C(3)-C(8)	126.0	C(30')-C(31')-C(36')	97.6
C(4)-C(3)-C(8)	126.0	C(31)-C(31')-C(30)	45.4
C(2)-C(3)-Lu(1)	74.6(2)	C(32)-C(31')-C(30)	120.4
C(4)-C(3)-Lu(1)	75.1(2)	C(32')-C(31')-C(30)	91.3
C(8)-C(3)-Lu(1)	116.44(18)	C(30')-C(31')-C(30)	17.4
C(5)-C(4)-C(3)	108.0	C(36')-C(31')-C(30)	114.5
C(5)-C(4)-C(9)	126.0	C(31)-C(31')-C(33)	122.4
C(3)-C(4)-C(9)	126.0	C(32)-C(31')-C(33)	43.4
C(5)-C(4)-Lu(1)	74.93(19)	C(32')-C(31')-C(33)	14.1
C(3)-C(4)-Lu(1)	74.24(19)	C(30')-C(31')-C(33)	94.5
C(9)-C(4)-Lu(1)	116.88(18)	C(36')-C(31')-C(33)	166.2
C(4)-C(5)-C(1)	108.0	C(30)-C(31')-C(33)	77.2
C(4)-C(5)-C(10)	126.0	C(31)-C(31')-C(36)	44.3

C(1)-C(5)-C(10)	126.0	C(32)-C(31')-C(36)	149.3
C(4)-C(5)-Lu(1)	74.46(19)	C(32')-C(31')-C(36)	177.0
C(1)-C(5)-Lu(1)	74.4(2)	C(30')-C(31')-C(36)	72.5
C(10)-C(5)-Lu(1)	117.14(18)	C(36')-C(31')-C(36)	25.4
N(2)-C(11)-C(12)	123.1(14)	C(30)-C(31')-C(36)	89.7
C(13)-C(12)-C(11)	119.1(16)	C(33)-C(31')-C(36)	166.6
C(12)-C(13)-C(14)	119.4(15)	C(31)-C(31')-C(37)	152.9
C(13)-C(14)-C(15)	118.5(15)	C(32)-C(31')-C(37)	40.6
N(2)-C(15)-C(14)	124.8(12)	C(32')-C(31')-C(37)	69.8
N(1)-C(16)-C(17)	125.0(12)	C(30')-C(31')-C(37)	178.3
C(16)-C(17)-C(18)	119.2(13)	C(36')-C(31')-C(37)	83.9
C(19)-C(18)-C(17)	116.5(13)	C(30)-C(31')-C(37)	160.9
C(18)-C(19)-C(20)	122.2(16)	C(33)-C(31')-C(37)	83.9
N(1)-C(20)-C(19)	122.1(13)	C(36)-C(31')-C(37)	109.1
Si(1)-C(21)-Lu(1)	141.3(7)	C(31)-C(31')-Lu(2)	92.9(2)
C(24')-C(24)-Si(1)	53(10)	C(32)-C(31')-Lu(2)	88.0(2)
Si(2)-C(25)-Lu(1)	125.7(5)	C(32')-C(31')-Lu(2)	74.5(2)
C(26')-C(26)-Si(2)	97(10)	C(30')-C(31')-Lu(2)	76.6(2)
C(27')-C(27)-Si(2)	78(9)	C(36')-C(31')-Lu(2)	119.1(2)
C(33')-C(29)-C(29')	149.3	C(30)-C(31')-Lu(2)	72.6(2)
C(33')-C(29)-C(30)	127.9	C(33)-C(31')-Lu(2)	70.3(2)
C(29')-C(29)-C(30)	22.8	C(36)-C(31')-Lu(2)	108.4(2)
C(33')-C(29)-C(33)	20.1	C(37)-C(31')-Lu(2)	103.4(2)
C(29')-C(29)-C(33)	130.1	C(32)-C(32')-C(33)	174.4
C(30)-C(29)-C(33)	108.0	C(32)-C(32')-C(31')	34.1
C(33')-C(29)-C(34)	106.1	C(33)-C(32')-C(31')	141.3
C(29')-C(29)-C(34)	103.6	C(32)-C(32')-C(33')	145.4
C(30)-C(29)-C(34)	126.0	C(33)-C(32')-C(33')	29.9
C(33)-C(29)-C(34)	126.0	C(31')-C(32')-C(33')	111.4
C(33')-C(29)-C(38')	74.7	C(32)-C(32')-C(37')	124.0
C(29')-C(29)-C(38')	135.6	C(33)-C(32')-C(37')	60.1
C(30)-C(29)-C(38')	157.2	C(31')-C(32')-C(37')	157.3
C(33)-C(29)-C(38')	94.2	C(33')-C(32')-C(37')	89.7
C(34)-C(29)-C(38')	32.1	C(32)-C(32')-C(31)	48.4
C(33')-C(29)-C(32')	42.3	C(33)-C(32')-C(31)	126.8
C(29')-C(29)-C(32')	107.8	C(31')-C(32')-C(31)	14.5
C(30)-C(29)-C(32')	85.6	C(33')-C(32')-C(31)	97.0
C(33)-C(29)-C(32')	22.4	C(37')-C(32')-C(31)	167.4
C(34)-C(29)-C(32')	148.4	C(32)-C(32')-C(29)	127.9
C(38')-C(29)-C(32')	116.6	C(33)-C(32')-C(29)	47.3
C(33')-C(29)-C(30')	111.8	C(31')-C(32')-C(29)	94.0
C(29')-C(29)-C(30')	38.2	C(33')-C(32')-C(29)	17.5
C(30)-C(29)-C(30')	16.0	C(37')-C(32')-C(29)	106.7
C(33)-C(29)-C(30')	92.1	C(31)-C(32')-C(29)	79.5
C(34)-C(29)-C(30')	141.9	C(32)-C(32')-C(37)	39.6
C(38')-C(29)-C(30')	172.9	C(33)-C(32')-C(37)	145.1

