Supporting Information for

Investigation of the Electronic Structure of Mono(1,1'-Diamidoferrocene) Uranium(IV) Complexes

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SYNTHESIS

Potassium 2,6-di-tert-butylphenoxide. A hexanes solution of 2,6-di-*tert*-butylphenol (HOAr) was filtered through alumina and stored at –35 ºC for 24 h. Pale yellow-green crystals (85 mg, 0.41 mmol, 1 equiv) were dissolved in Et_2O and cooled for 15 min. Solid KCH_2Ph (53 mg, 0.41 mmol, 1 equiv) was added to the stirring solution of the phenol and the reaction mixture was allowed to stir at room temperature for 90 min. The initially bright orange gradually faded to a very light pink color. The resulting suspension was filtered through a medium-porosity frit, and the light pink solid was washed with fresh Et_2O and dried. Yield: 98 mg, 97%.

Potassium diphenylamide. In a 20 mL scintillation vial, solid KH (85.2 mg, 2.1 mmol, 1.2 equiv) was added to a cold diethyl ether solution of $HNPh_2$ (302.8 mg, 1.8 mmol, 1 equiv). After the white suspension was allowed to stir for 10 min, it was placed at -40 ºC to allow the precipitate to settle. The solvent was decanted, after which the solid was washed with cold diethyl ether and dried under reduced pressure. Yield: 320.7 mg, 86 %.

^{1}H NMR SPECTROSCOPY

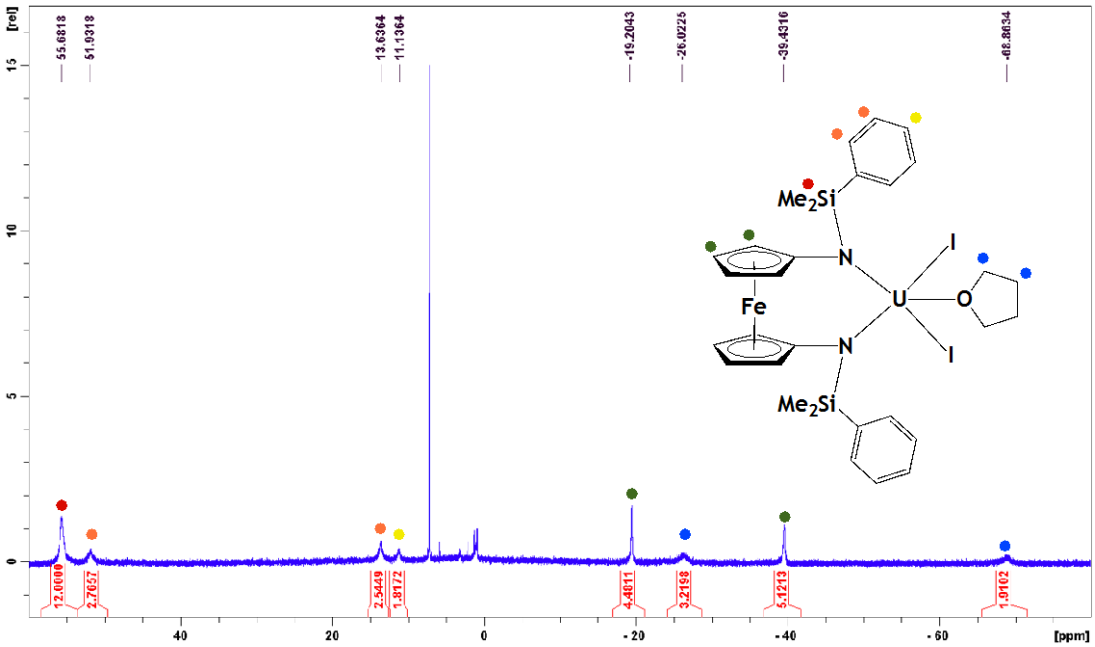


Figure S1. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of (NN^{DMP})UI_2(THF); δ, ppm: 55.7 (s, 12H, $LW_{1/2}$ = 144 Hz, -Si(C*H*$_3$)$_2$), 51.9 (s, 4H, $LW_{1/2}$ = 206 Hz, Si(C_6H_5)), 13.6 (s, 4H, $LW_{1/2}$ = 199 Hz, Si(C_6H_5)), 11.1 (s, 2H, $LW_{1/2}$ = 123 Hz, Si(C_6H_5)), -19.2 (s, 4H, $LW_{1/2}$ = 47 Hz, Cp*H*), -26.0 (s, 4H, $LW_{1/2}$ = 371 Hz, OC_4H_8), -39.4 (s, 4H, $LW_{1/2}$ = 36 Hz, Cp*H*), -68.9 (s, 4H, $LW_{1/2}$ = 414 Hz, OC_4H_8).

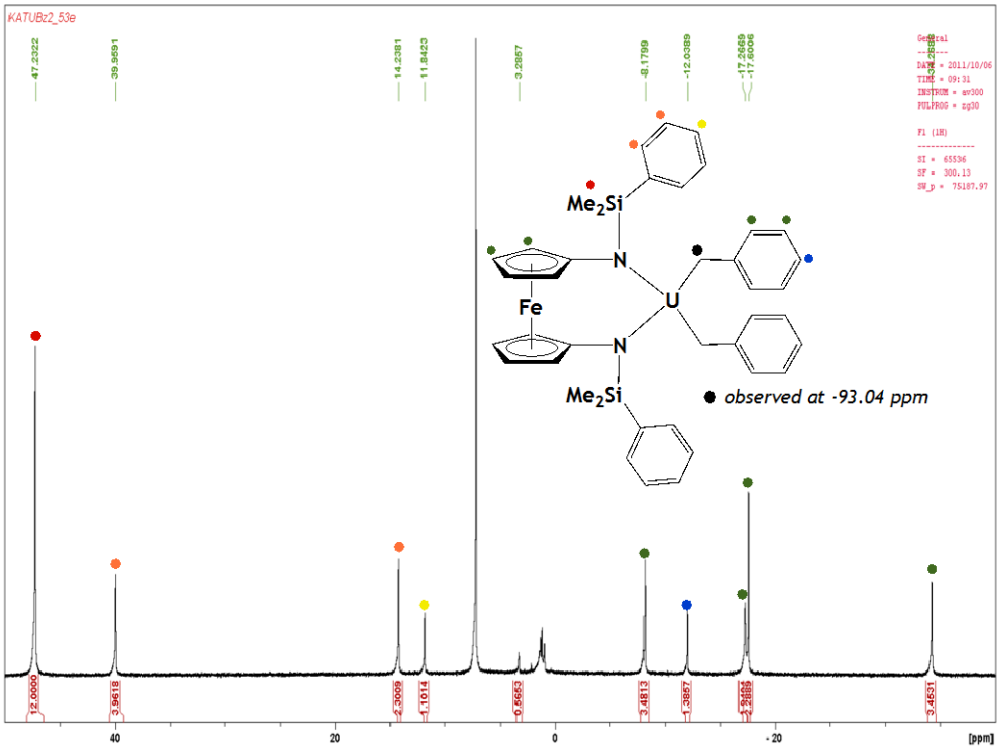


Figure S2. ^{1}H NMR spectrum (300 MHz, C_6D_6) of (NN^{DMP})$U(CH_2Ph)_2$; δ, ppm: 47.2 (s, 12H, Si(C*H*$_3$)$_2$), 39.9 (s, 4H, Si(C_6H_5)), 14.2 (s, 4H, Si(C_6H_5)), 11.8 (s, 2H, Si(C_6H_5)), -8.2 (s, 4H), -12.0 (s, 2H, CH_2(C_6H_5)), -17.3 (s, 4H), -17.6 (s, 4H), -34.3 (s, 4H).

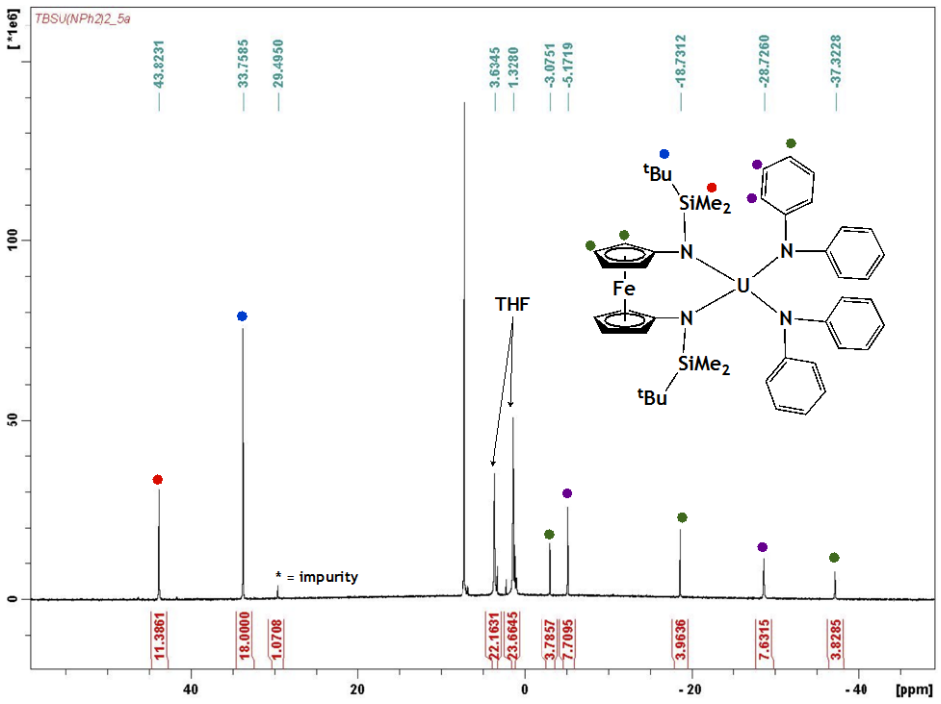


Figure S3. ^{1}H NMR spectrum (300 MHz, C_6D_6) of (NN^{TBS})U(NPh_2)$_2$; δ, ppm: 43.8 (s, 12H, Si(CH_3)$_2$), 33.7 (s, 18H, SiC(CH_3)$_3$), -3.1 (s, 4H), -5.2 (s, 8H), -18.7 (s, 4H), -28.7 (s, 8H), -37.3 (s, 4H).

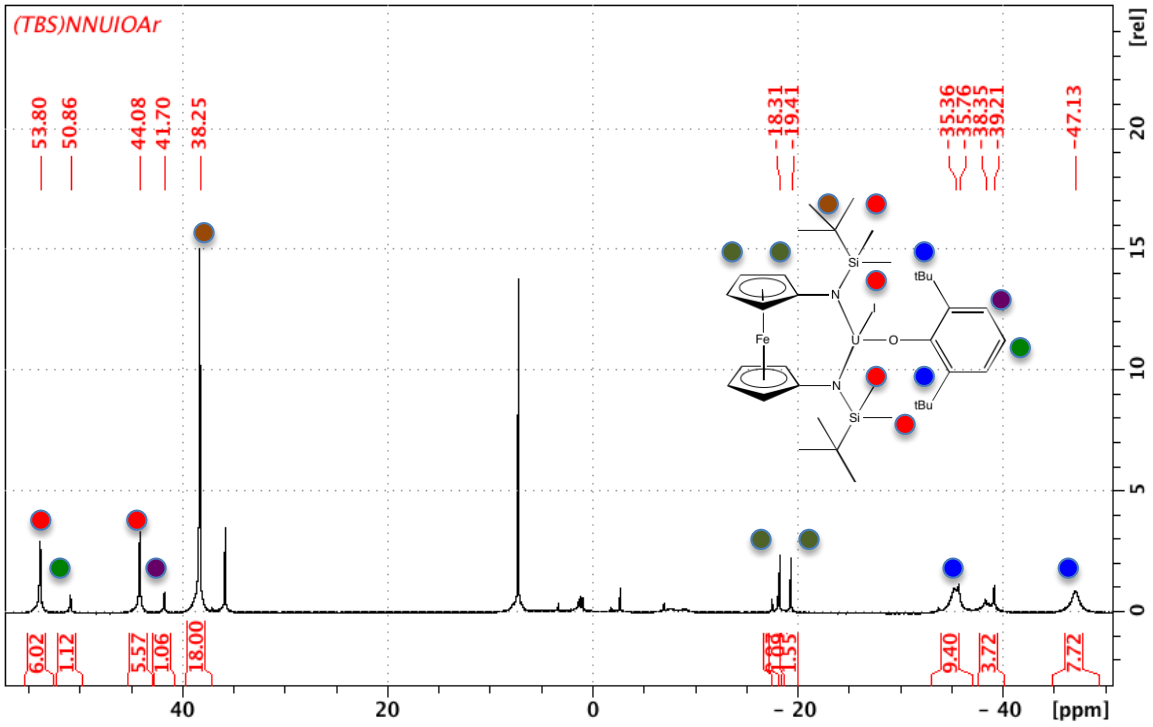


Figure S4. ^{1}H NMR spectrum (300 MHz, C_6D_6) of (NN^{TBS})UI(OAr); δ, ppm: 53.8 (s, 6H, Si(CH_3)$_2$), 50.9 (s, (1H, C_6H_3), 44.1 (s, 6H, Si(CH_3)$_2$), 41.7 (s, 1H, C_6H_3), 38.3 (s, 18H, Si(C(CH_3)$_3$)$_2$, -18.3 (s, 4H, C_5H_4), -19.4 (s, 4H, C_5H_4), -35.4 (s, 9H, OC_6H_3-C(CH_3)$_3$), -47.1 (s, 9H, OC_6H_3-C(CH_3)$_3$).

CYCLIC VOLTAMMETRY

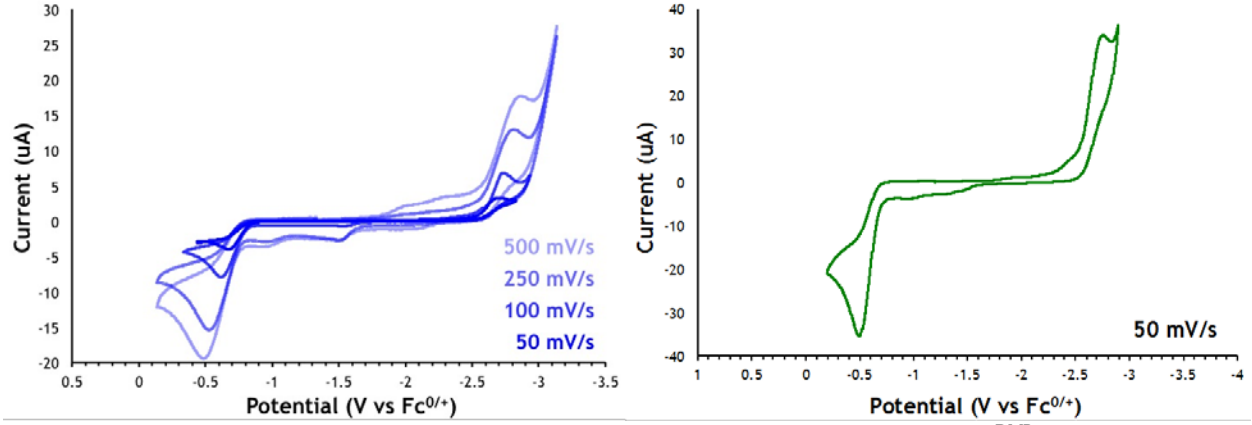


Figure S5. Cyclic voltammograms of a 4 mM (left) and 1.7 mM (right) TFT solution of $(NN^{DMP})U(CH_2Ph)_2$ with $TPABAr^F$ as the supporting electrolyte.

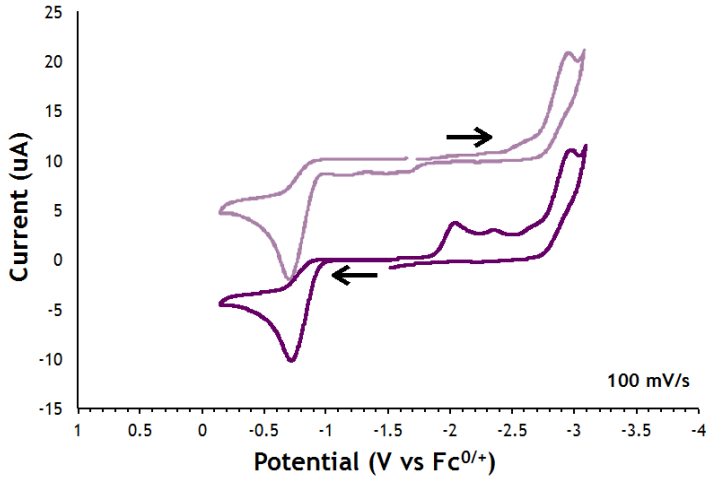


Figure S6. Cyclic voltammogram of a 5.5 mM TFT solution of $(NN^{TMS})U(CH_2Ph)_2$ with $TPABAr^F$ as the supporting electrolyte.

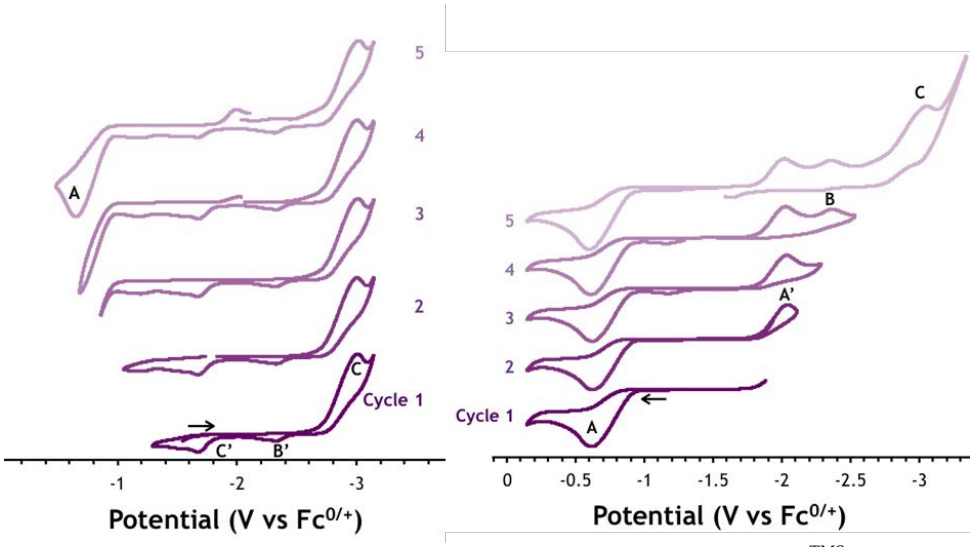


Figure S7. Effect of switching potential on reduction (left) and oxidation (right) of $(NN^{TMS})U(CH_2Ph)_2$ in TFT with $TPABAr^F$ as the supporting electrolyte.

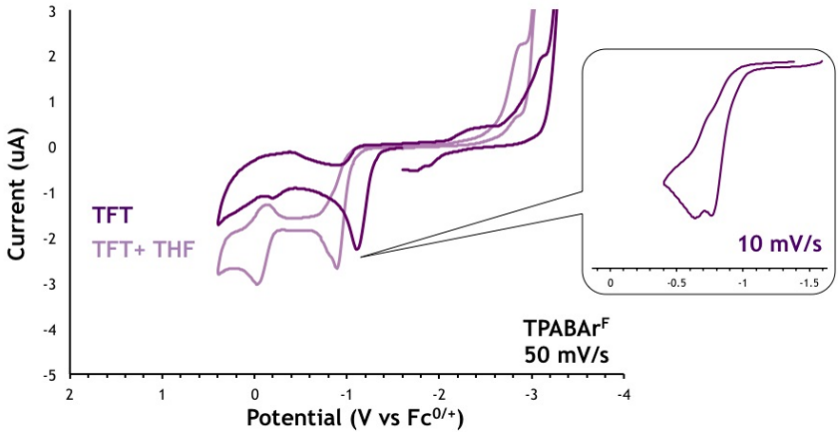


Figure S8. Oxidation of $(NN^{TMS})U(CH_2Ph)_2$ in TFT before and after addition of THF.

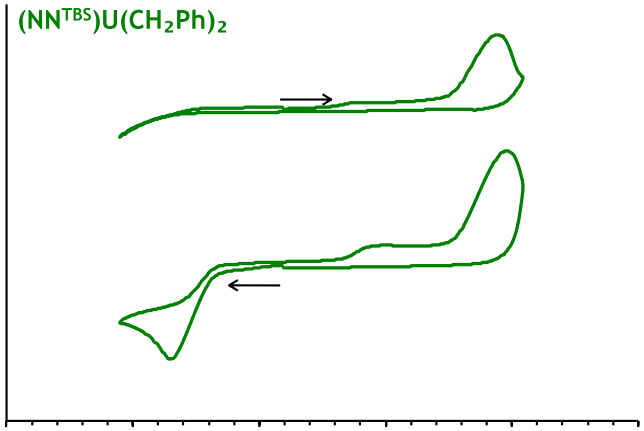


Figure S9. Cyclic voltammogram of $(NN^{TBS})U(CH_2Ph)_2$ in Et_2O with $NaBAr^F$ as the supporting electrolyte.

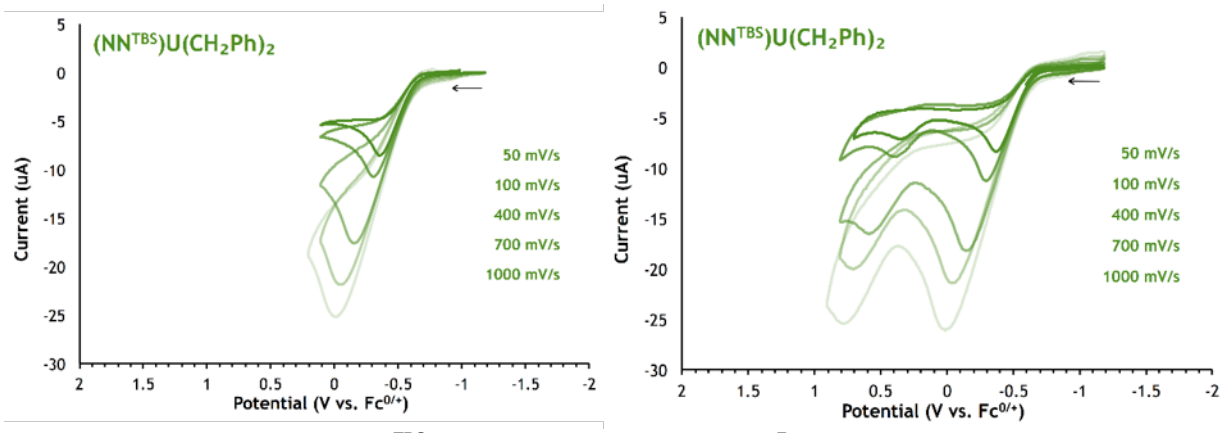


Figure S10. Oxidation events of $(NN^{TBS})U(CH_2Ph)_2$ in Et_2O with $NaBAr^F$ as the supporting electrolyte.