C(32')-C(29)-C(30')	69.7	C(31')-C(32')-C(37)	73.6
C(33')-C(29)-Lu(2)	79.8(2)	C(33')-C(32')-C(37)	175.0
C(29')-C(29)-Lu(2)	80.9(2)	C(37')-C(32')-C(37)	85.3
C(30)-C(29)-Lu(2)	76.4(2)	C(31)-C(32')-C(37)	88.0
C(33)-C(29)-Lu(2)	74.9(2)	C(29)-C(32')-C(37)	167.5
C(34)-C(29)-Lu(2)	115.0(2)	C(32)-C(32')-C(38)	146.1
C(38')-C(29)-Lu(2)	115.6(2)	C(33)-C(32')-C(38)	38.6
C(32')-C(29)-Lu(2)	67.8(2)	C(31')-C(32')-C(38)	179.16(8)
C(30')-C(29)-Lu(2)	69.3(2)	C(33')-C(32')-C(38)	68.5
C(30')-C(30)-C(29')	151.9	C(37')-C(32')-C(38)	23.2
C(30')-C(30)-C(29)	126.9	C(31)-C(32')-C(38)	165.4
C(29')-C(30)-C(29)	27.6	C(29)-C(32')-C(38)	85.9
C(30')-C(30)-C(31)	20.0	C(37)-C(32')-C(38)	106.5
C(29')-C(30)-C(31)	134.8	C(32)-C(32')-Lu(2)	93.0(3)
C(29)-C(30)-C(31)	108.0	C(33)-C(32')-Lu(2)	87.9(3)
C(30')-C(30)-C(35)	106.8	C(31')-C(32')-Lu(2)	77.7(2)
C(29')-C(30)-C(35)	98.9	C(33')-C(32')-Lu(2)	75.5(3)
C(29)-C(30)-C(35)	126.0	C(37')-C(32')-Lu(2)	117.1(2)
C(31)-C(30)-C(35)	126.0	C(31)-C(32')-Lu(2)	75.0(2)
C(30')-C(30)-C(31')	38.2	C(29)-C(32')-Lu(2)	71.9(2)
C(29')-C(30)-C(31')	115.8	C(37)-C(32')-Lu(2)	106.0(3)
C(29)-C(30)-C(31')	89.1	C(38)-C(32')-Lu(2)	101.5(2)
C(31)-C(30)-C(31')	19.0	C(29)-C(33')-C(33)	145.2
C(35)-C(30)-C(31')	144.9	C(29)-C(33')-C(32')	120.2
C(30')-C(30)-C(33')	111.5	C(33)-C(33')-C(32')	25.4
C(29')-C(30)-C(33')	42.6	C(29)-C(33')-C(29')	17.7
C(29)-C(30)-C(33')	15.4	C(33)-C(33')-C(29')	128.4
C(31)-C(30)-C(33')	92.6	C(32')-C(33')-C(29')	103.1
C(35)-C(30)-C(33')	141.4	C(29)-C(33')-C(38')	83.8
C(31')-C(30)-C(33')	73.7	C(33)-C(33')-C(38')	129.7
C(30')-C(30)-C(34')	145.3	C(32')-C(33')-C(38')	154.8
C(29')-C(30)-C(34')	60.4	C(29')-C(33')-C(38')	101.3
C(29)-C(30)-C(34')	87.2	C(29)-C(33')-C(34)	54.1
C(31)-C(30)-C(34')	164.8	C(33)-C(33')-C(34)	160.1
C(35)-C(30)-C(34')	38.8	C(32')-C(33')-C(34)	174.2
C(31')-C(30)-C(34')	176.1	C(29')-C(33')-C(34)	71.3
C(33')-C(30)-C(34')	102.6	C(38')-C(33')-C(34)	30.4
C(30')-C(30)-C(35')	46.6	C(29)-C(33')-C(30)	36.7
C(29')-C(30)-C(35')	158.8	C(33)-C(33')-C(30)	108.8
C(29)-C(30)-C(35')	173.4	C(32')-C(33')-C(30)	83.5
C(31)-C(30)-C(35')	65.4	C(29')-C(33')-C(30)	19.7
C(35)-C(30)-C(35')	60.6	C(38')-C(33')-C(30)	120.4
C(31')-C(30)-C(35')	84.4	C(34)-C(33')-C(30)	90.8
C(33')-C(30)-C(35')	158.0	C(29)-C(33')-C(38)	168.9
C(34')-C(30)-C(35')	99.3	C(33)-C(33')-C(38)	44.9
C(30')-C(30)-Lu(2)	79.2(2)	C(32')-C(33')-C(38)	70.3