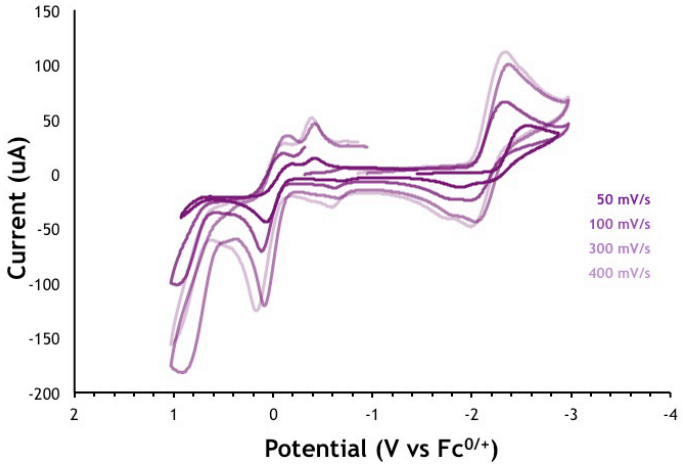


Figure S11. Cyclic voltammogram of a 2.8 mM THF solution of $(NN^{TMS})UI_2(THF)$ with $TPABAr^F$ as the supporting electrolyte.

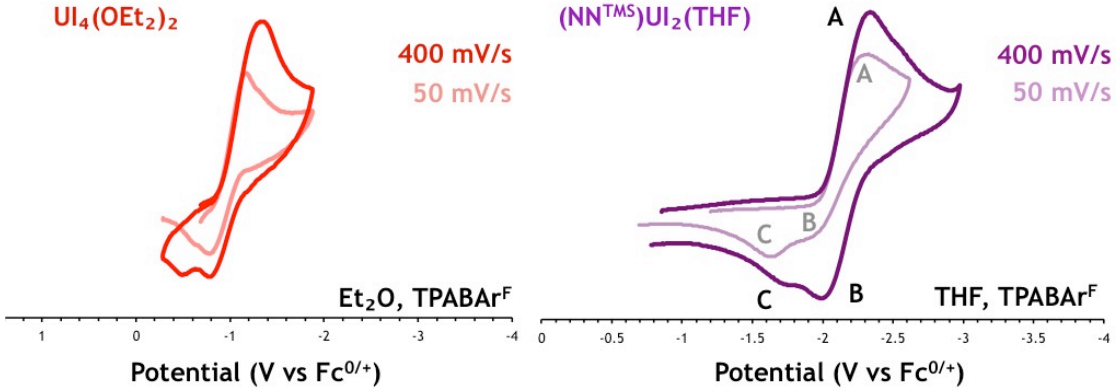


Figure S12. Reduction of $UI_4(Et_2O)_2$ (left) and $(NN^{TMS})UI_2(THF)$ (right). For clarity, the height of 50 mV/s scans was scaled by a factor of 0.5 and 3 in $UI_4(Et_2O)_2$ and $(NN^{TMS})UI_2(THF)$, respectively.

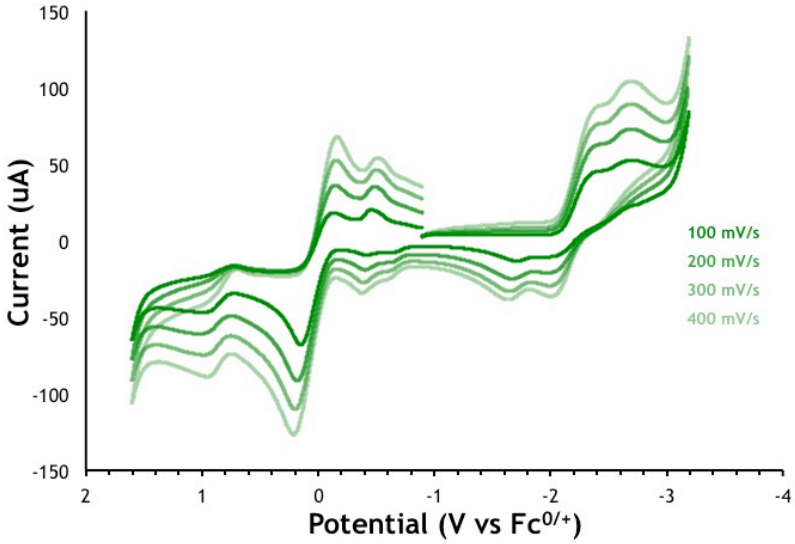


Figure S13. Cyclic voltammogram of a 3.6 mM THF solution of $(NN^{TBS})UI_2(THF)$ with $TPABAr^F$ as the supporting electrolyte**.**

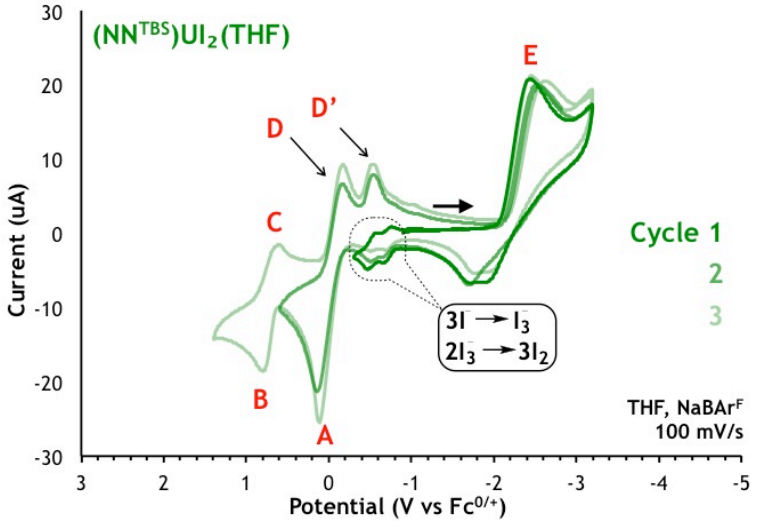


Figure S14. Effect of anodic switching potential on reduction of $(NN^{TBS})UI_2(THF)$.

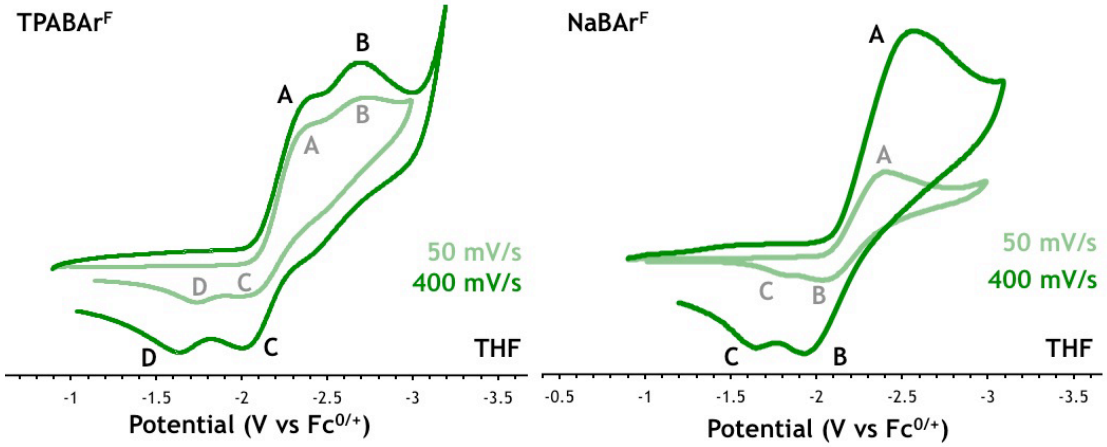


Figure S15. Reduction of $(NN^{TBS})UI_2(THF)$ in THF with $TPABAr^F$ (left) and $NaBAr^F$ (right). For clarity, the plot on the left corresponding to 50 mV/s was scaled by a factor of 2.

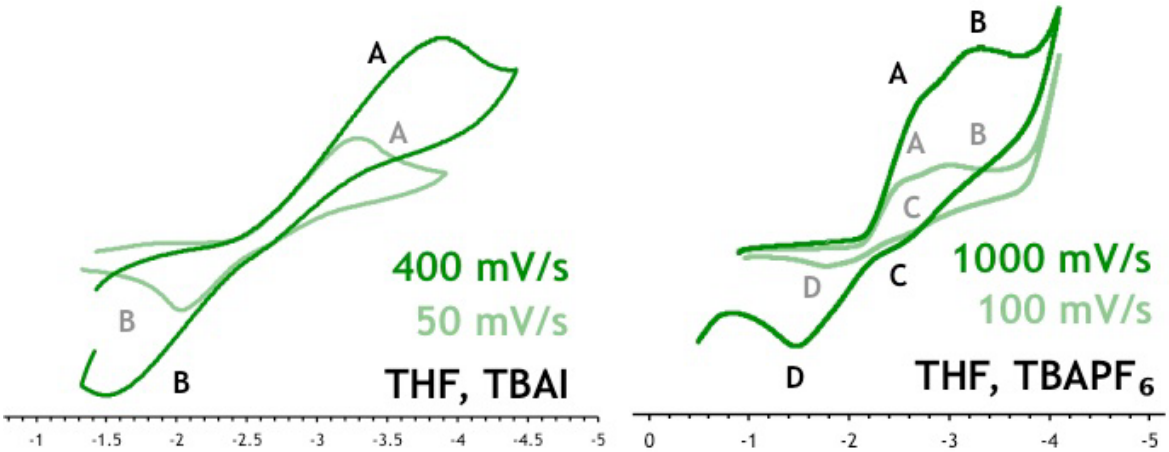


Figure S16. Reduction of $(NN^{TBS})UI_2(THF)$ in THF solutions of tetrabutylammonium iodide (left) and tetrabutylammonium hexafluorophosphate (right).

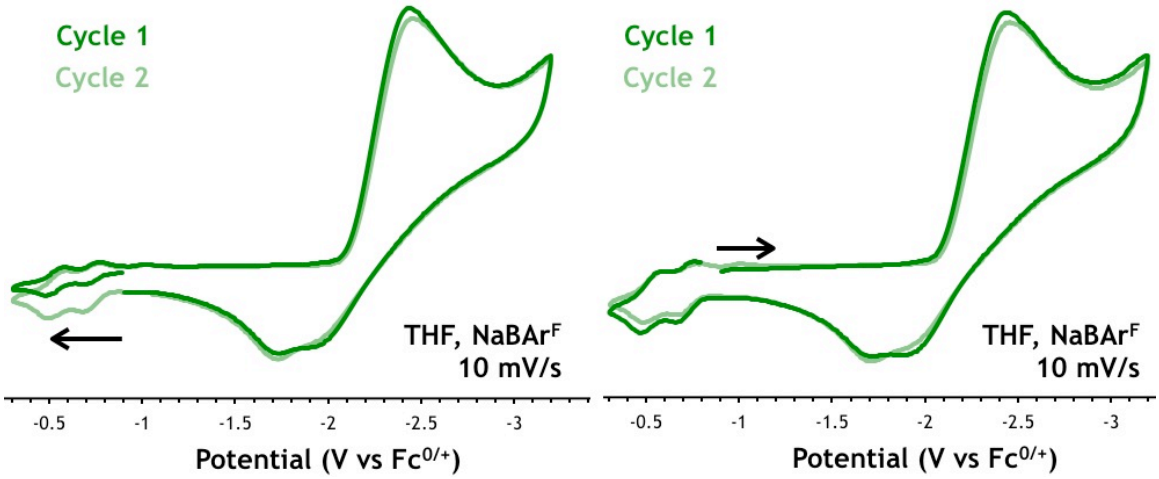


Figure S17. Oxidative and reductive potential scans in THF solution of (NN^{TBS})UI_2(THF).

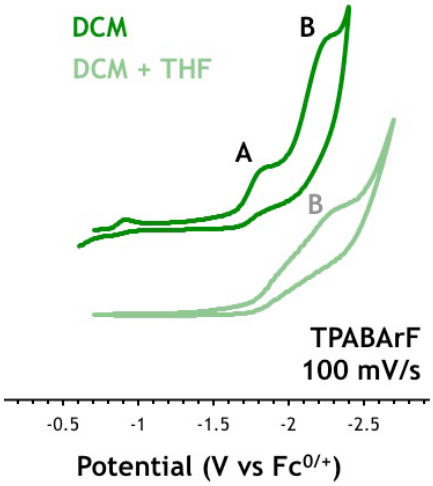


Figure S18. Reduction of (NN^{TBS})UI_2(THF) in CH_2Cl_2 before and after addition of THF.

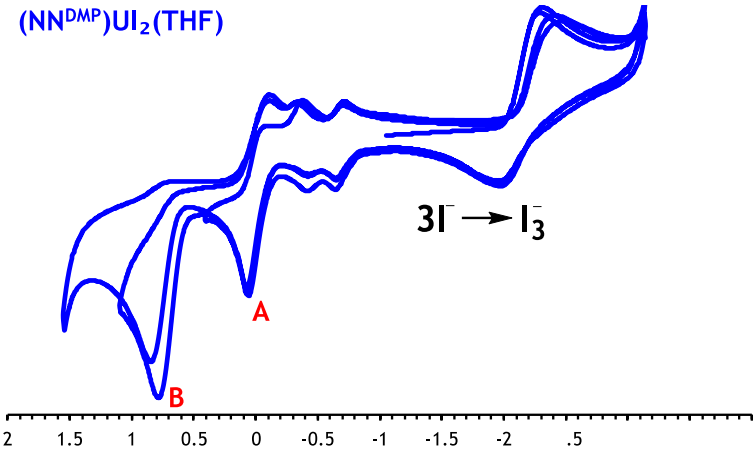


Figure S19. Effect of anodic switching potential on reduction of (NN^{DMP})UI_2(THF).

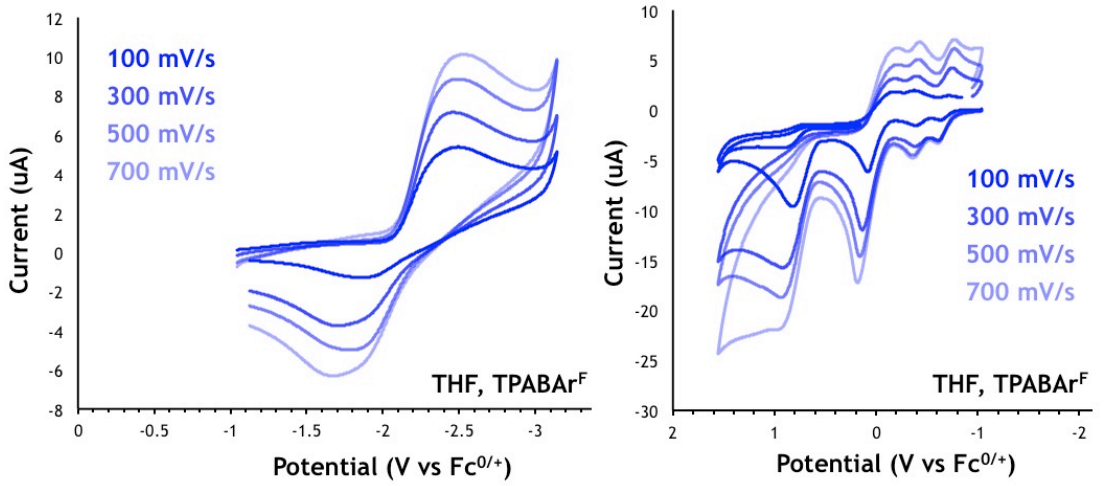


Figure S20. Cyclic voltammogram of a 1.2 mM THF solution of (NN^{DMP})UI_2(THF) with $TPABAr^F$ as the supporting electrolyte.

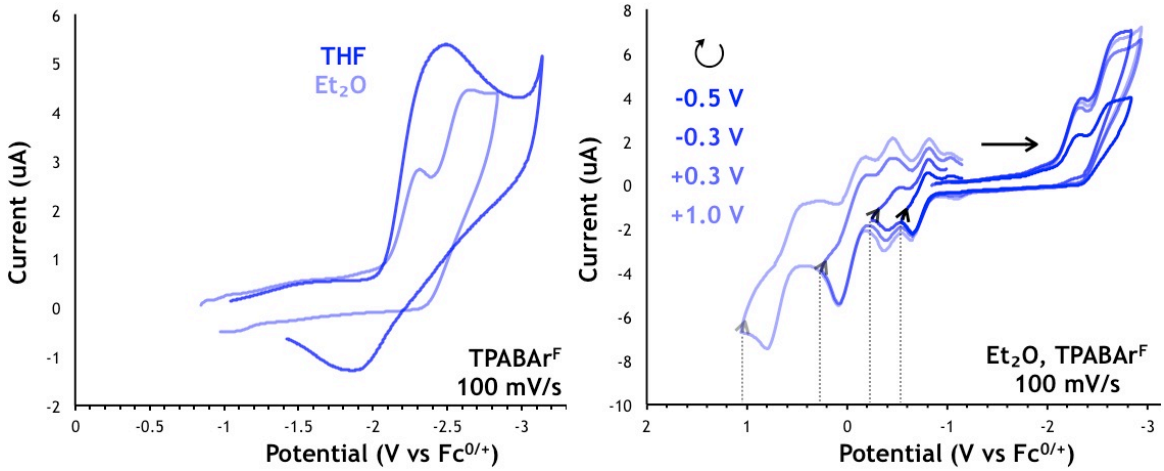


Figure S21. Cyclic voltammogram of a 1.8 mM Et_2O solution of (NN^{DMP})UI_2(THF) with $TPABAr^F$ as the supporting electrolyte: effect of switching potential (left) and addition of THF (right).

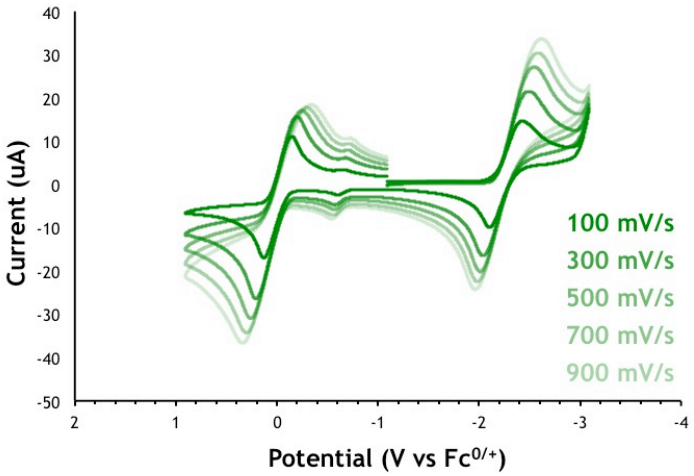


Figure S22. Cyclic voltammogram of a 3.4 mM THF solution of (NN^{TBS})UI(OAr) with $TPABAr^F$ as the supporting electrolyte.

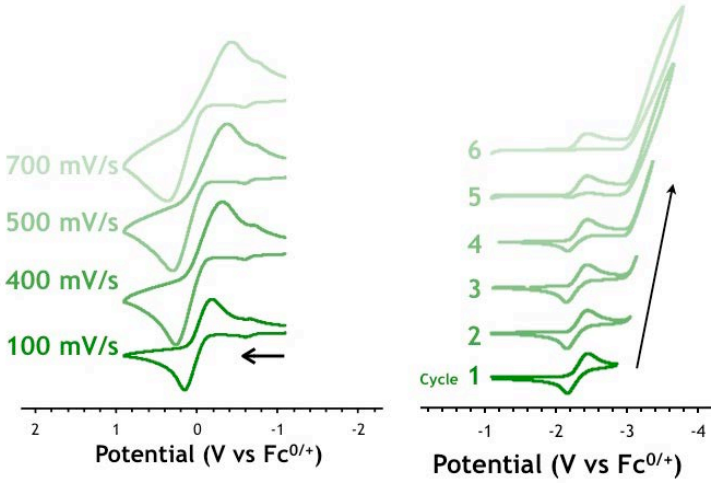


Figure S23. Effect of scan rate and negative switching potential on oxidation and reduction of (NN^{TBS})UI(OAr), respectively.

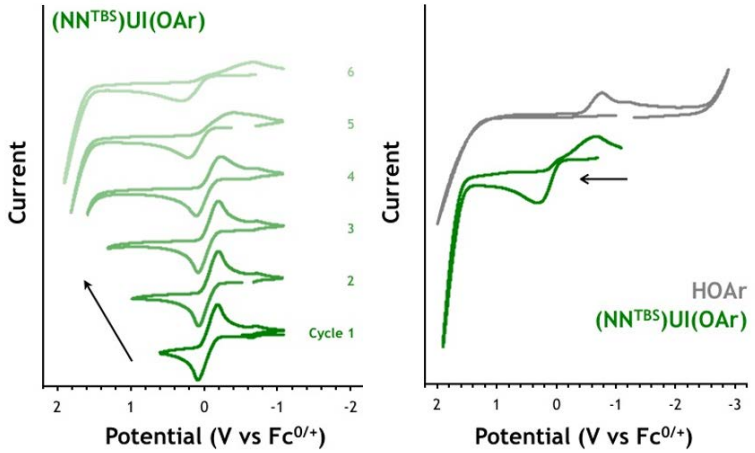


Figure S24. Effect of positive switching potential on oxidation in (NN^{TBS})UI(OAr) and its decomposition via dissociation of ArO^-.

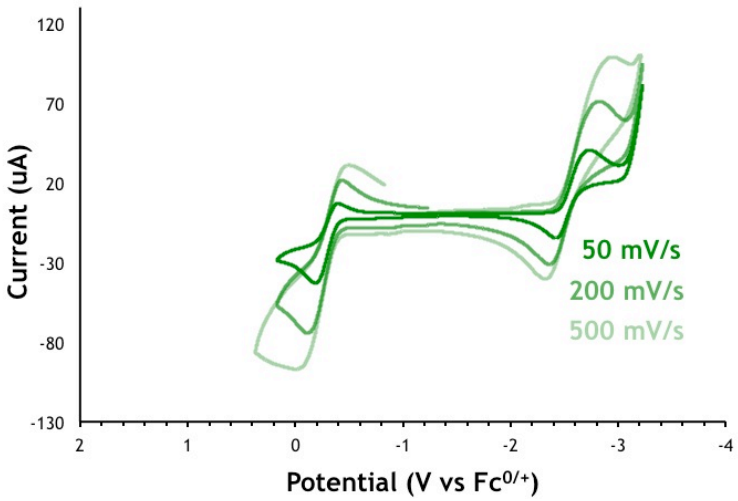


Figure S25. Cyclic voltammogram of a 3.6 mM THF solution of (NN^{TBS})U(NPh_2)$_2$ with $TPABAr^F$ as the supporting electrolyte.

UV-VIS-NIR SPECTROSCOPY

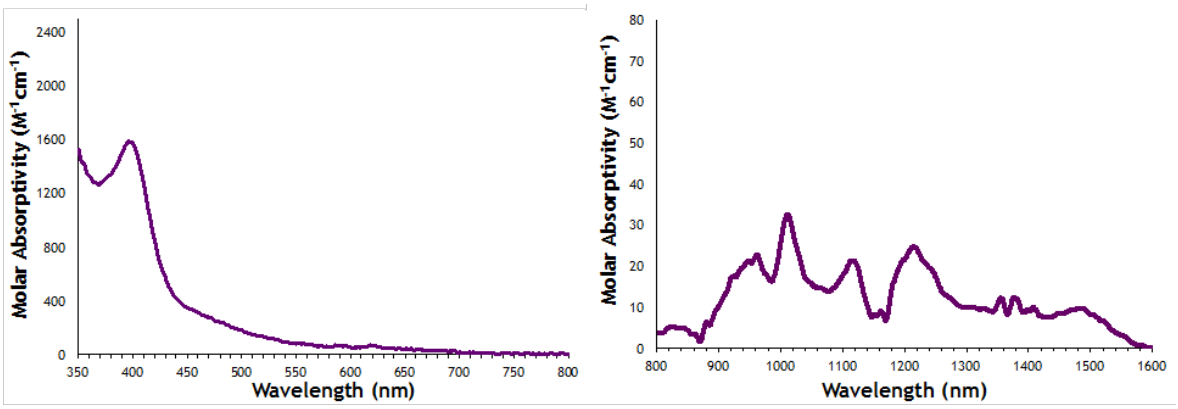


Figure S26. UV-Vis and NIR spectra of (NN^{TMS})UI_2(THF) in THF (0.53 mM and 19 mM, respectively).

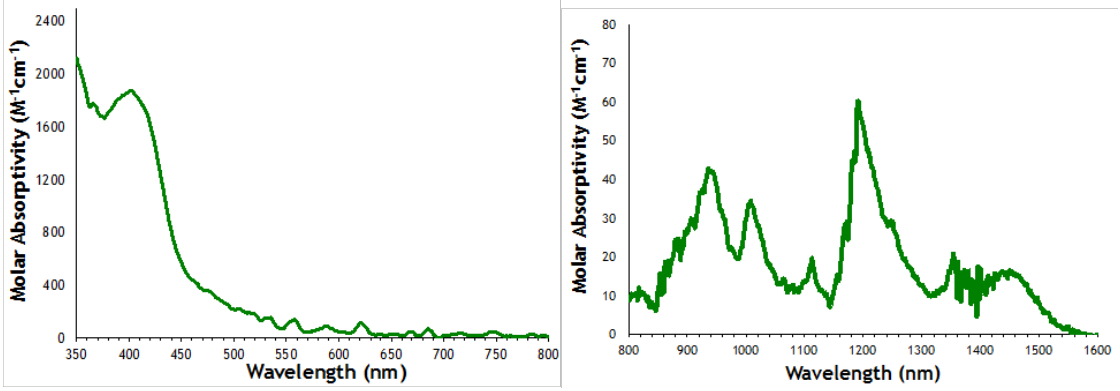


Figure S27. UV-Vis and NIR spectra of (NN^{TBS})UI_2(THF) in THF (0.38 mM and 2.6 mM, respectively).

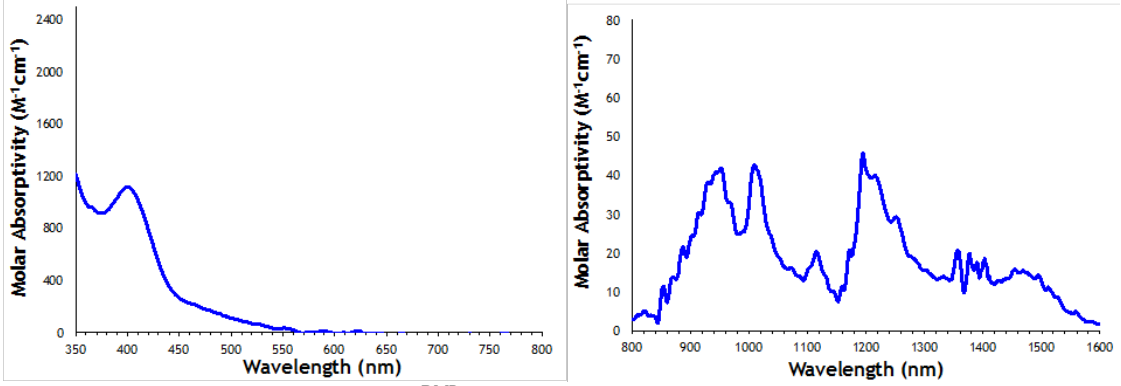


Figure S28. UV-Vis and NIR spectra of (NN^{DMP})UI_2(THF) in THF (0.67 mM and 12.2 mM, respectively).

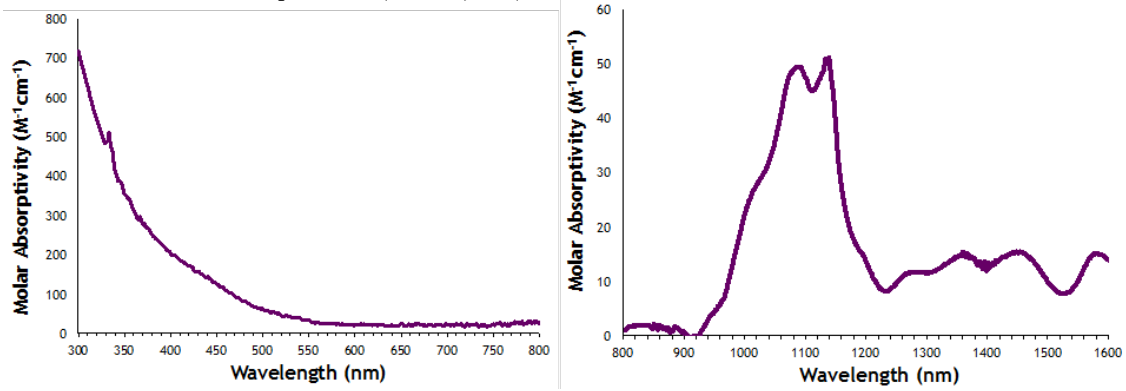


Figure S29. UV-Vis and NIR spectra of (NN^{TMS})$U(CH_2Ph)_2$ in toluene (1.0 mM and 15.9 mM, respectively).

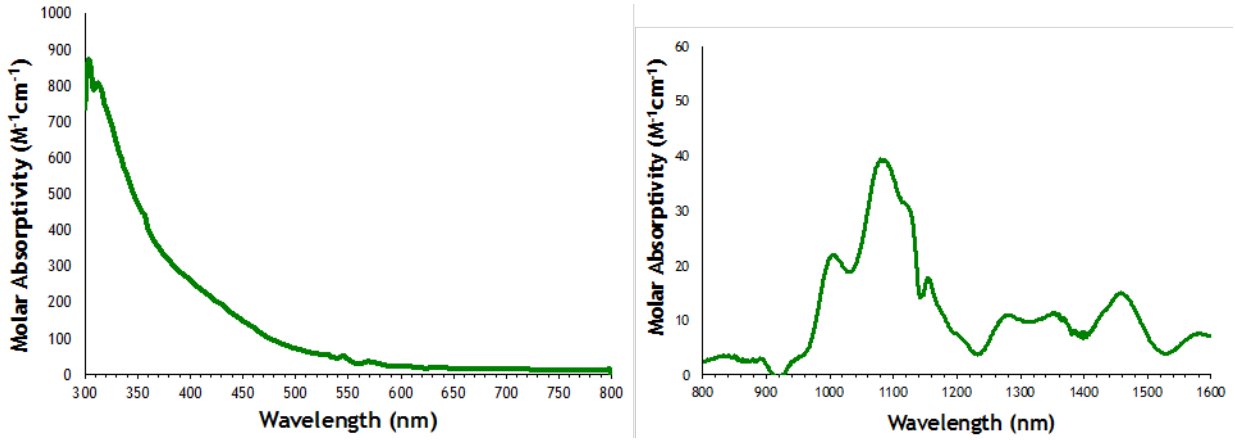


Figure S30. UV-Vis and NIR spectra of $(NN^{TBS})U(CH_2Ph)_2$ in toluene (5.0 mM and 23.4 mM, respectively).

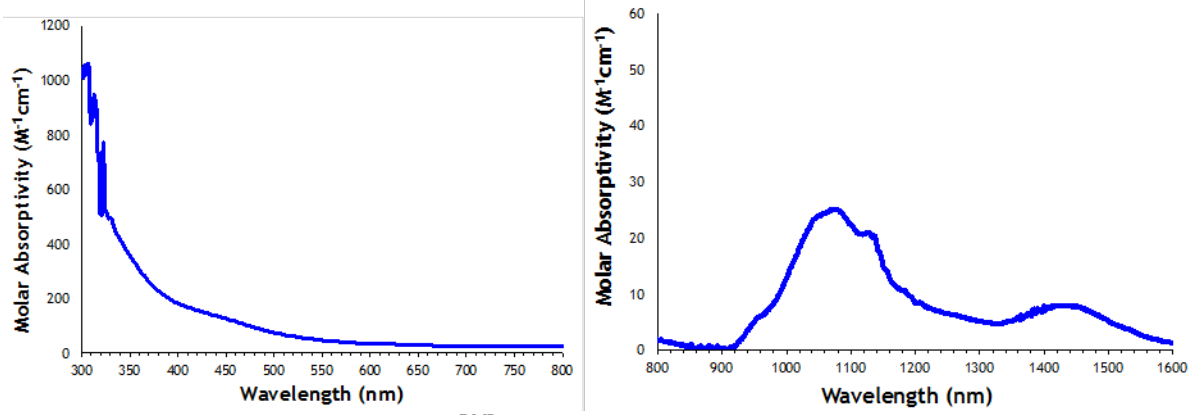


Figure S31. UV-Vis and NIR spectra of $(NN^{DMP})U(CH_2Ph)_2$ in toluene (1 mM and 22.7 mM, respectively).

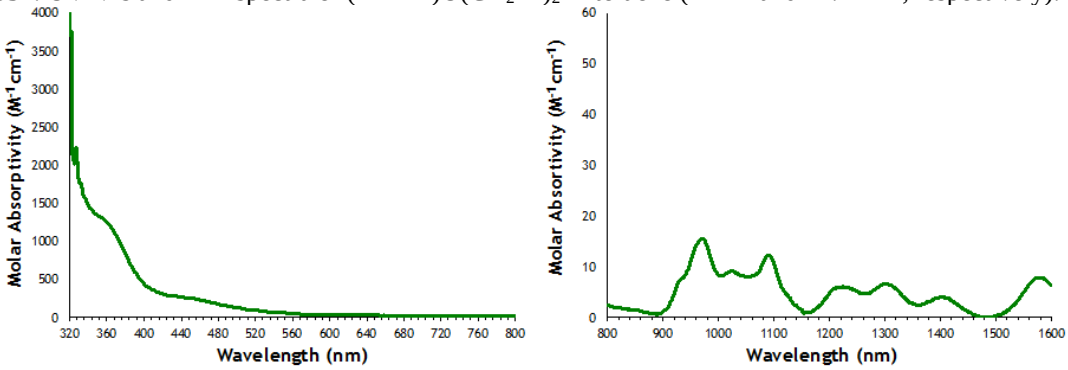


Figure S32. UV-Vis and NIR spectra of $(NN^{TBS})UI(OAr)$ in toluene (0.23 mM and 17.9 mM, respectively).

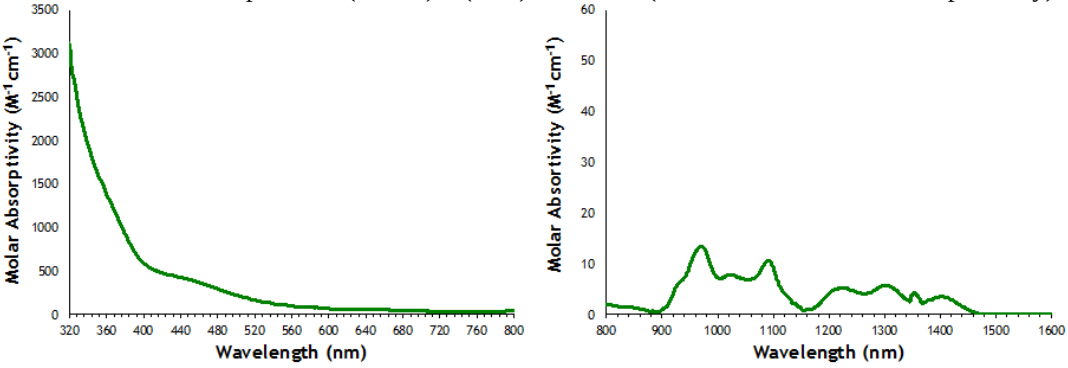


Figure S33. UV-Vis and NIR spectra of $(NN^{TBS})U(CH_2Ph)(OAr)$ in toluene (0.25 mM and 23 mM, respectively).

IR SPECTROSCOPY

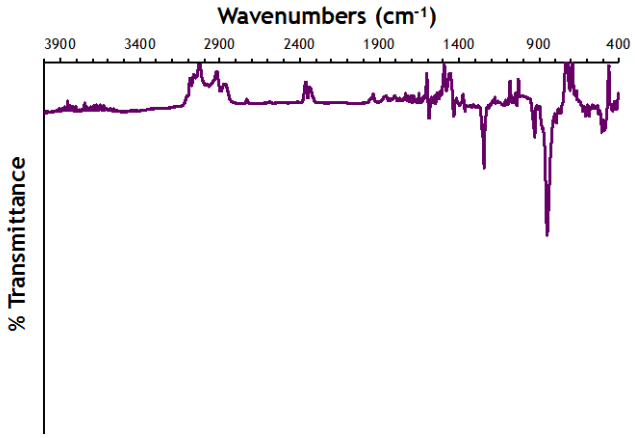


Figure S34. IR spectrum of $(NN^{TMS})U(CH_2Ph)_2$ in toluene.

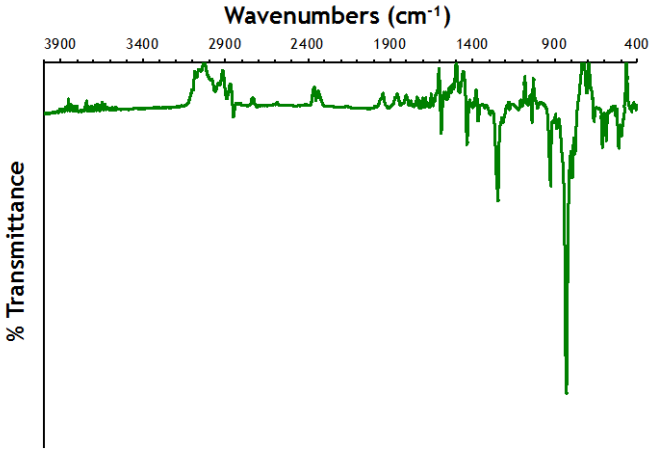


Figure S35. IR spectrum of $(NN^{TBS})U(CH_2Ph)_2$ in toluene.

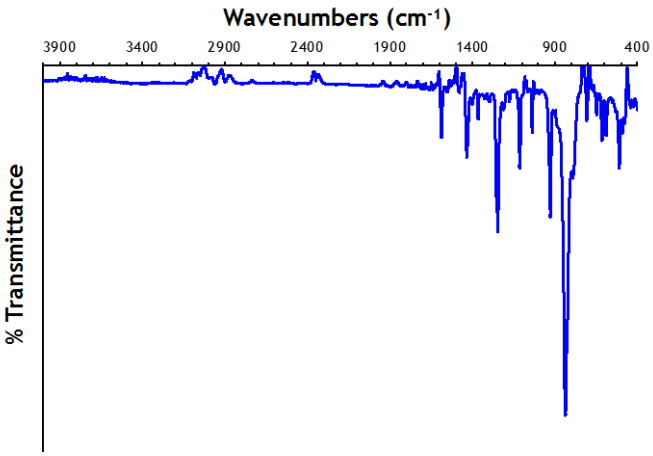


Figure S36. IR spectrum of $(NN^{DMP})U(CH_2Ph)_2$ in toluene.

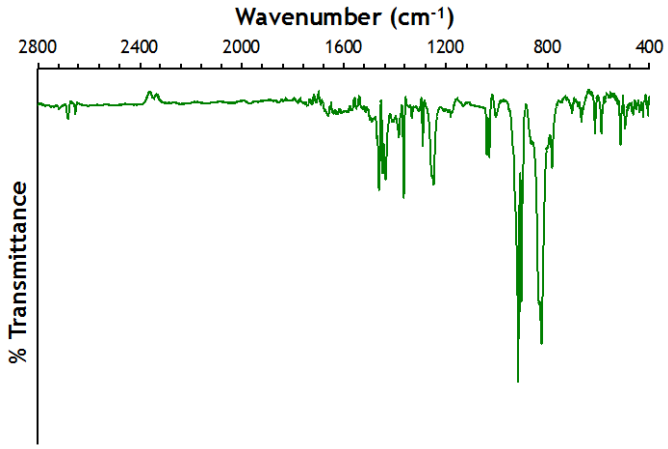


Figure S37. IR spectrum of $(NN^{TBS})UI_2(THF)$ in THF.

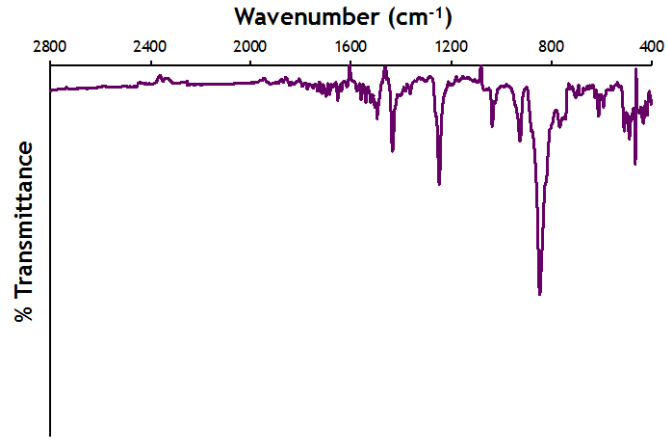


Figure S38. IR spectrum of $(NN^{TMS})UI_2(THF)$ in THF.

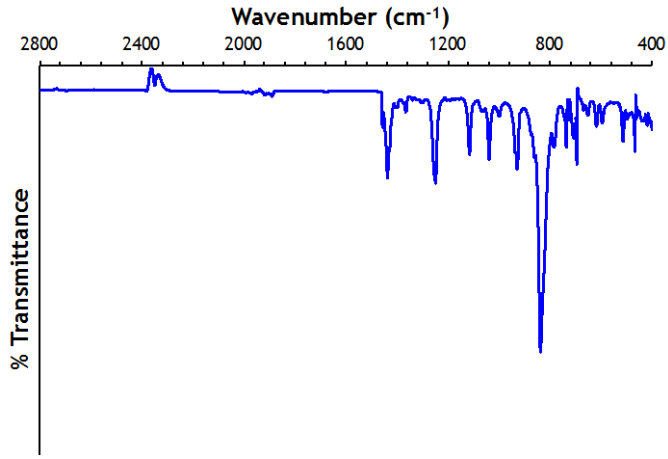


Figure S39. IR spectrum of $(NN^{DMP})UI_2(THF)$ in THF.

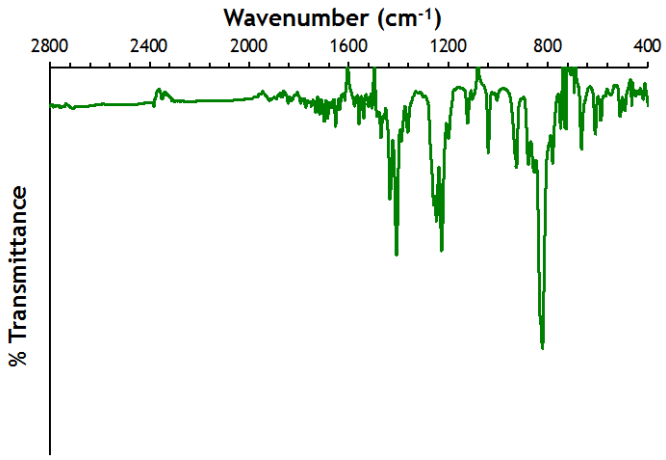


Figure S40. IR spectrum of (NN^{TBS})UI(OAr) in toluene.

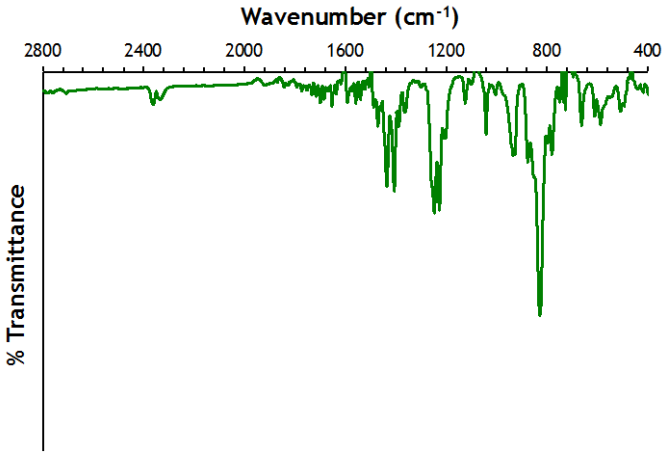


Figure S41. IR spectrum of (NN^{TBS})U(CH_2Ph)(OAr) in toluene.