C(29')-C(30)-Lu(2)	79.1(2)	C(29')-C(33')-C(38)	173.3
C(29)-C(30)-Lu(2)	73.0(2)	C(38')-C(33')-C(38)	85.4
C(31)-C(30)-Lu(2)	76.2(2)	C(34)-C(33')-C(38)	115.3
C(35)-C(30)-Lu(2)	116.9(2)	C(30)-C(33')-C(38)	153.7
C(31')-C(30)-Lu(2)	68.0(2)	C(29)-C(33')-C(32)	109.0
C(33')-C(30)-Lu(2)	67.1(2)	C(33)-C(33')-C(32)	36.5
C(34')-C(30)-Lu(2)	109.6(2)	C(32')-C(33')-C(32)	11.2
C(35')-C(30)-Lu(2)	104.5(2)	C(29')-C(33')-C(32)	91.9
C(31')-C(31)-C(30')	129.7	C(38')-C(33')-C(32)	164.9
C(31')-C(31)-C(32)	8.8	C(34)-C(33')-C(32)	163.1
C(30')-C(31)-C(32)	122.6	C(30)-C(33')-C(32)	72.3
C(31')-C(31)-C(30)	115.6	C(38)-C(33')-C(32)	81.4
C(30')-C(31)-C(30)	15.4	C(29)-C(33')-Lu(2)	86.5(3)
C(32)-C(31)-C(30)	108.0	C(33)-C(33')-Lu(2)	83.7(3)
C(31')-C(31)-C(36)	118.2	C(32')-C(33')-Lu(2)	73.1(3)
C(30')-C(31)-C(36)	111.2	C(29')-C(33')-Lu(2)	75.8(2)
C(32)-C(31)-C(36)	126.0	C(38')-C(33')-Lu(2)	119.6(2)
C(30)-C(31)-C(36)	126.0	C(34)-C(33')-Lu(2)	106.5(3)
C(31')-C(31)-C(36')	88.1	C(30)-C(33')-Lu(2)	71.8(2)
C(30')-C(31)-C(36')	141.9	C(38)-C(33')-Lu(2)	101.1(2)
C(32)-C(31)-C(36')	95.5	C(32)-C(33')-Lu(2)	70.3(2)
C(30)-C(31)-C(36')	156.2	C(35)-C(34')-C(29')	73.8
C(36)-C(31)-C(36')	30.7	C(35)-C(34')-C(30)	52.2
C(31')-C(31)-C(32')	29.0	C(29')-C(34')-C(30)	21.7
C(30')-C(31)-C(32')	101.5	C(36)-C(35')-C(30')	76.4
C(32)-C(31)-C(32')	21.2	C(36)-C(35')-C(35)	140.4
C(30)-C(31)-C(32')	86.8	C(30')-C(35')-C(35)	64.0
C(36)-C(31)-C(32')	147.2	C(36)-C(35')-C(31)	50.4
C(36')-C(31)-C(32')	116.6	C(30')-C(35')-C(31)	26.1
C(31')-C(31)-C(35')	171.6	C(35)-C(35')-C(31)	90.0
C(30')-C(31)-C(35')	56.8	C(36)-C(35')-C(30)	93.5
C(32)-C(31)-C(35')	179.5	C(30')-C(35')-C(30)	17.2
C(30)-C(31)-C(35')	71.5	C(35)-C(35')-C(30)	46.9
C(36)-C(31)-C(35')	54.5	C(31)-C(35')-C(30)	43.1
C(36')-C(31)-C(35')	85.0	C(36)-C(36')-C(31)	70.8
C(32')-C(31)-C(35')	158.3	C(36)-C(36')-C(31')	93.2
C(31')-C(31)-C(29')	100.9	C(31)-C(36')-C(31')	22.8
C(30')-C(31)-C(29')	29.4	C(38)-C(37')-C(33)	76.4
C(32)-C(31)-C(29')	93.4	C(38)-C(37')-C(32')	100.5
C(30)-C(31)-C(29')	14.8	C(33)-C(37')-C(32')	25.5
C(36)-C(31)-C(29')	140.6	C(34)-C(38')-C(33')	82.8
C(36')-C(31)-C(29')	170.9	C(34)-C(38')-C(29)	61.8
C(32')-C(31)-C(29')	72.2	C(33')-C(38')-C(29)	21.5
C(35')-C(31)-C(29')	86.1	C(40)-C(39)-N(3)	123.0(17)
C(31')-C(31)-Lu(2)	73.5(2)	C(39)-C(40)-C(41)	118.8(18)
C(30')-C(31)-Lu(2)	75.8(2)	C(42)-C(41)-C(40)	118.1(17)