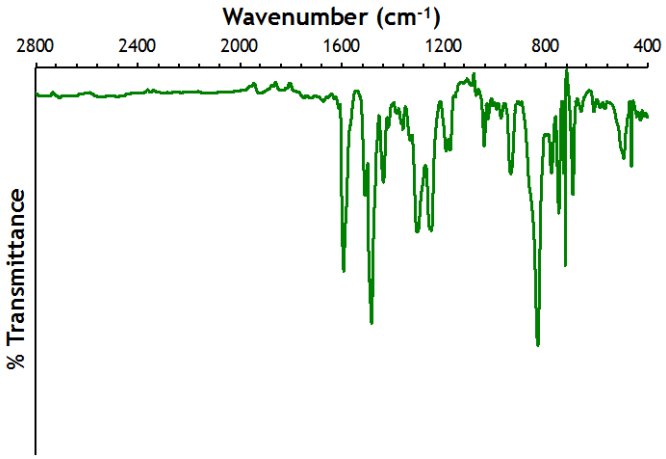


Figure S42. IR spectrum of (NN^{TBS})U(NPh_2)$_2$ in toluene.

X-RAY CRYSTALLOGRAPHY DATA

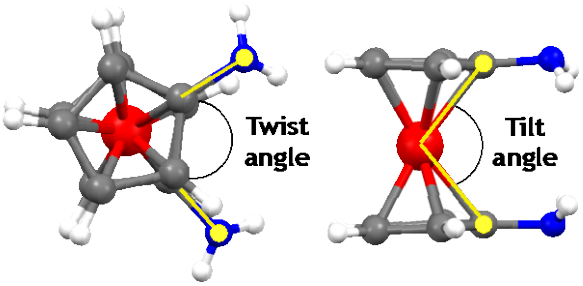


Figure S43. Graphical definitions of twist and tilt angles.

$(NN^{TBS})U(CH_2Ph)_2$

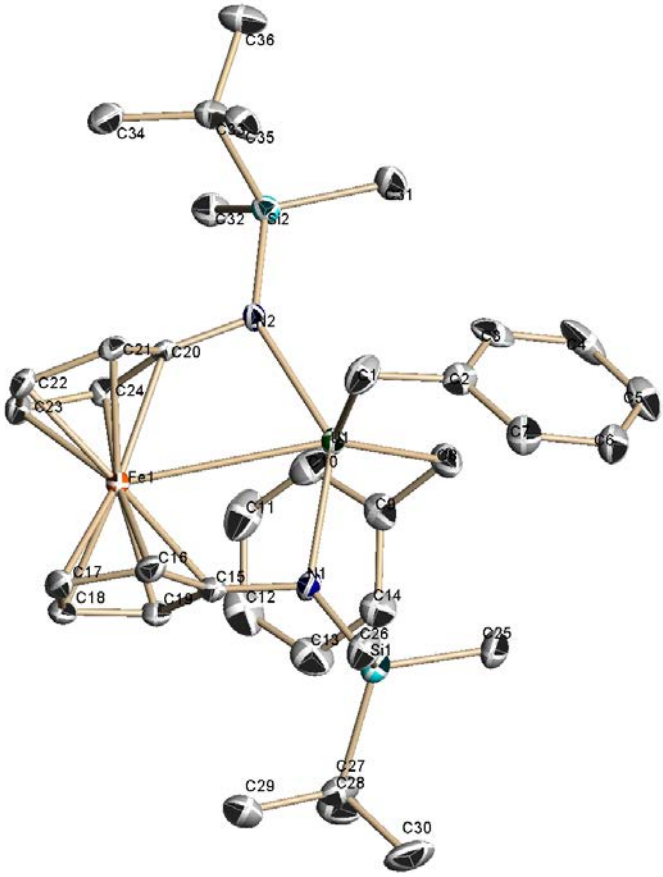


Figure S44. Thermal-ellipsoid (50% probability) representation of $(NN^{TBS})U(CH_2Ph)_2$. Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a hexanes solution at -35 ºC. A total of 15747 reflections ($-15 \le h \le 15$, $-15 \le k \le 15$, $-20 \le l \le 20$) were collected at T = 100(2) K with $2\theta_{max}$ = 56.42°, of which 8486 were unique. The residual peak and hole electron density were 2.04 and -0.67 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0289 and GOF = 1.015. Crystal and refinement data for $(NN^{TBS})U(CH_2Ph)_2$: formula $C_{36}H_{52}N_2Si_2FeU$, space group *P*-1, a = 11.8173(9), b = 11.8863(9), c = 15.3471(17), α = 105.126(1), β = 98.308(1), γ = 116.362(1)°, V = 1778.1(3) $Å^3$, Z = 2, μ = 5.050 mm^{-1}, F(000) = 856, R_1 = 0.0371 and wR_2 = 0.0617 (based on all data, $I > 2\sigma(I)$).

(NN^{DMP})U(CH$_2$Ph)$_2$

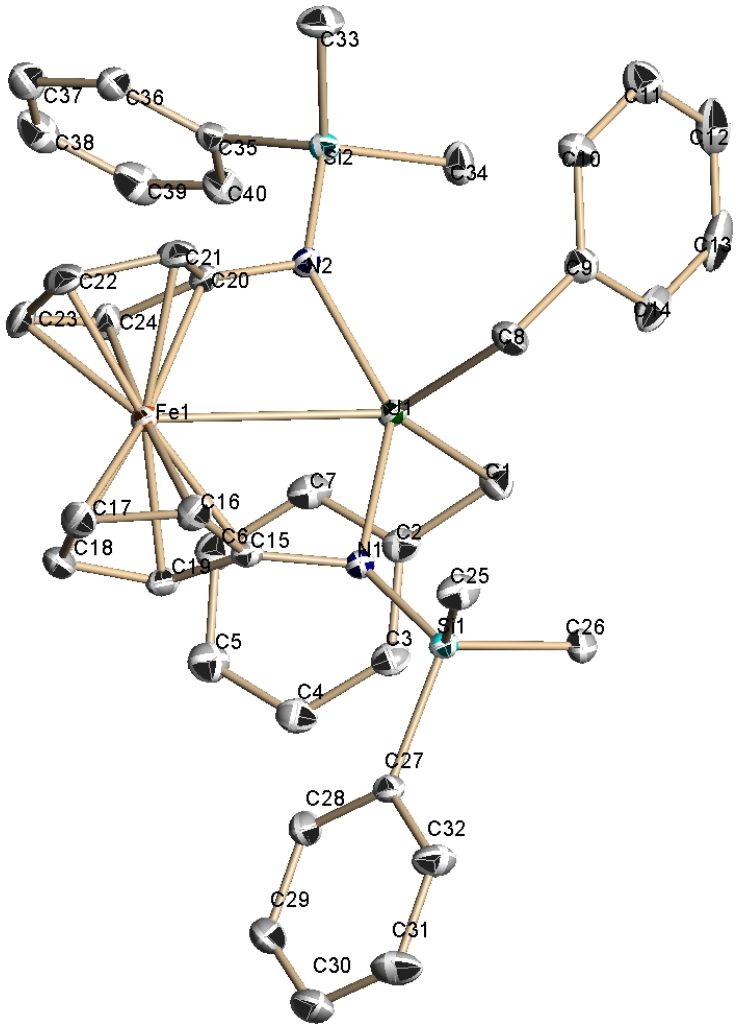


Figure S45. Thermal-ellipsoid (50% probability) representation of (NN^{DMP})U(CH$_2$Ph)$_2$. Hydrogen atoms were omitted for clarity.

Single crystals suitable for X-ray diffraction were grown from a hexanes solution at -35 ºC. A total of 18095 reflections ($-13 \le h \le 13$, $-16 \le k \le 17$, $-24 \le l \le 24$) were collected at T = 100(2) K with $2\theta_{max}$ = 61.48°, of which 10020 were unique. The residual peak and hole electron density were 1.46 and -1.30 eA^{-3}. The least-squares refinement converged normally with residuals of R_1 = 0.0188 and GOF = 1.036. Crystal and refinement data for (NN^{DMP})U(CH$_2$Ph)$_2$: formula $C_{40}H_{44}N_2Si_2FeU$, space group P-1, a = 9.8812(12), b = 11.9049(15), c = 17.141(2), α = 69.958(1), β = 75.045(1), γ = 74.617(1)°, V = 1795.1(4) Å^3, Z = 2, μ = 5.007 mm^{-1}, F(000) = 888, R_1 = 0.0201 and wR_2 = 0.0467 (based on all data, I > 2$\sigma(I)$).

DFT CALCULATIONS

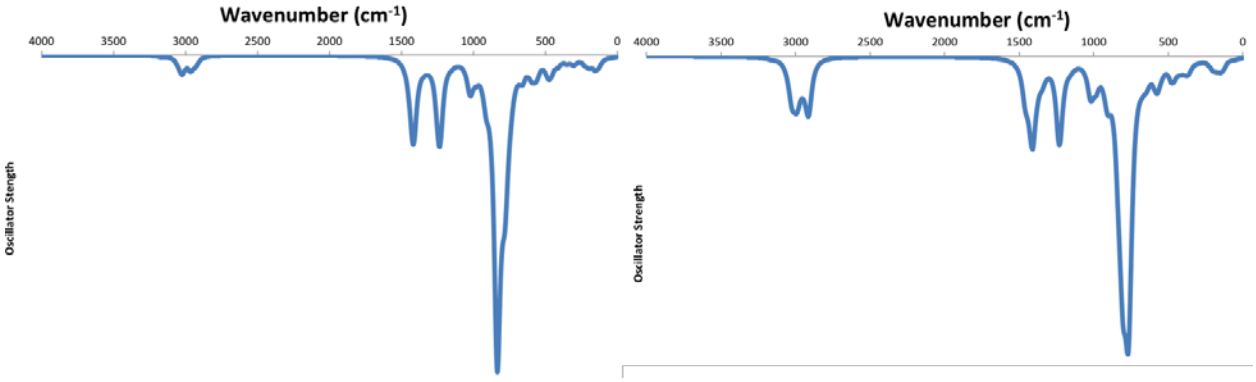


Figure S46. Calculated IR spectrum of (NN^{TMS})UI_2(THF) (left) and (NN^{TBS})UI_2(THF) (right) in the gas phase.

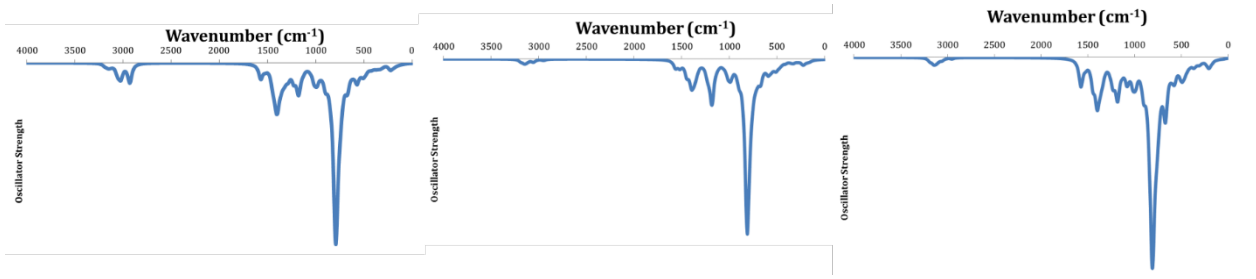


Figure S47. Calculated IR spectrum of (NN^{DMP})$U(CH_2Ph)_2$ (left), (NN^{DMP})$U(CH_2Ph)_2$ (center), and (NN^{DMP})$U(CH_2Ph)_2$ (right) in the gas phase.

Table S1. Comparison of metrical parameters from calculated (ADF) and X-ray crystal structures (experimental); distances in Å, angles in º.

	$(NN^{TBS})U(CH_2Ph)_2$		**$(NN^{DMP})U(CH_2Ph)_2$**		**$(NN^{TBS})UI_2(THF)$**		**$(NN^{TMS})UI_2(THF)$**		**$(NN^{TBS})U(CH_2Ph)(OAr)$**	
Parameter	**Exp.**	**Calc.**	**Exp.**	**Calc.**	**Exp.**	**Calc.**	**Exp.**	**Calc.**	**Exp.**	**Calc.**
Fe-U	3.19	3.21	3.19	3.21	3.18	3.20	3.23	3.26	3.20	3.24
U-N(1)	2.22	2.23	2.22	2.23	2.18	2.21	2.18	2.22	2.24	2.31
U-N(2)	2.23	2.28	2.21	2.26	2.17	2.21	2.18	2.20	2.24	2.29
U-C(1)/I(1)/C(1)	2.51	2.51	2.48	2.51	3.08	3.11	3.04	3.11	2.48	2.51
U-C(8)/I(2)/O(1)	2.48	2.50	2.47	2.52	3.07	3.11	3.03	3.09	2.14	2.11
U-C(1)-C(2)	87.6	83.6	91.6	88.4	-	-	-	-	-	-
U-C(8)-C(9)	93.0	89.2	100.6	90.5	-	-	-	-	-	-
N(1)-U-N(2)	139.8	140.5	139.1	140.0	139.7	140.1	137.4	138.0	138.6	140.6
U-N(1)-C(15)	100.8	99.7	100.9	100.0	101.6	102.0	102.4	102.8	100.5	98.8
U-N(2)-C(20)	99.0	98.6	100.3	99.8	101.7	101.9	102.5	102.7	99.6	99.5
Fe-C(20)-N(2)	128.5	129.3	128.1	129.2	127.8	129.1	128.9	129.2	129.9	129.1
Fe-C(5)-N(1)	130.4	129.9	128.9	129.2	127.4	128.8	128.3	129.2	128.9	129.3
U-N(2)-Si(2)	143.2	143.3	141.1	142.4	136.3	137.0	138.9	139.6	139.5	139.3
U-N(1)-Si(1)	133.8	139.9	131.8	139	132.9	135.2	138.9	139.4	140.3	141.9
C(15)-Fe-C(20)	121.1	121.1	121.5	121.2	121.3	121.1	120.3	120.9	121.5	121.4

Table S2. Calculated parameters for $(NN^{TMS})UI_2$**(**THF) and $(NN^{TBS})U(CH_2Ph)$(OAr).

		$(NN^{TMS})UI_2$(THF)	**$(NN^{TBS})UI_2$(THF)**	**$(NN^{DMP})UI_2$(THF)**	**$(NN^{TBS})U(CH_2Ph)$(OAr)**
Mulliken Charges	U	1.21	1.23	1.08	2.29
	Fe	0.36	0.34	0.47	0.35
Hirschfeld Charge	U	0.53	0.53	0.20	0.71
	Fe	0.06	0.06	0.07	0.06
Natural Charge	U	1.26	1.23	1.27	1.55
	Fe	0.23	0.23	0.24	0.21
Net Overlap	Fe-U	0.12	0.14	0.11	0.00
Natural bond order	Fe-U	0.17	0.22	0.15	0.03

Natural Localized Molecular Orbitals (NLMOs) of (NN^R)U(CH_2Ph)$_2$ complexes

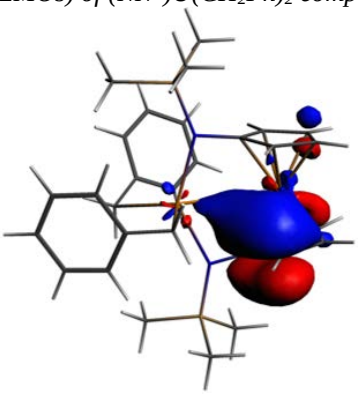


Figure S48. NLMO-189 of (NN^{TMS})U(CH_2Ph)$_2$.

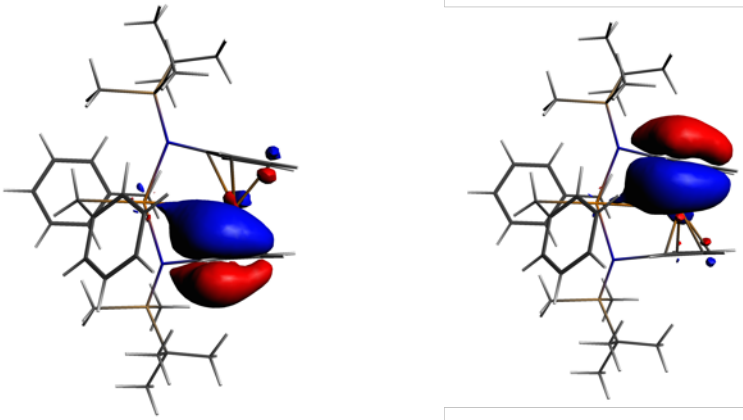


Figure S49. NLMO-213 (left) and NLMO-214 (right) of (NN^{TBS})U(CH_2Ph)$_2$.

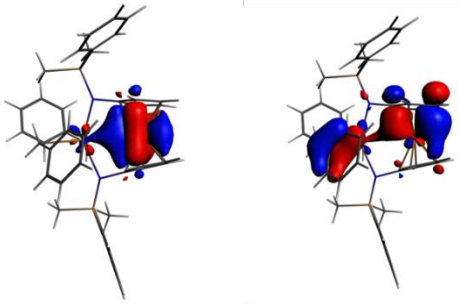


Figure S50. NLMO-212 (left) and NLMO-219 (right) of (NN^{DMP})U(CH_2Ph)$_2$.

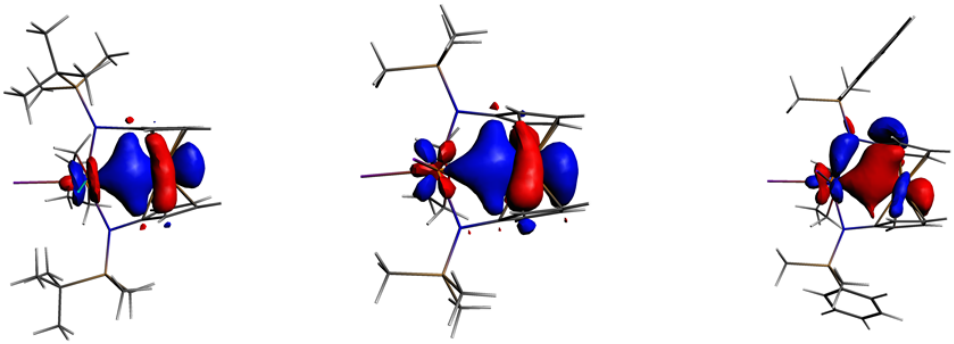


Figure S51. NLMO-212 of (NN^{TBS})UI_2(THF) (left), NLMO-232 of (NN^{TMS})UI_2(THF) (center), and NLMO-240 of (NN^{DMP})UI_2(THF) (right).

Bader Analysis of (NN^R)UX_2 complexes

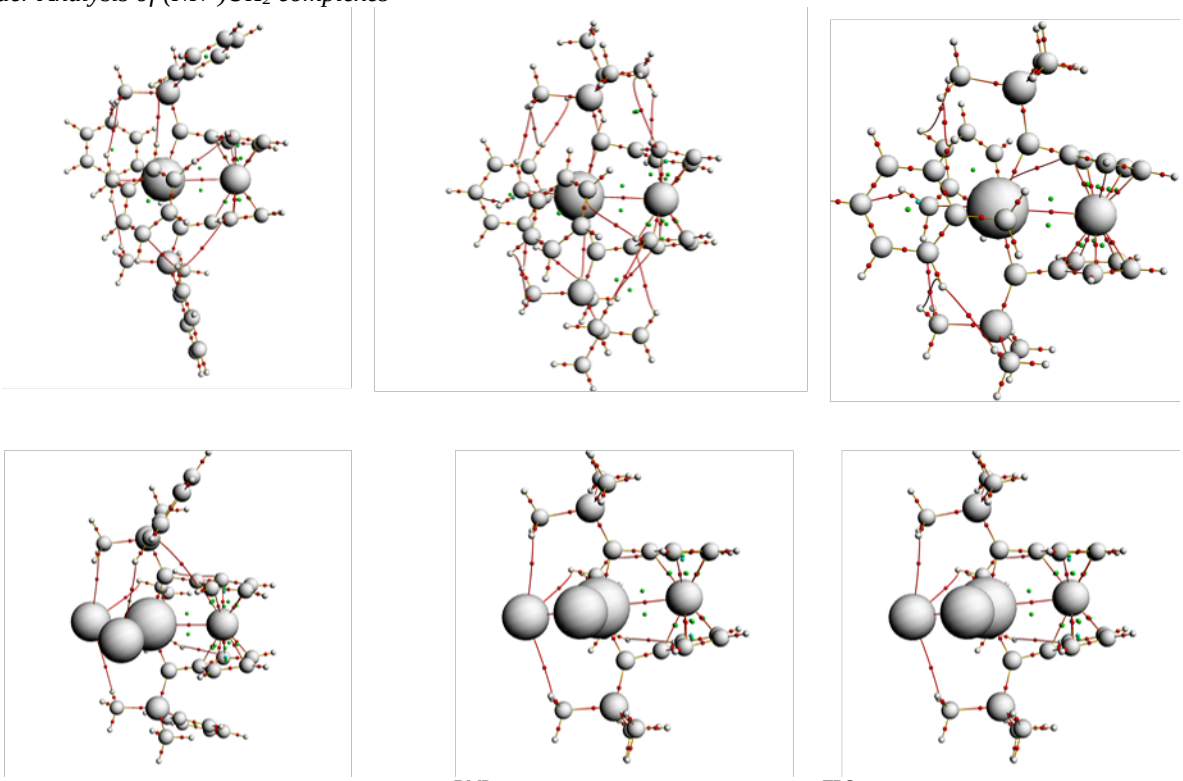


Figure S52. Plot of critical points for (NN^{DMP})$U(CH_2Ph)_2$ (upper left), (NN^{TBS})$U(CH_2Ph)_2$ (upper middle), and (NN^{TMS})$U(CH_2Ph)_2$ (upper right). Critical points for (NN^{DMP})UI_2(THF) (lower left), (NN^{TMS})UI_2(THF) (lower middle) and (NN^{TBS})UI_2(THF) (lower right).

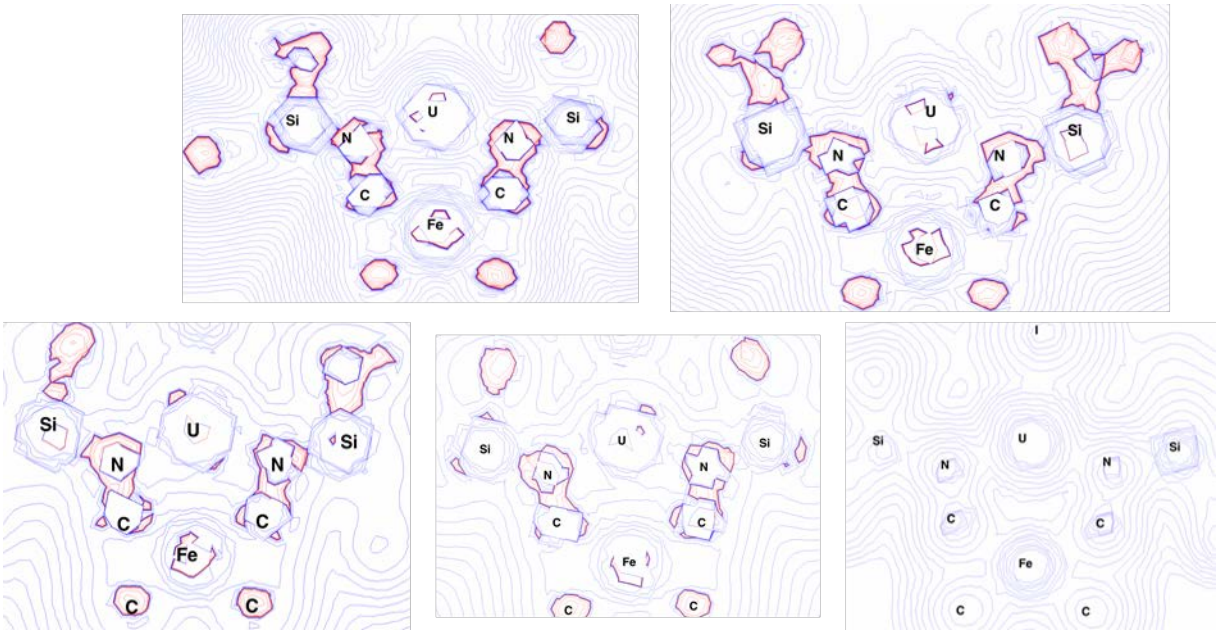


Figure S53. Contour plot of the Laplacian for (NN^{DMP})$U(CH_2Ph)_2$ (top left), (NN^{TMS})$U(CH_2Ph)_2$ (top right), (NN^{DMP})UI_2THF (bottom left), (NN^{TMS})UI_2THF (bottom center), and (NN^{TBS})UI2THF (bottom right). The cut plane is taken through the common plane of the iron, uranium and nitrogens for each complex.

Molecular Orbitals for $(NN^R)U(CH_2Ph)_2$ complexes

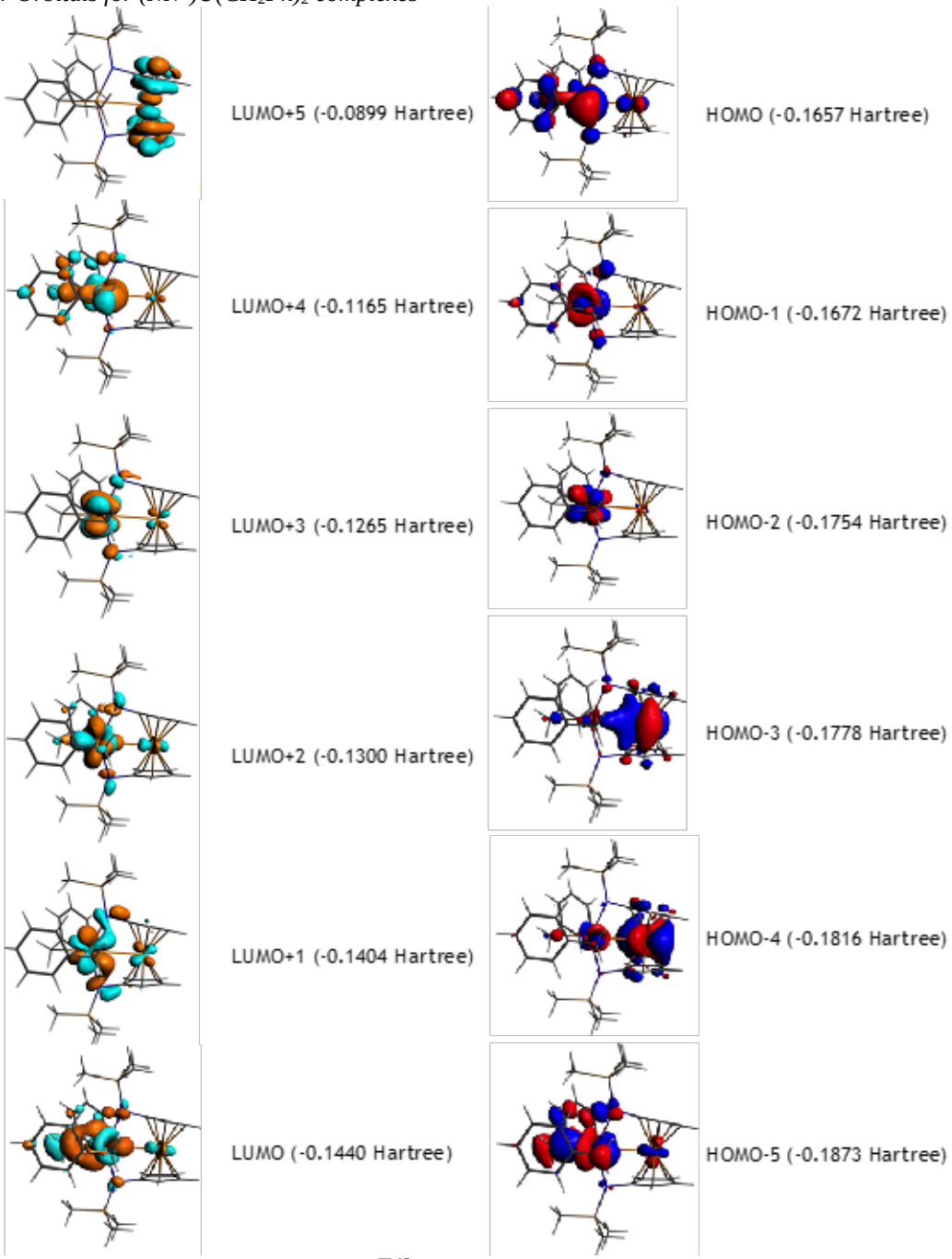


Figure S54. Selected molecular orbitals of $(NN^{TMS})U(CH_2Ph)_2$.

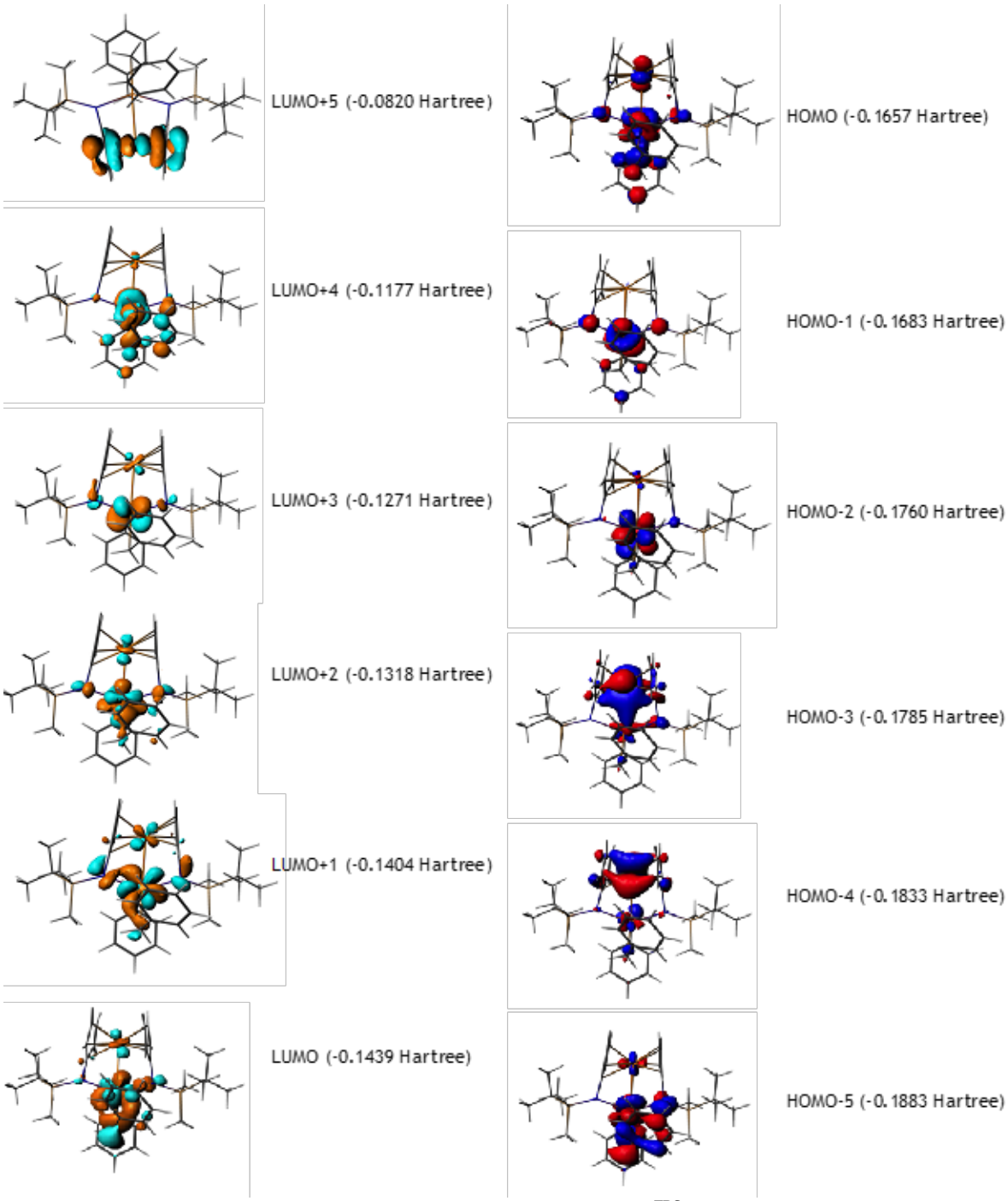


Figure S55. Selected molecular orbitals (isosurface value = 0.02) for $(NN^{TBS})U(CH_2Ph)_2$.

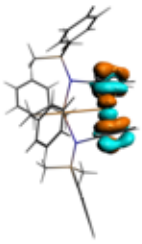
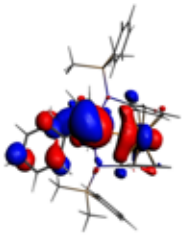
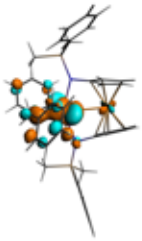
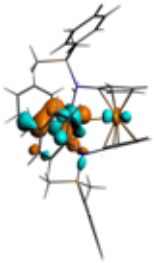
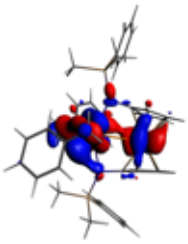
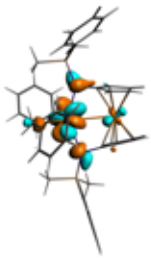
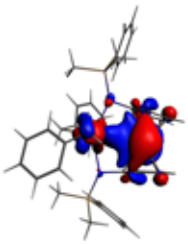
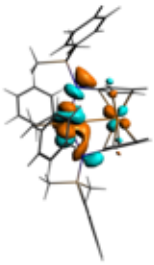
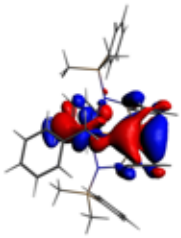
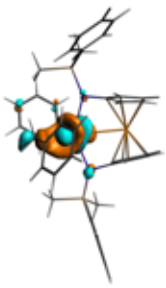
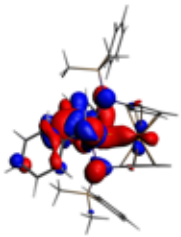
	MO	Energy (Hartree)		MO	Energy (Hartree)
	LUMO+5	-0.0810		HOMO	-0.1645
	LUMO+4	-0.1242		HOMO-1	-0.1737
	LUMO+3	-0.1348		HOMO-2	-0.1773
	LUMO+2	-0.1383		HOMO-3	-0.1800
	LUMO+1	-0.1438		HOMO-4	-0.1830
	LUMO	-0.1440		HOMO-5	-0.1928

Figure S56. Selected molecular orbitals for $(NN^{DMP})U(CH_2Ph)_2$.

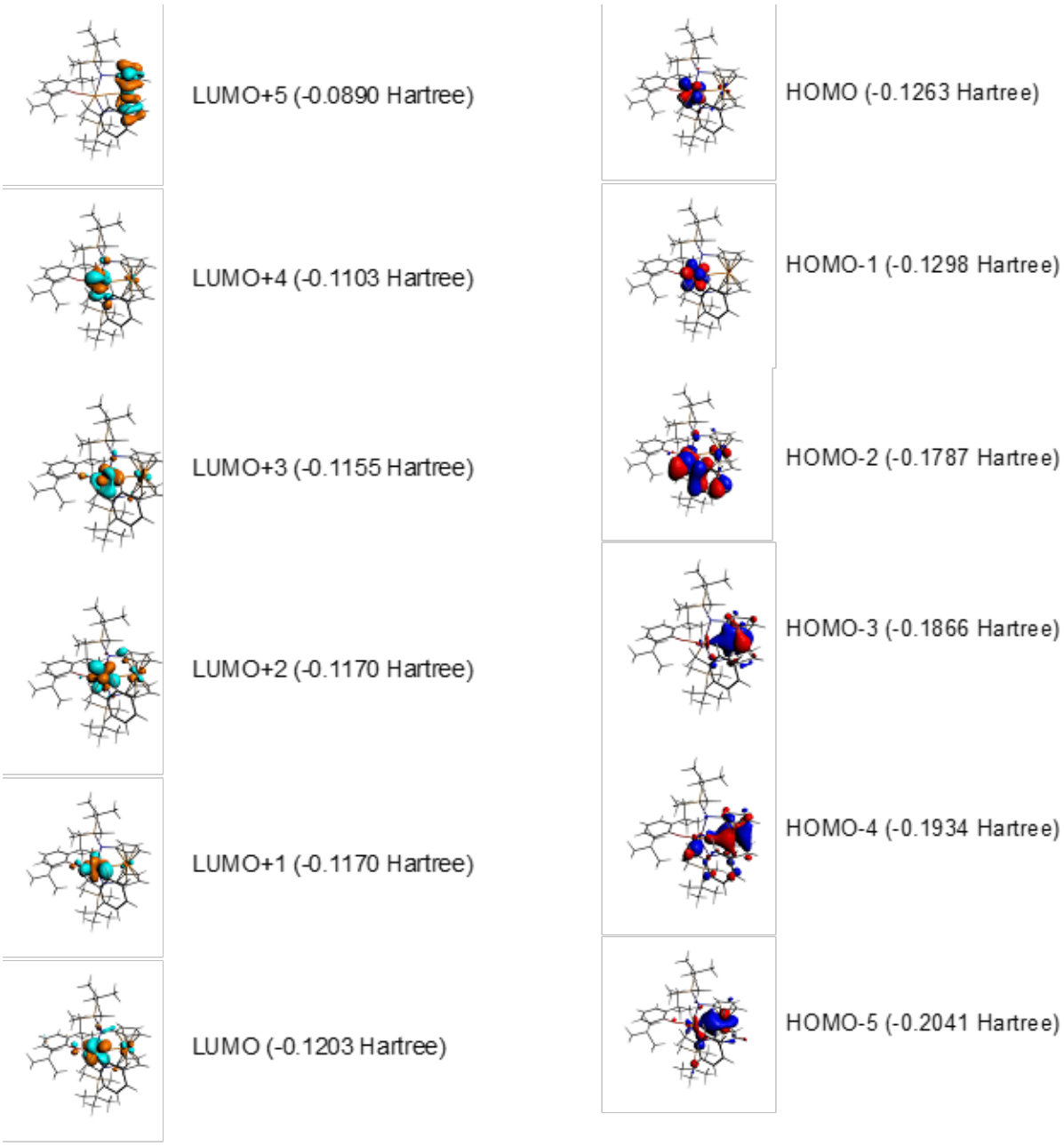


Figure S57. Selected molecular orbitals for (NN^{TBS})U(CH_2Ph)(OAr).

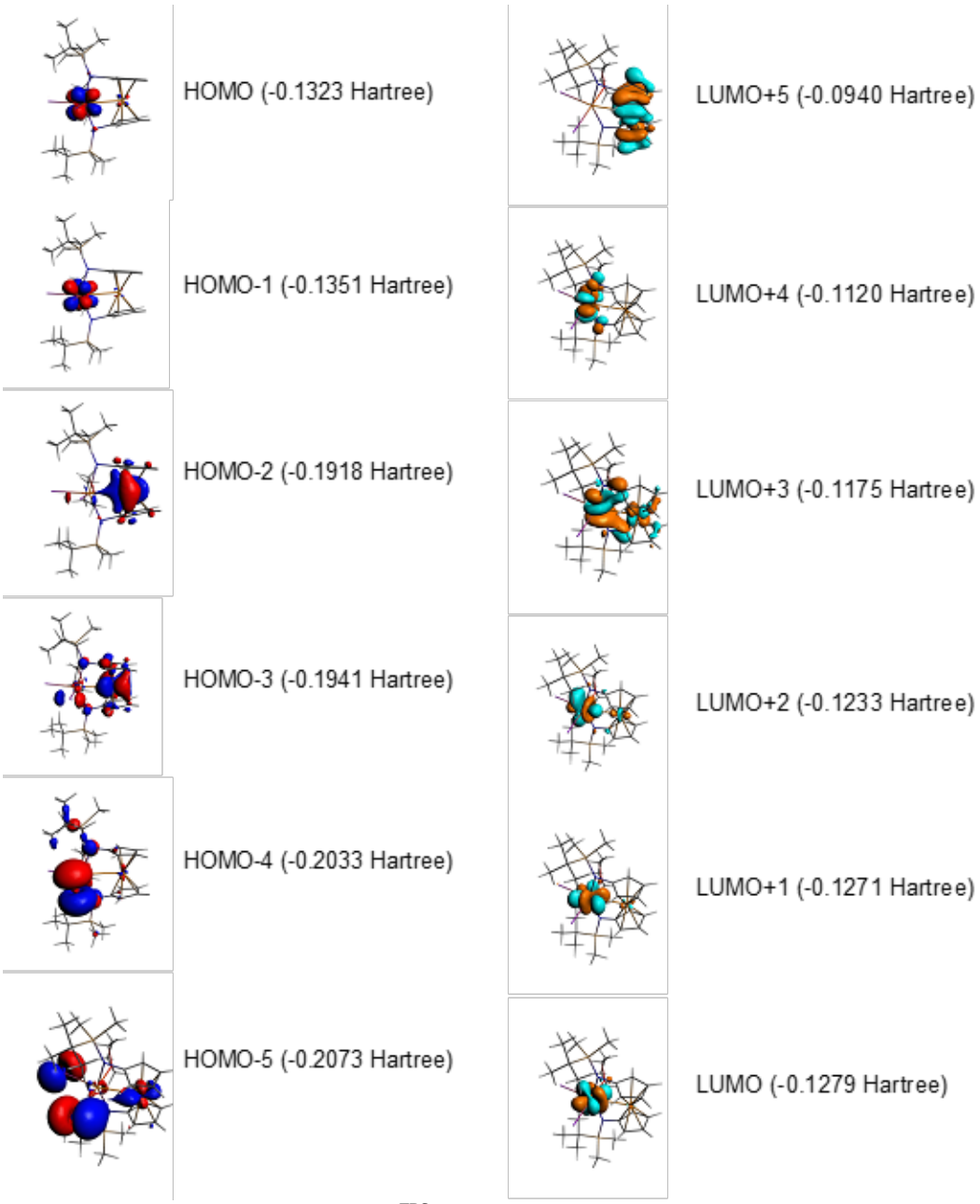


Figure S58. Selected molecular orbitals for $(NN^{TBS})UI_2(THF)$.

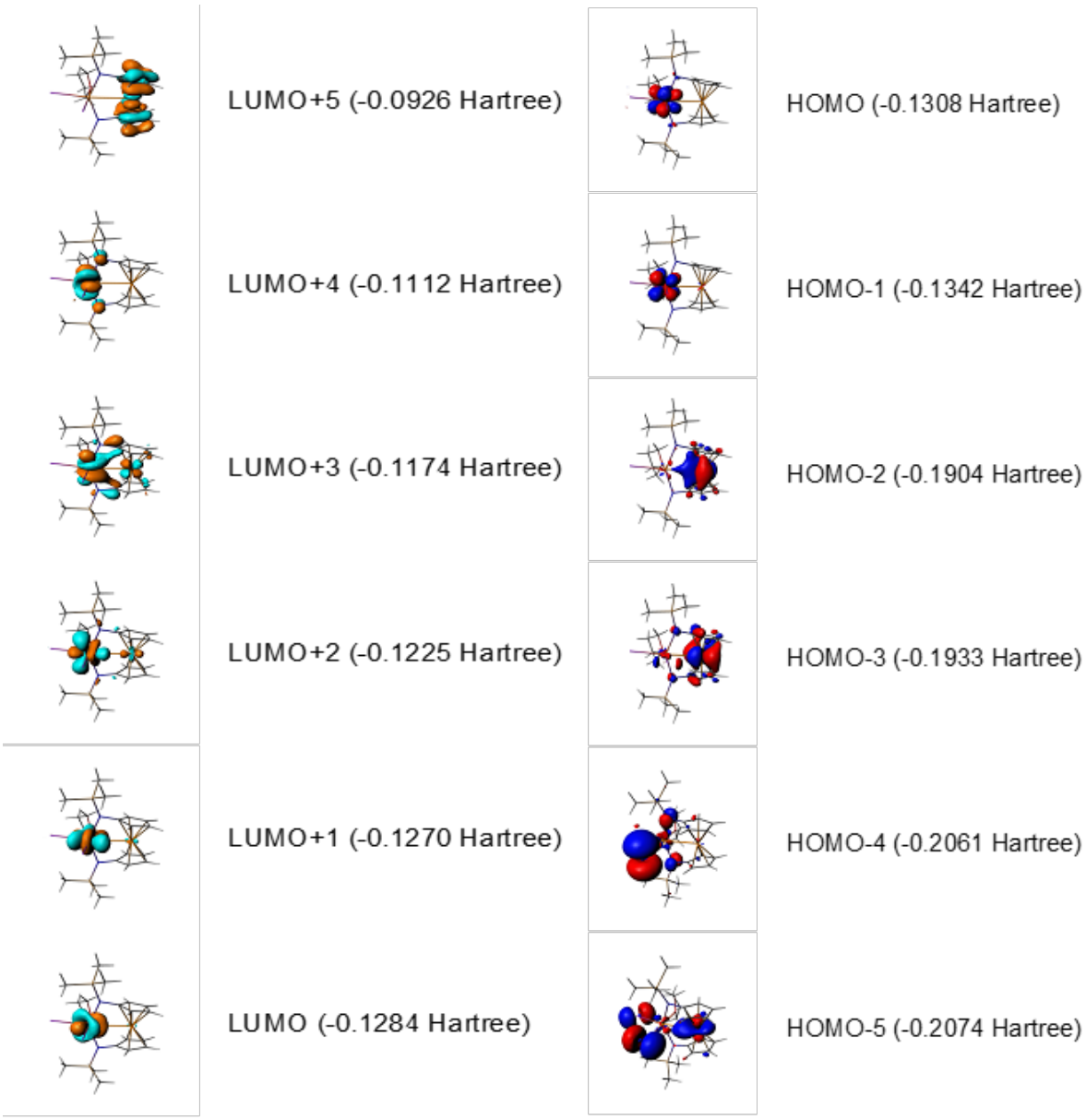


Figure S59. Selected molecular orbitals for $(NN^{TMS})UI_2(THF)$.