C(32)-C(31)-Lu(2)	74.1(2)	C(41)-C(42)-C(43)	119.6(19)
C(30)-C(31)-Lu(2)	73.6(2)	N(3)-C(43)-C(42)	121.4(15)
C(36)-C(31)-Lu(2)	118.3(2)	N(4)-C(44)-C(45)	123.1(16)
C(36')-C(31)-Lu(2)	118.1(2)	C(46)-C(45)-C(44)	120(4)
C(32')-C(31)-Lu(2)	66.1(2)	C(46)-C(45)-C(46')	4(7)
C(35')-C(31)-Lu(2)	105.7(2)	C(44)-C(45)-C(46')	117(4)
C(29')-C(31)-Lu(2)	66.4(2)	C(45)-C(46)-C(47)	120(3)
C(32')-C(32)-C(31')	116.6	C(46')-C(47)-C(48)	134(5)
C(32')-C(32)-C(31)	110.5	C(46')-C(47)-C(46)	17(5)
C(31')-C(32)-C(31)	7.2	C(48)-C(47)-C(46)	118(2)
C(32')-C(32)-C(33)	2.9	N(4)-C(48)-C(47)	122.0(16)
C(31')-C(32)-C(33)	114.3	Si(4)-C(49)-Lu(2)	140.8(6)
C(31)-C(32)-C(33)	108.0	Si(3)-C(53)-Lu(2)	122.7(6)
C(32')-C(32)-C(37)	123.5	C(54')-C(54)-Si(3)	68(10)
C(31')-C(32)-C(37)	119.6	C(24)-C(24')-Si(1)	113(10)
C(31)-C(32)-C(37)	126.0	C(26)-C(26')-Si(2)	65(10)
C(33)-C(32)-C(37)	126.0	C(27)-C(27')-Si(2)	78(10)
C(32')-C(32)-C(30')	89.9	C(47)-C(46')-C(45)	107(5)
C(31')-C(32)-C(30')	26.9	C(54)-C(54')-Si(3)	97(10)

Crystallographic Details for (C_5Me_5)Lu(η^2-(N,C)-NC_5H_5)(CH_2SiMe_3)(NC_5H_5) (3). A dark orange crystal grown from concentrated hexanes solution of **3** at –35 °C was mounted from Paratone N oil (Hampton Research) onto a glass fiber under argon gas flow and placed on a Bruker P4/CCD diffractometer, equipped with a Bruker LT-2 temperature device. A hemisphere of data was collected using φ scans, with 30 s frame exposures, and 0.3° frame widths. Data collection and initial indexing and cell refinement were handled using SMART software. Frame integration and final cell parameter calculations were carried out using SAINT software. The data were corrected for absorption using the SADABS program. Decay of reflection data was monitored by analysis of redundant frames. The structure was solved using Patterson techniques, completed by subsequent difference Fourier techniques, and refined by full-matrix least-squares procedures. All non-hydrogen atoms were refined anisotropically, and hydrogen atoms were treated as idealized contributions. Structure solution, refinement, and creation of publication materials were performed using SHELXTL. The figure was made using ORTEP-3.

Table S4. Crystal Data and Structure Refinement for Complex 3.

Identification code	kjLuCHpya	
Empirical formula	$C_{24}H_{35}N_2LuSi$	
Formula weight	554.60 g/mol	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.734(3) Å	
	b = 7.955(2) Å	β = 102.850(4) °
	c = 15.068(5) Å	
Volume	1254.4(6) Å^3	
Z	2	
Density (calculated)	1.468 g cm^{-3}	
Absorption coefficient	3.994 mm^{-1}	
F(000)	556	
Crystal size	0.2 × 0.3 × 0.3 mm^3	
Theta range for data collection	1.4-27.9°	
Index ranges	$-14 \le h \le 14$, $-10 \le k \le 10$, $-15 \le l \le 19$	
Reflections collected	8803	
Independent reflections	5322 (R_{int} = 0.0554)	
Max. and min. transmission	0.5022 and 0.3804	
Refinement method	full-matrix least-squares on F^2	
Data/restraints/parameters	5322/1/ 261	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2σ(I)]	R1 = 0.0413, wR2 = 0.0957	
R indices (all data)	R1 = 0.0523, wR2 = 0.1012	
Largest diff. peak and hole	1.477 and -2.842 e.Å^{-3}	

Table S5. Bond lengths (Å) for 3.

Lu(1)-N(2)	2.270(6)	C(1)-C(5)	1.427(14)
Lu(1)-C(20)	2.340(8)	C(1)-C(6)	1.490(13)
Lu(1)-C(21)	2.379(9)	C(2)-C(3)	1.420(13)
Lu(1)-N(1)	2.396(8)	C(2)-C(7)	1.517(13)
Lu(1)-C(2)	2.611(9)	C(3)-C(4)	1.419(13)
Lu(1)-C(5)	2.618(9)	C(3)-C(8)	1.505(12)
Lu(1)-C(3)	2.621(9)	C(4)-C(5)	1.439(12)
Lu(1)-C(4)	2.626(9)	C(4)-C(9)	1.495(12)
Lu(1)-C(1)	2.637(11)	C(5)-C(10)	1.495(14)
N(1)-C(11)	1.331(13)	C(11)-C(12)	1.368(14)
N(1)-C(15)	1.351(13)	C(12)-C(13)	1.344(16)
N(2)-C(20)	1.356(13)	C(13)-C(14)	1.390(15)
N(2)-C(19)	1.365(12)	C(14)-C(15)	1.389(13)
Si(1)-C(24)	1.851(12)	C(16)-C(20)	1.403(13)
Si(1)-C(21)	1.851(9)	C(16)-C(17)	1.403(17)
Si(1)-C(22)	1.873(13)	C(17)-C(18)	1.371(16)
Si(1)-C(23)	1.892(11)	C(18)-C(19)	1.370(15)
C(1)-C(2)	1.409(14)		

Table S6. Bond Angles (°) for 3.