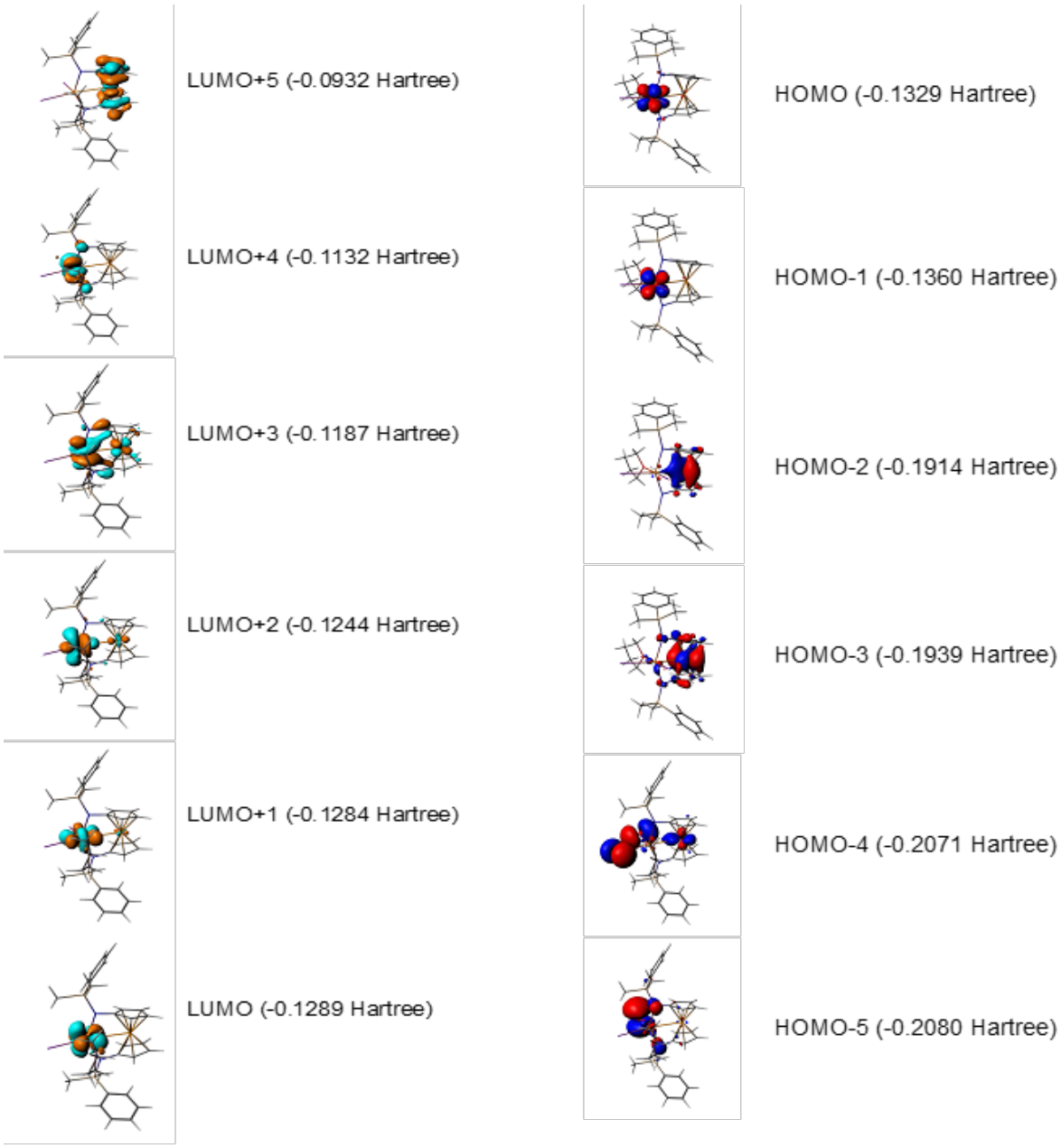


Figure S60. Selected molecular orbitals for $(NN^{DMP})UI_2(THF)$.

Optimized coordinates

Table S3. (NN^{TMS})U(CH_2Ph)$_2$

Atom	X	Y	Z
U	5.004389	3.399709	10.63334
Fe	6.114172	6.308625	11.562887
Si	1.792509	5.28991	9.720324
Si	8.436721	2.092874	11.725662
N	3.446102	4.986723	10.288532
N	7.140406	3.243373	11.357909
C	4.065333	2.761863	12.883313
C	7.981437	5.603174	10.936548
C	4.874071	7.885902	12.066369
C	3.713436	1.566386	12.163723
C	4.649076	0.510665	11.970515
C	8.19939	0.532477	10.695065
C	4.357449	-0.589644	11.168613
C	5.406247	8.073548	10.7485
C	3.146415	-0.674498	10.481971
C	1.132502	3.775817	8.812307
C	2.230978	0.372556	10.606325
C	4.977522	6.984026	9.937593
C	2.511023	1.475623	11.407264
C	8.421142	1.660127	13.569357
C	5.08645	1.741071	8.748776
C	7.376139	4.570237	11.745047
C	7.088836	5.166317	13.031038
C	5.248777	2.850515	7.845753
C	6.386874	3.699877	7.944366
C	10.117243	2.849647	11.300251
C	6.487218	4.879106	7.198952
C	7.567035	6.50885	13.024325
C	5.465896	5.262971	6.338048
C	1.775825	6.763223	8.536992
C	4.335344	4.439984	6.220538
C	8.121784	6.777408	11.730413
C	4.223591	3.274872	6.957024
C	0.67871	5.670712	11.203596
C	4.13272	6.124782	10.734915
C	4.114535	6.679806	12.06961
H	3.232508	3.397584	13.201566
H	4.845973	2.650673	13.643458
H	8.314047	5.472145	9.910393
H	5.029037	8.548069	12.914807
H	5.578569	0.530019	12.541511
H	8.963198	-0.211004	10.981451
H	8.323704	0.732487	9.61907
H	7.21323	0.06918	10.840435
H	5.08616	-1.397461	11.083864
H	6.033718	8.901636	10.427723
H	2.919767	-1.540468	9.860413
H	1.548661	3.716466	7.795757
H	0.035245	3.852726	8.721846
H	1.36282	2.831666	9.325852
H	1.277452	0.32467	10.077507
H	5.197086	6.823371	8.884005
H	1.75932	2.256755	11.533537
H	9.228793	0.948045	13.812212
H	7.468804	1.20159	13.879904
H	8.57724	2.559364	14.187954
H	4.248585	1.062386	8.56109
H	6.011074	1.206416	9.006136
H	6.617114	4.649475	13.862777
H	7.234223	3.377073	8.554321
H	10.294399	3.789736	11.848591
H	10.207212	3.064318	10.22271
H	10.927577	2.149596	11.567976
H	7.388328	5.489413	7.27929
H	7.518962	7.210047	13.853942
H	5.551455	6.172915	5.743866
H	2.112452	7.691792	9.026718
H	0.755145	6.935968	8.153666
H	2.434666	6.577431	7.672686
H	3.537593	4.715637	5.528644
H	8.56605	7.716948	11.410706
H	3.348441	2.635183	6.837535
H	0.635068	4.82487	11.908613
H	-0.352187	5.883301	10.871209
H	1.036105	6.55435	11.757418
H	3.577243	6.251246	12.911803

Table S4. (NN^{TBS})U(CH_2Ph)$_2$

Atom	X	Y	Z
U	4.982705	3.433941	10.670898
Fe	6.099121	6.309963	11.539004
Si	1.716543	5.189734	9.835573
Si	8.49434	2.122361	11.569252
N	3.450055	5.032395	10.185593
N	7.100526	3.217533	11.496841
C	3.892467	2.791933	12.84344
C	3.558885	1.582678	12.131454
C	4.517639	0.547382	11.9531
C	4.255663	-0.566433	11.159304
C	3.047597	-0.686826	10.474674
C	2.10108	0.332572	10.599937
C	2.352777	1.447111	11.391993
C	4.95652	1.805667	8.769434
C	5.328627	2.875756	7.875875
C	6.581349	3.532777	8.02174
C	6.909156	4.664463	7.269447
C	6.00538	5.190424	6.353422
C	4.760701	4.563247	6.194875
C	4.424636	3.448312	6.941289
C	4.165914	6.169265	10.573762
C	4.100618	6.855105	11.845253
C	4.938958	8.005435	11.780092
C	5.579438	8.018951	10.498079
C	5.131507	6.88112	9.767196
C	7.307968	4.544666	11.895229
C	6.854475	5.158836	13.124441
C	7.348949	6.494591	13.17535
C	8.075177	6.745247	11.966339
C	8.017461	5.570306	11.163302
C	1.191691	3.667907	8.844202
C	0.744294	5.265667	11.464725
C	1.274071	6.755916	8.793551
C	2.099253	6.798209	7.496629
C	1.497721	8.063193	9.574478
C	-0.219671	6.666657	8.418913
C	8.052351	0.515275	10.681897
C	9.990289	2.864098	10.668072
C	9.000504	1.745123	13.396797
C	9.677364	2.971647	14.037519
C	7.764187	1.36333	14.226404
C	9.998562	0.572052	13.428846
H	4.639711	2.676154	13.637164
H	3.050029	3.426987	13.138415
H	5.445647	0.601481	12.523627
H	5.00501	-1.355507	11.077925
H	2.844072	-1.561199	9.856823
H	1.146742	0.254865	10.076305
H	1.579875	2.208171	11.5088
H	5.777507	1.136783	9.061019
H	4.044634	1.249976	8.527518
H	7.334941	3.094725	8.679104
H	7.892602	5.122073	7.388351
H	6.265704	6.061913	5.752376
H	4.049371	4.956744	5.467601
H	3.457096	2.966283	6.796165
H	3.479364	6.551989	12.684358
H	5.079595	8.741071	12.568583
H	6.284668	8.768036	10.145899
H	5.418153	6.600657	8.754942
H	6.277046	4.654723	13.895335
H	7.203152	7.200135	13.989689
H	8.568906	7.677206	11.702074
H	8.467283	5.435504	10.183581
H	1.750526	2.768778	9.141647
H	1.362067	3.822526	7.767493
H	0.118299	3.459901	8.987953
H	0.945008	4.380428	12.088988
H	-0.34331	5.303658	11.284219
H	1.013484	6.154356	12.057957
H	1.808197	7.679517	6.894514
H	1.93145	5.905044	6.874983
H	3.178109	6.869423	7.697985
H	1.17374	8.92257	8.957432
H	2.556452	8.221985	9.830384
H	0.911065	8.090516	10.506877
H	-0.498551	7.54333	7.804949
H	-0.871313	6.66934	9.307723
H	-0.448374	5.765272	7.827767
H	7.84242	0.693125	9.615454
H	7.182861	-0.001002	11.112056
H	8.910376	-0.175729	10.727343
H	9.773943	3.010408	9.596524
H	10.852433	2.177961	10.731754
H	10.303716	3.832727	11.087781
H	9.942645	2.74501	15.087362
H	9.023095	3.857354	14.044639
H	10.608399	3.243184	13.514861
H	8.05272	1.17156	15.276619
H	7.284276	0.446051	13.849594
H	7.011236	2.164645	14.22524
H	10.321648	0.386663	14.470325
H	10.905914	0.783194	12.839553
H	9.553234	-0.362063	13.051661

Table S5. (NN^{DMP})U(CH_2Ph)$_2$

Atom	X	Y	Z
U	12.148563	12.055158	10.689361
Fe	10.085119	13.655705	12.55376
Si	14.436869	15.031617	11.010221
Si	9.562192	9.253408	10.69451
N	13.102693	13.966648	11.428933
N	10.244677	10.865264	10.931471
C	13.993191	10.332492	10.736736
C	14.105351	10.472345	12.170648
C	15.254169	11.019525	12.800607
C	15.29211	11.253237	14.164273
C	14.176244	10.992491	14.973447
C	13.028377	10.474328	14.385124
C	12.98937	10.217054	13.01165
C	11.500581	13.23083	8.56074
C	11.816778	12.017038	7.842173
C	10.824315	11.169192	7.280469
C	11.153715	9.962556	6.690461
C	12.483368	9.512616	6.661201
C	13.47229	10.301612	7.232793
C	13.148581	11.529181	7.820073
C	12.069108	14.45879	12.234428
C	11.032022	15.387463	11.845871
C	10.232162	15.671749	12.989984
C	10.724355	14.887998	14.08395
C	11.833075	14.12458	13.619357
C	9.48641	11.777079	11.679508
C	8.708241	12.880316	11.163817
C	8.042146	13.510941	12.254601
C	8.416901	12.82961	13.458495
C	9.324863	11.788572	13.115883
C	13.865681	16.573375	10.078279
C	15.608471	14.038537	9.914896
C	15.332885	15.589969	12.584868
C	15.398048	14.742189	13.702595
C	16.071303	15.121065	14.862347
C	16.698322	16.364336	14.930709
C	16.642746	17.225441	13.835922
C	15.964661	16.841834	12.678471
C	8.064905	9.350472	9.550329
C	10.885288	8.12814	9.97964
C	9.001664	8.553634	12.369224
C	7.695083	8.759207	12.844635
C	7.289233	8.274353	14.087274
C	8.185834	7.568042	14.88809
C	9.486814	7.347544	14.437552
C	9.885309	7.834795	13.193222
H	16.564386	14.576021	9.80018
H	15.194995	13.888358	8.904556
H	15.834706	13.054392	10.352381
H	14.930608	10.44255	10.181394
H	13.424665	9.453568	10.397712
H	14.729454	17.164681	9.729711
H	13.246411	17.226616	10.713384
H	13.278622	16.299931	9.187052
H	11.308156	8.543306	9.05098
H	10.440903	7.148045	9.736563
H	11.717013	7.944006	10.676766
H	8.381088	9.652508	8.539098
H	7.328192	10.090583	9.903071
H	7.556729	8.374579	9.473654
H	16.13738	11.225418	12.193141
H	16.207831	11.64313	14.611654
H	14.216702	11.172743	16.047781
H	12.1564	10.239453	14.997359
H	12.101902	9.738823	12.592031
H	12.250431	14.027142	8.457751
H	10.480427	13.607996	8.430409
H	9.787534	11.509222	7.28509
H	10.369397	9.354661	6.236312
H	12.734036	8.561674	6.191159
H	14.51218	9.973316	7.215408
H	13.955114	12.16975	8.186934
H	10.920401	15.814898	10.852919
H	9.387712	16.355518	13.026879
H	10.320954	14.877592	15.093354
H	12.439529	13.437144	14.205161
H	8.624505	13.142797	10.112352
H	7.36607	14.359861	12.186412
H	8.075153	13.073941	14.461133
H	9.778845	11.075149	13.798627
H	14.912631	13.767836	13.661931
H	16.104324	14.445869	15.718719
H	17.225379	16.664155	15.837681
H	17.126185	18.202043	13.885347
H	15.928485	17.538538	11.838625
H	6.974499	9.308882	12.235906
H	6.267789	8.444848	14.430599
H	7.868755	7.182072	15.857964
H	10.191751	6.786455	15.052713
H	10.905922	7.636606	12.861176

Table S6. (NN^{TMS})UI_2(THF)

Atom	X	Y	Z
U	12.427329	9.864066	4.245982
I	7.84874	6.715483	2.879376
I	13.374531	12.162593	-0.955609
Fe	12.748027	8.231771	10.092795
Si	7.631066	14.654996	6.1326
Si	15.987663	3.97014	2.71996
O	16.183519	12.708926	5.133324
N	10.188072	12.520178	6.608259
N	14.90395	6.498081	4.663542
C	12.473128	12.119983	10.815457
H	13.938869	13.527191	10.518465
C	12.068147	10.692555	13.06158
H	13.190264	10.796795	14.779901
C	9.923628	9.088148	12.662342
H	9.14591	7.760689	14.024535
C	9.00601	9.515229	10.168837
H	7.414513	8.585032	9.262909
C	10.526556	11.470913	9.011787
C	16.440271	7.112078	9.16892
H	18.043572	8.335276	8.78239
C	15.709816	6.140769	11.570777
H	16.635387	6.52368	13.365035
C	13.534155	4.568519	11.214422
H	12.523371	3.562814	12.694059
C	12.911277	4.574486	8.596379
H	11.347032	3.592512	7.6975
C	14.762884	6.089057	7.272608
C	4.619455	13.305316	7.48645
H	4.746021	13.006392	9.543583
H	4.153637	11.487072	6.585225
H	3.032328	14.612989	7.137624
C	8.401783	17.738151	7.773488
H	10.076592	18.650281	6.935801
H	8.773656	17.443	9.803229
H	6.811364	19.078482	7.616201
C	7.2851	15.143714	2.635798
H	6.790927	13.368182	1.669256
H	9.016362	15.880793	1.749104
H	5.752439	16.510267	2.270496
C	14.267193	0.951922	3.531852
H	12.213072	1.179855	3.278757
H	14.626155	0.339834	5.489642
H	14.89656	-0.583743	2.268092
C	19.492076	3.534834	3.283379
H	19.892131	3.157179	5.293949
H	20.572616	5.224002	2.720003
H	20.224007	1.920836	2.183522
C	15.356247	4.845491	-0.658978
H	16.300302	6.609007	-1.22801
H	13.319306	5.081419	-1.012362
H	16.042824	3.322757	-1.907975
C	15.895731	15.47411	5.147226
H	14.838945	15.968291	6.856955
H	14.81205	16.007227	3.454328
C	18.577067	16.483503	5.035076
H	18.647421	18.423966	4.297703
H	19.45352	16.454373	6.924445
C	19.848596	14.558886	3.282368
H	21.921275	14.562139	3.417814
H	19.301155	14.925511	1.308644
C	18.711669	12.069049	4.156156
H	18.475465	10.691224	2.628233
H	19.77277	11.219256	5.728916

Table S7. (NN^{DMP})UI_2(THF)

Atom	X	Y	Z
U	12.24494	10.14684	4.170736
I	8.825178	6.457274	1.439687
I	12.36028	14.08462	-
Fe	13.02783	6.831719	9.188076
Si	6.629036	13.12664	7.300965
Si	18.05430	6.84428	1.592708
O	15.21463	13.40990	6.049729
N	9.349635	11.21108	7.053617
N	15.72487	7.801152	3.800397
C	11.61385	9.990717	11.11355
C	17.98953	3.297612	1.214495
C	11.61172	7.81846	12.70120
C	18.44375	16.52153	5.467177
C	10.04548	5.940013	11.54643
C	16.77716	17.22037	7.728917
C	9.070125	6.946547	9.25241
H	4.613808	8.03844	6.012687
C	9.961282	9.518366	8.993533
C	16.88422	7.16912	8.433717
H	21.77374	10.99869	0.341331
C	16.43602	5.22058	10.23651
C	17.76198	13.77095	4.963601
C	14.84260	3.357627	9.086768
H	-	11.36003	12.78019
C	14.30481	4.150684	6.573496
H	-	7.172253	10.83036
C	15.64117	6.485624	6.097955
C	7.173435	15.84148	9.569307
C	14.35886	15.81777	7.10966
C	17.42453	8.470464	-
H	0.945585	5.535996	7.436188
C	5.877777	14.35832	4.059043
C	3.896265	11.18615	8.526584
C	2.298479	12.06590	10.45250
C	0.240011	10.63861	11.27957
C	-	8.293202	10.18994
C	1.319143	7.377635	8.282641
C	3.372946	8.810199	7.467915
H	2.657787	13.89289	11.33894
C	21.24448	7.845647	2.900113
C	22.34030	6.549185	4.946367
C	24.62407	7.333356	6.001138
C	25.87683	9.435925	5.02339
C	24.83572	10.74216	2.985726
C	22.54711	9.951763	1.941393
H	21.40418	4.889612	5.736297
H	25.4389	6.287809	7.579644
H	27.67014	10.04373	5.837347
H	25.81815	12.37285	2.195549
H	12.60091	11.75640	11.46935
H	19.45861	2.69309	-
H	16.13782	2.674501	0.499664
H	18.34287	2.301251	3.009218
H	12.62973	7.615447	14.47421
H	20.47127	16.75082	5.846432
H	17.93359	17.69449	3.827601
H	9.666932	4.064672	12.29439
H	17.59910	16.50709	9.50308
H	16.47362	19.26704	7.903724
H	7.837234	6.001005	7.918168
H	5.505965	12.79643	2.735062
H	18.04624	8.840443	8.707037
H	17.15754	5.161284	12.15954
H	17.66042	13.33365	2.942105
H	19.02179	12.42783	5.916025
H	14.13950	1.652301	9.991824
H	13.12613	3.180733	5.197019
H	7.450939	15.19214	11.52576
H	5.550761	17.14823	9.527095
H	8.849235	16.94789	9.018702
H	13.16228	15.37581	8.739255
H	13.25034	16.81420	5.656979
H	17.09728	10.51526	-1.29927
H	15.73678	7.667611	-
H	19.02516	8.201331	-
H	7.407284	15.51169	3.252906
H	4.149118	15.51776	4.151522