N(2)-Lu(1)-C(20)	34.2(3)	C(21)-Si(1)-C(23)	114.8(5)
N(2)-Lu(1)-C(21)	103.8(3)	C(22)-Si(1)-C(23)	106.4(5)
C(20)-Lu(1)-C(21)	120.0(3)	C(2)-C(1)-C(5)	107.4(9)
N(2)-Lu(1)-N(1)	125.9(4)	C(2)-C(1)-C(6)	125.8(10)
C(20)-Lu(1)-N(1)	93.4(3)	C(5)-C(1)-C(6)	126.7(10)
C(21)-Lu(1)-N(1)	92.4(3)	C(2)-C(1)-Lu(1)	73.4(5)
N(2)-Lu(1)-C(2)	113.5(4)	C(5)-C(1)-Lu(1)	73.5(6)
C(20)-Lu(1)-C(2)	134.5(3)	C(6)-C(1)-Lu(1)	121.7(7)
C(21)-Lu(1)-C(2)	93.7(3)	C(1)-C(2)-C(3)	109.1(8)
N(1)-Lu(1)-C(2)	116.5(3)	C(1)-C(2)-C(7)	125.6(10)
N(2)-Lu(1)-C(5)	115.1(3)	C(3)-C(2)-C(7)	125.0(10)
C(20)-Lu(1)-C(5)	104.6(3)	C(1)-C(2)-Lu(1)	75.4(6)
C(21)-Lu(1)-C(5)	135.4(3)	C(3)-C(2)-Lu(1)	74.6(5)
N(1)-Lu(1)-C(5)	82.3(3)	C(7)-C(2)-Lu(1)	121.1(6)
C(2)-Lu(1)-C(5)	51.8(3)	C(4)-C(3)-C(2)	108.1(8)
N(2)-Lu(1)-C(3)	85.0(4)	C(4)-C(3)-C(8)	124.7(9)
C(20)-Lu(1)-C(3)	103.2(3)	C(2)-C(3)-C(8)	127.1(9)
C(21)-Lu(1)-C(3)	114.4(3)	C(4)-C(3)-Lu(1)	74.5(5)
N(1)-Lu(1)-C(3)	133.9(3)	C(2)-C(3)-Lu(1)	73.9(5)
C(2)-Lu(1)-C(3)	31.5(3)	C(8)-C(3)-Lu(1)	121.0(6)
C(5)-Lu(1)-C(3)	52.1(3)	C(3)-C(4)-C(5)	107.2(8)
N(2)-Lu(1)-C(4)	85.6(3)	C(3)-C(4)-C(9)	126.3(9)

C(20)-Lu(1)-C(4)	86.9(3)	C(5)-C(4)-C(9)	126.4(9)
C(21)-Lu(1)-C(4)	144.6(3)	C(3)-C(4)-Lu(1)	74.1(5)
N(1)-Lu(1)-C(4)	109.8(3)	C(5)-C(4)-Lu(1)	73.8(5)
C(2)-Lu(1)-C(4)	52.1(3)	C(9)-C(4)-Lu(1)	120.2(6)
C(5)-Lu(1)-C(4)	31.8(3)	C(1)-C(5)-C(4)	108.3(9)
C(3)-Lu(1)-C(4)	31.4(3)	C(1)-C(5)-C(10)	125.7(9)
N(2)-Lu(1)-C(1)	135.5(4)	C(4)-C(5)-C(10)	125.6(9)
C(20)-Lu(1)-C(1)	135.7(3)	C(1)-C(5)-Lu(1)	75.0(5)
C(21)-Lu(1)-C(1)	104.3(3)	C(4)-C(5)-Lu(1)	74.4(5)
N(1)-Lu(1)-C(1)	86.5(3)	C(10)-C(5)-Lu(1)	122.0(6)
C(2)-Lu(1)-C(1)	31.1(3)	N(1)-C(11)-C(12)	123.9(10)
C(5)-Lu(1)-C(1)	31.5(3)	C(13)-C(12)-C(11)	119.9(10)
C(3)-Lu(1)-C(1)	52.0(3)	C(12)-C(13)-C(14)	118.7(9)
C(4)-Lu(1)-C(1)	52.4(3)	C(15)-C(14)-C(13)	118.3(9)
C(11)-N(1)-C(15)	116.2(9)	N(1)-C(15)-C(14)	122.9(9)
C(11)-N(1)-Lu(1)	122.1(7)	C(20)-C(16)-C(17)	120.2(11)
C(15)-N(1)-Lu(1)	121.2(7)	C(18)-C(17)-C(16)	119.9(10)
C(20)-N(2)-C(19)	122.2(9)	C(19)-C(18)-C(17)	119.1(10)
C(20)-N(2)-Lu(1)	75.7(5)	N(2)-C(19)-C(18)	120.9(11)
C(19)-N(2)-Lu(1)	160.9(9)	N(2)-C(20)-C(16)	117.6(9)
C(24)-Si(1)-C(21)	109.6(5)	N(2)-C(20)-Lu(1)	70.1(4)
C(24)-Si(1)-C(22)	109.3(6)	C(16)-C(20)-Lu(1)	169.3(7)
C(21)-Si(1)-C(22)	110.8(5)	Si(1)-C(21)-Lu(1)	119.4(4)
C(24)-Si(1)-C(23)	105.6(6)		

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