Table S8. (NN^{TBS})UI_2(THF)

Atom	X	Y	Z
U	12.34001	9.814907	4.323358
I	7.949502	6.283605	3.271572
I	12.28977	12.50350	-
Fe	12.97400	8.171764	10.01554
Si	8.070754	15.16313	6.637769
Si	16.19906	3.869548	2.73911
O	16.20902	12.61359	4.956709
N	10.19022	12.52364	6.744188
N	14.99008	6.525209	4.462704
C	12.60285	12.02350	10.86393
H	14.01856	13.48095	10.56317
C	12.30445	10.52238	13.07606
H	13.47205	10.60708	14.76477
C	10.19837	8.866076	12.68596
H	9.498439	7.473482	14.02520
C	9.192105	9.344718	10.23690
H	7.597254	8.394366	9.360119
C	10.61911	11.37754	9.097556
C	16.66218	7.189117	8.929357
H	18.21112	8.463113	8.49235
C	16.06774	6.173067	11.34871
H	17.05692	6.574353	13.10456
C	13.93535	4.527729	11.06884
H	13.02101	3.477489	12.57998
C	13.20227	4.533346	8.480721
H	11.62905	3.514151	7.641195
C	14.94154	6.126014	7.092237
C	7.897783	16.57612	9.923132
H	9.791089	17.11623	10.60669
H	7.084211	15.26001	11.31857
H	6.725694	18.29902	9.905848
C	9.392746	17.60382	4.398299
H	9.911343	16.77774	2.559711
H	11.07932	18.52201	5.204494
H	7.983249	19.09934	4.049652
C	14.13488	1.004513	3.293396
H	12.13022	1.437272	2.938602
H	14.31615	0.314879	5.250101
H	14.69506	-	2.03482
C	19.48995	3.182728	3.982407
H	19.45080	2.943289	6.053453
H	20.83852	4.709517	3.547815
H	20.23982	1.417186	3.167624
C	15.99392	15.39351	4.929182
H	15.20048	15.97513	6.752218
H	14.68991	15.88677	3.391518
C	18.65190	16.36657	4.423033
H	18.62439	18.19782	3.443582
H	19.71591	16.58253	6.200199
C	19.78520	14.23467	2.822798
H	21.86111	14.26619	2.7572
H	19.04137	14.31705	0.880978
C	18.77170	11.91133	4.154917
H	18.61649	10.22555	2.968553
H	19.87303	11.46978	5.867148
C	16.35607	4.592296	-
C	13.69491	4.830862	-
C	17.86593	7.016643	-
C	17.71911	2.367332	-
H	12.58794	3.087792	-
H	12.60450	6.391081	-
H	13.83185	5.21024	-4.00016
H	19.78689	6.92594	-
H	18.06133	7.300589	-
H	16.90053	8.702219	-
H	17.77954	2.705966	-
H	19.68315	2.154964	-
H	16.73219	0.558777	-1.81253
C	4.746033	14.21237	5.510272
C	4.803389	13.54091	2.684029
C	3.743919	11.93196	7.005036
C	2.940316	16.46219	5.90918
H	5.384558	15.15711	1.509626
H	6.087661	11.95754	2.28301
H	2.898218	12.95502	2.057343
H	3.748871	12.27002	9.060693
H	1.772571	11.52852	6.440785
H	4.858322	10.22671	6.600451
H	1.050589	15.97546	5.162377
H	2.711598	16.9342	7.924328
H	3.574731	18.17444	4.906553

Table S9. (NN^{TBS})$U(CH_2Ph)(OAr)$

Atom	X	Y	Z
U	8.407981	10.331498	23.34270
Fe	10.581025	10.301133	28.98069
Si	15.262696	9.654505	21.11515
Si	1.992103	11.800581	26.16031
O	7.735173	12.312861	19.85633
N	12.655089	9.640736	23.23161
N	5.325642	11.480948	26.10325
C	13.089562	9.408494	25.83088
C	12.569552	7.231107	27.39949
C	7.486792	14.044063	17.97859
C	13.399451	7.759706	29.90497
C	6.54583	13.220561	15.57887
C	14.364829	10.287255	29.95764
C	6.250639	15.016544	13.67193
C	14.100578	11.331568	27.49127
C	0.457542	9.056699	27.87676
C	8.383126	10.065629	32.20525
C	6.849571	17.548646	14.03821
C	9.18474	12.618756	31.79767
C	2.395579	17.149526	26.63811
C	8.20203	13.433193	29.42670
C	7.786568	18.305063	16.35661
C	6.695217	11.412474	28.36762
C	6.909394	9.301263	30.08849
C	9.950932	0.695302	25.39309
C	14.451282	11.796905	18.38710
C	8.144318	16.618966	18.36998
C	5.865079	10.441906	15.03115
C	8.206791	8.749055	15.36097
C	18.197231	10.912331	22.73293
C	11.821339	19.054288	20.14704

C	0.943784	14.902356	27.76690
C	-1.902455	15.314785	27.31135
C	15.93513	6.306818	19.84061
C	16.36255	4.447987	22.03288
C	3.71304	9.559277	16.77481
C	9.245257	17.839192	20.78626
C	6.609625	6.153827	22.13911
C	13.678651	5.411323	18.24809
C	8.521441	0.397396	27.59082
C	4.941613	10.065391	12.30191
C	9.312659	2.523994	23.61630
C	18.309628	6.331651	18.15850
C	0.938385	11.786704	22.75932
C	1.406407	14.793466	30.63775
C	9.705186	16.069455	23.03274
C	7.219016	4.145482	23.95456
C	5.784633	3.779271	26.17446
C	7.422313	19.91483	21.72421
C	6.418232	1.949191	27.95092
H	11.763964	5.455031	26.74222
H	13.316028	6.460347	31.49356
H	15.137381	11.247501	31.60157
H	5.53261	14.44002	11.83629
H	14.659849	13.218569	26.90274
H	0.737124	7.276395	26.83418
H	-1.600294	9.349146	28.04402
H	1.214217	8.805974	29.79987
H	8.843059	8.90412	33.83618
H	6.593688	18.913741	12.51710
H	10.344902	13.737048	33.07235

H	4.442612	16.975934	26.95271
H	1.766688	18.936081	27.52229
H	2.072257	17.322017	24.58907
H	8.435518	15.29686	28.59580
H	8.266781	20.288366	16.62075
H	5.240184	1.709487	29.62762
H	6.061969	7.453515	29.79686
H	11.575047	-0.528479	25.04723
H	15.804169	11.557935	16.82074
H	14.552062	13.78941	18.97835
H	12.544415	11.470806	17.62947
H	9.709772	9.330302	14.04260
H	7.71582	6.764959	14.96194
H	8.953857	8.851747	17.28552
H	18.727937	9.801619	24.41291
H	17.937089	12.889043	23.33533
H	19.80613	10.87989	21.40764
H	13.149774	17.624962	19.42971
H	12.63913	19.927471	21.85254
H	11.644154	20.530069	18.69729
H	-2.526603	17.048882	28.29726
H	-3.052698	13.741572	28.04647
H	-2.345948	15.554957	25.29194
H	16.760906	2.538382	21.28023
H	14.691855	4.306131	23.26039
H	17.983881	5.000802	23.21758
H	4.249923	9.709327	18.76207
H	3.239649	7.57106	16.37590
H	2.011119	10.718803	16.47160
H	7.266416	5.70553	20.21456

H	4.557342	6.524454	22.06050
H	13.968292	3.4381	17.62189
H	13.421845	6.577668	16.54452
H	11.906597	5.472578	19.33088
H	9.012746	-1.04646	28.97574
H	6.394276	10.590401	10.90844
H	3.209234	11.148149	11.91058
H	4.49956	8.051608	12.02399
H	10.435321	2.690642	21.89659
H	20.018833	6.846817	19.22938
H	18.125706	7.646705	16.55414
H	18.626173	4.425686	17.36105
H	1.908726	13.222282	21.60876
H	-1.109462	12.141065	22.62293
H	1.285581	9.933381	21.88045
H	3.41157	14.495276	31.10929
H	0.303763	13.272602	31.53614
H	0.814016	16.595151	31.51780
H	11.082695	14.574645	22.56479
H	7.90834	15.284367	23.74604
H	10.530479	17.167881	24.59726
H	4.112783	4.946621	26.47442
H	8.196615	20.825528	23.43075
H	5.567331	19.104835	22.19629
H	7.126592	21.38931	20.29205

Bond Order Analyses for $(NN^R)U(CH_2Ph)_2$ complexes

Table S10. $(NN^{TMS})U(CH_2Ph)_2$						**BOND-ORDERS (THRESHOLD = 0.200)**				
Atom	No.		Atom	No.	DIST. [A]	MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
U	1	-	Fe	2	3.2492	0.3772	0.3169	0.5173	-0.0702	0.4650
U	1	-	N	5	2.2507	0.6675	1.0246	1.3741	1.7233	1.3914
U	1	-	N	6	2.2610	0.6291	0.9937	1.3353	1.6962	1.3546
U	1	-	C	7	2.5201	0.4463	0.6484	0.8506	1.2121	0.8481
U	1	-	C	10	2.7147	-0.0411	0.1837	0.2364	0.2148	0.2227
U	1	-	C	21	2.5119	0.5209	0.6567	0.8598	1.2116	0.8560
U	1	-	C	25	3.0384	0.0768	0.1787	0.2310	0.3953	0.2230
Fe	2	-	C	8	2.0920	0.3986	0.3411	0.4688	0.6212	0.4482
Fe	2	-	C	9	2.0686	0.3961	0.3422	0.4706	0.6107	0.4491
Fe	2	-	C	14	2.0687	0.3965	0.3420	0.4703	0.6101	0.4488
Fe	2	-	C	18	2.0952	0.4017	0.3413	0.4688	0.6159	0.4478
Fe	2	-	C	22	2.1559	0.3919	0.2494	0.3414	0.2929	0.3169
Fe	2	-	C	23	2.1001	0.3967	0.3361	0.4620	0.6175	0.4418
Fe	2	-	C	28	2.0704	0.3927	0.3400	0.4676	0.6081	0.4463
Fe	2	-	C	32	2.0684	0.3929	0.3402	0.4678	0.6081	0.4465
Fe	2	-	C	35	2.1553	0.3928	0.2507	0.3432	0.2944	0.3185
Fe	2	-	C	36	2.0960	0.3952	0.3404	0.4678	0.6223	0.4474
Si	3	-	N	5	1.7746	0.8695	0.8242	0.8990	1.3881	0.8382
Si	3	-	C	16	1.8848	0.8481	0.8958	0.9535	1.6540	0.9006
Si	3	-	C	30	1.8898	0.8422	0.8855	0.9423	1.6577	0.8915
Si	3	-	C	34	1.8936	0.8292	0.8734	0.9296	1.6529	0.8801
Si	4	-	N	6	1.7718	0.8853	0.8326	0.9099	1.4093	0.8515
Si	4	-	C	12	1.8850	0.8451	0.8959	0.9532	1.6564	0.9020
Si	4	-	C	20	1.8939	0.8325	0.8727	0.9283	1.6468	0.8795
Si	4	-	C	26	1.8915	0.8381	0.8858	0.9420	1.6561	0.8924
N	5	-	C	35	1.4021	1.0655	1.1033	1.1889	1.1588	1.2811
N	6	-	C	22	1.4021	1.0657	1.1034	1.1920	1.1592	1.2871
C	7	-	C	10	1.4390	1.1309	1.1925	1.2525	1.2162	1.3322
C	7	-	H	37	1.0950	0.9995	0.9260	0.9824	1.0221	0.9702
C	7	-	H	38	1.0953	0.9830	0.9252	0.9806	1.0195	0.9694
C	8	-	C	22	1.4447	1.0768	1.1772	1.2084	1.2104	1.2394
C	8	-	C	32	1.4243	1.1086	1.2714	1.3130	1.2325	1.3920
C	8	-	H	39	1.0866	1.0567	0.9224	0.9641	0.9874	0.9089
C	9	-	C	14	1.4336	1.0823	1.2433	1.2847	1.2106	1.3590
C	9	-	C	36	1.4253	1.1109	1.2720	1.3132	1.2318	1.3927
C	9	-	H	40	1.0873	1.0818	0.9237	0.9703	0.9915	0.9109
C	10	-	C	11	1.4238	1.1840	1.2449	1.2827	1.2789	1.3124
C	10	-	C	19	1.4235	1.1825	1.2464	1.2844	1.2806	1.3146
C	11	-	C	13	1.3924	1.2882	1.4433	1.4927	1.4470	1.5593
C	11	-	H	41	1.0910	0.9516	0.9242	0.9598	0.9754	0.9107
C	12	-	H	42	1.1037	1.0176	0.9409	1.0086	1.0592	1.0193
C	12	-	H	43	1.1015	0.9734	0.9445	1.0099	1.0575	1.0230
C	12	-	H	44	1.0992	0.9224	0.9436	1.0046	1.0482	1.0211
C	13	-	C	15	1.3947	1.2444	1.4115	1.4621	1.4156	1.5282
C	13	-	H	45	1.0912	1.0420	0.9244	0.9669	0.9780	0.9050
C	14	-	C	18	1.4242	1.1114	1.2720	1.3127	1.2349	1.3904
C	14	-	H	46	1.0874	1.0850	0.9236	0.9701	0.9912	0.9108
C	15	-	C	17	1.3964	1.2379	1.4028	1.4531	1.4053	1.5196
C	15	-	H	47	1.0898	1.0569	0.9268	0.9735	0.9904	0.9162
C	16	-	H	48	1.1000	0.9663	0.9439	1.0063	1.0515	1.0209
C	16	-	H	49	1.1037	1.0209	0.9422	1.0090	1.0582	1.0203
C	16	-	H	50	1.0992	0.9204	0.9419	1.0023	1.0460	1.0182
C	17	-	C	19	1.3916	1.2923	1.4522	1.5021	1.4544	1.5704
C	17	-	H	51	1.0914	1.0400	0.9245	0.9672	0.9790	0.9059
C	18	-	C	35	1.4449	1.0769	1.1761	1.2064	1.2087	1.2362
C	18	-	H	52	1.0881	1.0397	0.9159	0.9573	0.9803	0.8980
C	19	-	H	53	1.0914	0.9672	0.9243	0.9617	0.9778	0.9109
C	20	-	H	54	1.1038	1.0089	0.9423	1.0093	1.0580	1.0226
C	20	-	H	55	1.1017	0.9693	0.9479	1.0114	1.0534	1.0298
C	20	-	H	56	1.1026	0.9952	0.9453	1.0107	1.0574	1.0255

C	21	-	C	24	1.4397	1.1306	1.2057	1.2634	1.2332	1.3406
C	21	-	H	57	1.0945	0.9498	0.9253	0.9781	1.0189	0.9623
C	21	-	H	58	1.0986	0.9149	0.9056	0.9561	0.9972	0.9414
C	22	-	C	23	1.4462	1.0817	1.1766	1.2077	1.2096	1.2393
C	23	-	C	28	1.4252	1.1074	1.2729	1.3145	1.2325	1.3942
C	23	-	H	59	1.0869	1.0476	0.9203	0.9640	0.9883	0.9060
C	24	-	C	25	1.4235	1.1962	1.2654	1.3055	1.3027	1.3371
C	24	-	C	33	1.4216	1.1782	1.2649	1.3039	1.3024	1.3300
C	25	-	C	27	1.3987	1.2624	1.4051	1.4559	1.4057	1.5242
C	25	-	H	60	1.0928	0.9233	0.9076	0.9452	0.9636	0.8945
C	26	-	H	61	1.1026	0.9910	0.9446	1.0099	1.0582	1.0235
C	26	-	H	62	1.1024	0.9940	0.9475	1.0128	1.0574	1.0289
C	26	-	H	63	1.1038	1.0083	0.9427	1.0097	1.0586	1.0226
C	27	-	C	29	1.3898	1.2794	1.4493	1.5041	1.4553	1.5731
C	27	-	H	64	1.0913	1.0275	0.9255	0.9673	0.9787	0.9075
C	28	-	C	32	1.4332	1.0797	1.2445	1.2861	1.2117	1.3606
C	28	-	H	65	1.0873	1.0836	0.9235	0.9703	0.9916	0.9107
C	29	-	C	31	1.4033	1.2052	1.3677	1.4198	1.3701	1.4861
C	29	-	H	66	1.0901	1.0539	0.9281	0.9751	0.9924	0.9195
C	30	-	H	67	1.1024	0.9922	0.9449	1.0101	1.0579	1.0239
C	30	-	H	68	1.1039	1.0140	0.9430	1.0097	1.0575	1.0233
C	30	-	H	69	1.1025	0.9753	0.9453	1.0090	1.0547	1.0244
C	31	-	C	33	1.3829	1.3228	1.5039	1.5575	1.5131	1.6253
C	31	-	H	70	1.0914	1.0437	0.9252	0.9691	0.9814	0.9083
C	32	-	H	71	1.0873	1.0846	0.9236	0.9703	0.9915	0.9109
C	33	-	H	72	1.0906	1.0015	0.9245	0.9651	0.9791	0.9086
C	34	-	H	73	1.1020	0.9798	0.9479	1.0126	1.0559	1.0301
C	34	-	H	74	1.1038	1.0102	0.9428	1.0096	1.0575	1.0237
C	34	-	H	75	1.1024	0.9947	0.9457	1.0108	1.0566	1.0265
C	35	-	C	36	1.4456	1.0801	1.1764	1.2073	1.2093	1.2386
C	36	-	H	76	1.0870	1.0552	0.9207	0.9647	0.9889	0.9065
					Sum	83.6481	90.2393	97.4227	97.4227	97.4227

Table S11. $(NN^{TBS})U(CH_2Ph)_2$

						BOND-ORDERS (THRESHOLD = 0.200)				
Atom	**No.**		**Atom**	**No.**	**DIST. [A]**	**MAYER**	**G-J**	**N-M (1)**	**N-M (2)**	**N-M (3) (*)**
U	1	-	Fe	2	3.2049	0.3809	0.4266	0.7081	0.3140	0.6484
U	1	-	N	5	2.2671	0.7326	0.9725	1.3264	1.5272	1.3641
U	1	-	N	6	2.2835	0.7233	0.9566	1.3076	1.5138	1.3471
U	1	-	C	7	2.5141	0.3475	0.6663	0.8899	1.0854	0.9003
U	1	-	C	21	2.5035	0.4097	0.6940	0.9259	1.1093	0.9344
U	1	-	C	25	3.0957	-0.0279	0.1568	0.2064	0.2958	0.2032
Fe	2	-	C	35	2.1654	0.4560	0.2345	0.3228	0.2630	0.2986
Fe	2	-	C	36	2.0940	0.4441	0.3379	0.4671	0.6275	0.4457
Fe	2	-	C	38	2.0685	0.3757	0.3355	0.4640	0.6076	0.4417
Fe	2	-	C	40	2.0674	0.3914	0.3418	0.4728	0.6157	0.4501
Fe	2	-	C	42	2.0980	0.4528	0.3327	0.4597	0.6128	0.4382
Fe	2	-	C	44	2.1690	0.4473	0.2347	0.3232	0.2648	0.2990
Fe	2	-	C	45	2.0998	0.4493	0.3319	0.4589	0.6191	0.4378
Fe	2	-	C	47	2.0673	0.3875	0.3402	0.4706	0.6141	0.4480
Fe	2	-	C	49	2.0681	0.3812	0.3344	0.4625	0.6065	0.4403
Fe	2	-	C	51	2.0900	0.4409	0.3362	0.4647	0.6232	0.4432
Si	3	-	N	5	1.7755	0.8515	0.8615	0.9366	1.3513	0.8813
Si	3	-	C	53	1.8906	0.8500	0.9034	0.9564	1.5778	0.9136
Si	3	-	C	57	1.8987	0.8422	0.8769	0.9283	1.5676	0.8883
Si	3	-	C	61	1.9325	0.7145	0.8139	0.8407	0.8944	0.7386
Si	4	-	N	6	1.7741	0.8732	0.8700	0.9480	1.3726	0.8953
Si	4	-	C	74	1.8882	0.8604	0.9066	0.9594	1.5774	0.9174
Si	4	-	C	78	1.8974	0.8376	0.8859	0.9375	1.5755	0.8985
Si	4	-	C	82	1.9335	0.7293	0.8029	0.8291	0.8882	0.7296
N	5	-	C	35	1.3984	1.2710	1.1364	1.2282	1.2091	1.3139
N	6	-	C	44	1.4011	1.2582	1.1321	1.2267	1.2046	1.3153
C	7	-	H	8	1.0963	1.0512	0.9238	0.9786	1.0135	0.9618
C	7	-	H	9	1.0954	1.0509	0.9268	0.9832	1.0188	0.9651
C	7	-	C	10	1.4424	1.2881	1.2054	1.2705	1.2485	1.3388
C	10	-	C	11	1.4223	1.3193	1.2608	1.3042	1.3035	1.3288
C	10	-	C	19	1.4212	1.3141	1.2658	1.3093	1.3086	1.3343
C	11	-	H	12	1.0907	1.0167	0.9213	0.9579	0.9708	0.9070
C	11	-	C	13	1.3926	1.4351	1.4466	1.5024	1.4628	1.5644
C	13	-	H	14	1.0912	1.0385	0.9247	0.9664	0.9771	0.9063
C	13	-	C	15	1.3938	1.3743	1.4146	1.4727	1.4308	1.5352
C	15	-	H	16	1.0898	1.0474	0.9267	0.9754	0.9900	0.9174
C	15	-	C	17	1.3967	1.3572	1.3962	1.4536	1.4104	1.5164
C	17	-	H	18	1.0913	1.0399	0.9244	0.9671	0.9786	0.9067
C	17	-	C	19	1.3903	1.4457	1.4680	1.5248	1.4833	1.5891
C	19	-	H	20	1.0910	1.0278	0.9248	0.9634	0.9766	0.9113
C	21	-	H	22	1.0984	1.0196	0.9105	0.9621	0.9977	0.9400
C	21	-	H	23	1.0949	1.0326	0.9253	0.9797	1.0155	0.9562
C	21	-	C	24	1.4429	1.2903	1.2090	1.2724	1.2545	1.3363
C	24	-	C	25	1.4221	1.3242	1.2717	1.3159	1.3152	1.3419
C	24	-	C	33	1.4207	1.3033	1.2718	1.3152	1.3153	1.3372
C	25	-	H	26	1.0918	1.0098	0.9139	0.9504	0.9647	0.9006
C	25	-	C	27	1.3979	1.4138	1.4224	1.4784	1.4346	1.5426
C	27	-	H	28	1.0912	1.0433	0.9260	0.9673	0.9790	0.9099
C	27	-	C	29	1.3902	1.3924	1.4363	1.4965	1.4503	1.5631
C	29	-	H	30	1.0902	1.0493	0.9281	0.9766	0.9922	0.9210
C	29	-	C	31	1.4028	1.3303	1.3730	1.4309	1.3863	1.4938
C	31	-	H	32	1.0908	1.0398	0.9250	0.9673	0.9785	0.9072
C	31	-	C	33	1.3832	1.4580	1.4975	1.5560	1.5185	1.6181
C	33	-	H	34	1.0907	1.0355	0.9247	0.9660	0.9773	0.9090
C	35	-	C	36	1.4461	1.1450	1.1735	1.2070	1.2122	1.2362
C	35	-	C	42	1.4456	1.1525	1.1762	1.2091	1.2144	1.2368
C	36	-	H	37	1.0872	1.0792	0.9211	0.9636	0.9869	0.9089
C	36	-	C	38	1.4249	1.1784	1.2720	1.3159	1.2366	1.3943
C	38	-	H	39	1.0875	1.0894	0.9234	0.9689	0.9892	0.9115
C	38	-	C	40	1.4332	1.1427	1.2447	1.2887	1.2173	1.3616

C	40	-	H	41	1.0874	1.0881	0.9229	0.9688	0.9891	0.9110
C	40	-	C	42	1.4246	1.1775	1.2693	1.3129	1.2371	1.3894
C	42	-	H	43	1.0888	1.0703	0.9149	0.9541	0.9764	0.8980
C	44	-	C	45	1.4470	1.1585	1.1744	1.2081	1.2127	1.2375
C	44	-	C	51	1.4460	1.1465	1.1766	1.2099	1.2146	1.2391
C	45	-	H	46	1.0871	1.0813	0.9201	0.9618	0.9849	0.9078
C	45	-	C	47	1.4252	1.1819	1.2690	1.3136	1.2345	1.3918
C	47	-	H	48	1.0873	1.0886	0.9231	0.9693	0.9897	0.9114
C	47	-	C	49	1.4325	1.1403	1.2462	1.2905	1.2187	1.3637
C	49	-	H	50	1.0873	1.0878	0.9232	0.9690	0.9894	0.9113
C	49	-	C	51	1.4243	1.1752	1.2710	1.3148	1.2363	1.3928
C	51	-	H	52	1.0864	1.0764	0.9220	0.9626	0.9853	0.9093
C	53	-	H	54	1.0996	0.9939	0.9392	0.9981	1.0422	1.0104
C	53	-	H	55	1.1010	1.0175	0.9461	1.0066	1.0477	1.0209
C	53	-	H	56	1.1028	1.0382	0.9448	1.0089	1.0541	1.0197
C	57	-	H	58	1.1017	1.0212	0.9480	1.0084	1.0475	1.0256
C	57	-	H	59	1.1031	1.0324	0.9429	1.0068	1.0518	1.0194
C	57	-	H	60	1.1019	1.0284	0.9479	1.0095	1.0502	1.0254
C	61	-	C	62	1.5378	0.9877	1.0081	1.0483	0.9356	1.1303
C	61	-	C	66	1.5391	0.9847	1.0092	1.0497	0.9354	1.1326
C	61	-	C	70	1.5426	0.9834	1.0044	1.0443	0.9286	1.1274
C	62	-	H	63	1.1063	1.0052	0.9402	0.9838	1.0164	0.9697
C	62	-	H	64	1.1011	0.9972	0.9494	0.9913	1.0229	0.9777
C	62	-	H	65	1.0998	0.9893	0.9453	0.9878	1.0224	0.9701
C	66	-	H	67	1.1065	1.0008	0.9404	0.9844	1.0173	0.9707
C	66	-	H	68	1.1007	0.9931	0.9457	0.9885	1.0242	0.9704
C	66	-	H	69	1.1019	1.0048	0.9498	0.9945	1.0280	0.9791
C	70	-	H	71	1.1060	0.9980	0.9387	0.9830	1.0174	0.9682
C	70	-	H	72	1.1021	1.0050	0.9492	0.9940	1.0282	0.9784
C	70	-	H	73	1.1019	1.0047	0.9487	0.9935	1.0282	0.9773
C	74	-	H	75	1.1014	1.0164	0.9442	1.0060	1.0498	1.0181
C	74	-	H	76	1.0989	1.0082	0.9470	1.0062	1.0454	1.0222
C	74	-	H	77	1.1026	1.0414	0.9415	1.0063	1.0548	1.0145
C	78	-	H	79	1.1029	1.0277	0.9488	1.0112	1.0517	1.0276
C	78	-	H	80	1.1037	1.0323	0.9423	1.0068	1.0529	1.0189
C	78	-	H	81	1.1012	1.0243	0.9461	1.0088	1.0532	1.0223
C	82	-	C	83	1.5405	0.9827	1.0077	1.0483	0.9320	1.1318
C	82	-	C	87	1.5370	0.9857	1.0078	1.0481	0.9338	1.1305
C	82	-	C	91	1.5405	0.9822	1.0058	1.0461	0.9289	1.1298
C	83	-	H	84	1.1063	1.0007	0.9404	0.9846	1.0178	0.9708
C	83	-	H	85	1.1012	0.9928	0.9448	0.9879	1.0232	0.9707
C	83	-	H	86	1.1017	1.0060	0.9487	0.9942	1.0291	0.9770
C	87	-	H	88	1.1059	1.0050	0.9382	0.9825	1.0167	0.9662
C	87	-	H	89	1.1017	0.9967	0.9489	0.9913	1.0233	0.9773
C	87	-	H	90	1.0996	0.9845	0.9472	0.9882	1.0205	0.9742
C	91	-	H	92	1.1061	0.9969	0.9388	0.9836	1.0181	0.9684
C	91	-	H	93	1.1023	1.0046	0.9494	0.9945	1.0287	0.9789
C	91	-	H	94	1.1014	1.0032	0.9491	0.9941	1.0288	0.9778
					Sum	106.2983	108.3379	116.3759	116.3759	116.3759

Table S12. $(NN^{DMP})U(CH_2Ph)_2$						BOND-ORDERS (THRESHOLD = 0.200)				
Atom	**No.**		**Atom**	**No.**	**DIST. [A]**	**MAYER**	**G-J**	**N-M (1)**	**N-M (2)**	**N-M (3) (*)**
U	1	-	Fe	2	3.2094	0.4032	0.3603	0.5934	-0.0134	0.5328
U	1	-	N	5	2.2616	0.6206	0.9767	1.3326	1.7041	1.3478
U	1	-	N	6	2.2571	0.6130	0.9884	1.3471	1.7134	1.3613
U	1	-	C	7	2.5240	0.5155	0.6565	0.8740	1.2447	0.8690
U	1	-	C	13	3.0765	0.0598	0.1623	0.2131	0.3768	0.2051
U	1	-	C	14	2.5156	0.4592	0.6638	0.8842	1.2550	0.8793
Fe	2	-	C	21	2.1655	0.3918	0.2446	0.3335	0.2808	0.3095
Fe	2	-	C	22	2.0979	0.4011	0.3395	0.4647	0.6198	0.4447
Fe	2	-	C	23	2.0681	0.3992	0.3397	0.4651	0.6034	0.4440
Fe	2	-	C	24	2.0648	0.4009	0.3458	0.4735	0.6093	0.4519
Fe	2	-	C	25	2.0982	0.4023	0.3370	0.4610	0.6049	0.4404
Fe	2	-	C	26	2.1574	0.3875	0.2460	0.3354	0.2873	0.3114
Fe	2	-	C	27	2.1055	0.3948	0.3309	0.4528	0.6060	0.4332
Fe	2	-	C	28	2.0697	0.3940	0.3425	0.4690	0.6099	0.4479
Fe	2	-	C	29	2.0689	0.3921	0.3375	0.4621	0.5996	0.4411
Fe	2	-	C	30	2.0921	0.3931	0.3419	0.4678	0.6148	0.4472
Si	3	-	N	5	1.7571	0.9010	0.8551	0.9338	1.4226	0.8776
Si	3	-	C	31	1.8899	0.8367	0.8791	0.9342	1.6408	0.8889
Si	3	-	C	32	1.8863	0.8468	0.8906	0.9458	1.6354	0.8981
Si	3	-	C	33	1.8961	0.7794	0.8370	0.8712	1.0354	0.7690
Si	4	-	N	6	1.7665	0.9054	0.8367	0.9118	1.3972	0.8566
Si	4	-	C	39	1.8867	0.8277	0.8875	0.9419	1.6364	0.8961
Si	4	-	C	40	1.8781	0.8437	0.9090	0.9651	1.6455	0.9170
Si	4	-	C	41	1.8995	0.7888	0.8305	0.8642	1.0333	0.7639
N	5	-	C	21	1.3995	1.0606	1.1062	1.1960	1.1670	1.2906
N	6	-	C	26	1.4015	1.0619	1.1010	1.1888	1.1572	1.2826
C	7	-	C	8	1.4452	1.1180	1.1917	1.2512	1.2187	1.3302
C	7	-	H	50	1.0951	0.9825	0.9334	0.9873	1.0245	0.9783
C	7	-	H	51	1.1004	0.9045	0.9045	0.9555	0.9968	0.9434
C	8	-	C	9	1.4198	1.1873	1.2780	1.3175	1.3158	1.3444
C	8	-	C	13	1.4205	1.2010	1.2788	1.3196	1.3168	1.3505
C	9	-	C	10	1.3839	1.3203	1.4978	1.5511	1.5065	1.6188
C	9	-	H	61	1.0915	1.0192	0.9255	0.9669	0.9812	0.9110
C	10	-	C	11	1.4030	1.2084	1.3710	1.4232	1.3738	1.4895
C	10	-	H	62	1.0911	1.0283	0.9240	0.9671	0.9792	0.9052
C	11	-	C	12	1.3900	1.2773	1.4494	1.5045	1.4562	1.5733
C	11	-	H	63	1.0901	1.0519	0.9279	0.9751	0.9924	0.9195
C	12	-	C	13	1.3980	1.2654	1.4074	1.4587	1.4106	1.5255
C	12	-	H	64	1.0911	1.0258	0.9239	0.9666	0.9777	0.9043
C	13	-	H	65	1.0918	0.8875	0.9055	0.9393	0.9565	0.8920
C	14	-	C	15	1.4457	1.1151	1.1812	1.2412	1.2087	1.3198
C	14	-	H	66	1.0988	0.9365	0.9128	0.9654	1.0048	0.9552
C	14	-	H	67	1.0954	1.0187	0.9316	0.9868	1.0239	0.9781
C	15	-	C	16	1.4211	1.1819	1.2686	1.3082	1.3063	1.3353
C	15	-	C	20	1.4183	1.2036	1.2809	1.3212	1.3186	1.3511
C	16	-	C	17	1.3830	1.3244	1.5044	1.5582	1.5117	1.6277
C	16	-	H	68	1.0912	1.0113	0.9259	0.9666	0.9811	0.9120
C	17	-	C	18	1.4038	1.2056	1.3648	1.4164	1.3672	1.4823
C	17	-	H	69	1.0914	1.0399	0.9252	0.9693	0.9820	0.9085
C	18	-	C	19	1.3883	1.2851	1.4590	1.5138	1.4676	1.5815
C	18	-	H	70	1.0900	1.0544	0.9268	0.9744	0.9912	0.9167
C	19	-	C	20	1.3986	1.2534	1.3992	1.4492	1.4035	1.5141
C	19	-	H	71	1.0906	1.0353	0.9234	0.9677	0.9785	0.9038
C	20	-	H	72	1.0932	0.9201	0.9117	0.9474	0.9637	0.8981
C	21	-	C	22	1.4453	1.0760	1.1763	1.2078	1.2114	1.2384
C	21	-	C	25	1.4443	1.0707	1.1784	1.2093	1.2132	1.2374
C	22	-	C	23	1.4245	1.1058	1.2727	1.3141	1.2331	1.3934
C	22	-	H	73	1.0868	1.0510	0.9213	0.9650	0.9892	0.9074
C	23	-	C	24	1.4329	1.0772	1.2432	1.2846	1.2128	1.3576
C	23	-	H	74	1.0872	1.0831	0.9238	0.9703	0.9912	0.9106
C	24	-	C	25	1.4242	1.1029	1.2686	1.3090	1.2344	1.3849
C	24	-	H	75	1.0870	1.0860	0.9233	0.9700	0.9906	0.9094
C	25	-	H	76	1.0879	1.0297	0.9169	0.9579	0.9801	0.8983
C	26	-	C	27	1.4452	1.0801	1.1787	1.2105	1.2125	1.2416
C	26	-	C	30	1.4454	1.0733	1.1746	1.2058	1.2080	1.2356
C	27	-	C	28	1.4251	1.1076	1.2724	1.3140	1.2328	1.3934
C	27	-	H	77	1.0869	1.0427	0.9204	0.9633	0.9870	0.9063
C	28	-	C	29	1.4332	1.0794	1.2432	1.2848	1.2112	1.3587
C	28	-	H	78	1.0874	1.0883	0.9237	0.9704	0.9918	0.9111
C	29	-	C	30	1.4234	1.1079	1.2734	1.3145	1.2377	1.3917
C	29	-	H	79	1.0871	1.0853	0.9233	0.9700	0.9907	0.9099
C	30	-	H	80	1.0869	1.0479	0.9197	0.9615	0.9844	0.9022
C	31	-	H	52	1.1032	1.0003	0.9415	1.0076	1.0554	1.0218
C	31	-	H	53	1.1017	0.9961	0.9433	1.0102	1.0606	1.0222
C	31	-	H	54	1.1018	0.9738	0.9456	1.0110	1.0569	1.0265
C	32	-	H	47	1.1028	1.0111	0.9391	1.0076	1.0627	1.0142
C	32	-	H	48	1.1019	0.9302	0.9445	1.0060	1.0477	1.0235
C	32	-	H	49	1.1005	0.9176	0.9434	1.0057	1.0518	1.0197
C	33	-	C	34	1.4039	1.2742	1.4077	1.4583	1.3989	1.5348
C	33	-	C	38	1.4058	1.2792	1.4090	1.4599	1.3947	1.5394
C	34	-	C	35	1.3936	1.2539	1.4355	1.4855	1.4490	1.5446
C	34	-	H	81	1.0888	0.8908	0.9176	0.9518	0.9610	0.8930
C	35	-	C	36	1.3940	1.2397	1.4318	1.4829	1.4399	1.5469
C	35	-	H	82	1.0910	1.0354	0.9266	0.9703	0.9835	0.9115
C	36	-	C	37	1.3944	1.2378	1.4308	1.4817	1.4384	1.5458
C	36	-	H	83	1.0910	1.0465	0.9268	0.9726	0.9852	0.9106
C	37	-	C	38	1.3949	1.2545	1.4390	1.4892	1.4484	1.5518
C	37	-	H	84	1.0909	1.0469	0.9261	0.9717	0.9852	0.9108
C	38	-	H	85	1.0919	1.0047	0.9264	0.9657	0.9769	0.9086
C	39	-	H	58	1.1018	0.9801	0.9440	1.0077	1.0543	1.0221
C	39	-	H	59	1.1023	0.9982	0.9448	1.0093	1.0560	1.0236
C	39	-	H	60	1.1030	1.0137	0.9409	1.0087	1.0602	1.0190
C	40	-	H	55	1.1016	0.9046	0.9355	0.9982	1.0500	1.0079
C	40	-	H	56	1.1033	1.0285	0.9383	1.0070	1.0617	1.0139
C	40	-	H	57	1.1007	0.9467	0.9446	1.0064	1.0490	1.0230
C	41	-	C	42	1.4057	1.2734	1.4053	1.4565	1.3929	1.5352
C	41	-	C	46	1.4059	1.2771	1.4081	1.4596	1.3936	1.5397
C	42	-	C	43	1.3943	1.2539	1.4378	1.4875	1.4489	1.5484
C	42	-	H	86	1.0917	0.9968	0.9245	0.9637	0.9741	0.9043
C	43	-	C	44	1.3943	1.2376	1.4312	1.4821	1.4388	1.5462
C	43	-	H	87	1.0910	1.0471	0.9256	0.9713	0.9845	0.9100
C	44	-	C	45	1.3943	1.2385	1.4306	1.4815	1.4379	1.5459
C	44	-	H	88	1.0910	1.0441	0.9264	0.9724	0.9853	0.9102
C	45	-	C	46	1.3945	1.2567	1.4376	1.4877	1.4470	1.5501
C	45	-	H	89	1.091	1.0457	0.9251	0.9711	0.9846	0.9093
C	46	-	H	90	1.0913	0.976	0.9247	0.9624	0.9736	0.9058
					Sum	102.1968	112.1927	120.0941	120.0941	120.0941

Table S13. (NN^{TBS})UI_2(THF)							BOND-ORDERS (THRESHOLD = 0.200)			
Atom	No.		Atom	No.	DIST. [A]	MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
U	1	-	I	2	3.0331	1.247	1.0186	1.3649	1.4571	1.4401
U	1	-	I	3	3.0459	1.2248	1.0106	1.3556	1.449	1.4323
U	1	-	Fe	4	3.1531	0.3525	0.3876	0.6104	0.225	0.5578
U	1	-	O	7	2.549	0.2641	0.3655	0.4848	0.6392	0.4948
U	1	-	N	8	2.2338	0.6858	1.0569	1.3654	1.5799	1.4121
U	1	-	N	9	2.2366	0.6875	1.0493	1.3556	1.5717	1.4029
Fe	4	-	C	10	2.0963	0.4058	0.3396	0.4636	0.6153	0.4432
Fe	4	-	C	12	2.0726	0.3929	0.3365	0.4598	0.5993	0.4388
Fe	4	-	C	14	2.0711	0.3956	0.338	0.4618	0.5987	0.4406
Fe	4	-	C	16	2.0986	0.4028	0.3355	0.4579	0.6043	0.4375
Fe	4	-	C	18	2.1603	0.402	0.2424	0.3297	0.2767	0.3058
Fe	4	-	C	19	2.1	0.4005	0.3364	0.4593	0.6097	0.439
Fe	4	-	C	21	2.0728	0.3941	0.3377	0.4615	0.602	0.4405
Fe	4	-	C	23	2.0707	0.3896	0.3347	0.4573	0.5955	0.4363
Fe	4	-	C	25	2.0932	0.3992	0.3381	0.4614	0.6105	0.4409
Fe	4	-	C	27	2.1562	0.4007	0.2433	0.331	0.2843	0.3073
Si	5	-	N	8	1.7922	0.8179	0.8099	0.8791	1.3505	0.8233
Si	5	-	C	28	1.8947	0.8342	0.8952	0.9481	1.6296	0.9012
Si	5	-	C	32	1.8873	0.8282	0.8971	0.9501	1.6322	0.9033
Si	5	-	C	69	1.9247	0.763	0.8042	0.8308	0.9063	0.7245
Si	6	-	N	9	1.7934	0.8162	0.804	0.8728	1.3499	0.8177
Si	6	-	C	36	1.8915	0.8418	0.8903	0.9432	1.6334	0.897
Si	6	-	C	40	1.8967	0.8281	0.8847	0.9372	1.6266	0.891
Si	6	-	C	56	1.9188	0.7588	0.8237	0.8515	0.9225	0.7422
O	7	-	C	44	1.4755	0.7657	0.9005	1.0112	0.9556	1.0867
O	7	-	C	53	1.4687	0.7689	0.9067	1.0177	0.9643	1.093
N	8	-	C	18	1.4036	1.0777	1.0994	1.1844	1.1594	1.2738
N	9	-	C	27	1.4077	1.0744	1.0953	1.18	1.1495	1.2713
C	10	-	H	11	1.0869	1.0454	0.9233	0.964	0.9868	0.91
C	10	-	C	12	1.4235	1.1143	1.2755	1.3166	1.2375	1.395
C	10	-	C	18	1.4466	1.0757	1.1722	1.2026	1.2064	1.2321
C	12	-	H	13	1.0874	1.0848	0.9234	0.9703	0.9912	0.9102
C	12	-	C	14	1.4328	1.0822	1.2441	1.2855	1.2137	1.3587
C	14	-	H	15	1.0874	1.0884	0.9227	0.9696	0.9901	0.9084
C	14	-	C	16	1.4238	1.1151	1.2722	1.3126	1.2374	1.389
C	16	-	H	17	1.0865	1.023	0.912	0.9545	0.9775	0.8923
C	16	-	C	18	1.446	1.0827	1.1743	1.2046	1.2086	1.233
C	19	-	H	20	1.0862	1.0374	0.9225	0.9624	0.9848	0.9089
C	19	-	C	21	1.4238	1.1173	1.2749	1.3162	1.2373	1.3946
C	19	-	C	27	1.4459	1.0849	1.1744	1.2052	1.2069	1.2358
C	21	-	H	22	1.0874	1.086	0.9234	0.9703	0.9914	0.9104
C	21	-	C	23	1.4329	1.0846	1.2441	1.2858	1.213	1.3594
C	23	-	H	24	1.0874	1.0891	0.9226	0.9696	0.9904	0.9086
C	23	-	C	25	1.4235	1.1159	1.2743	1.3147	1.2376	1.3922
C	25	-	H	26	1.0869	1.0251	0.9112	0.9542	0.978	0.8914
C	25	-	C	27	1.4482	1.0801	1.1704	1.2005	1.2023	1.2308
C	28	-	H	29	1.1029	0.9903	0.9463	1.0102	1.0546	1.0255
C	28	-	H	30	1.1026	0.9868	0.9454	1.0098	1.0568	1.0231
C	28	-	H	31	1.1027	1.0104	0.9428	1.0086	1.0571	1.0206
C	32	-	H	33	1.1014	0.9245	0.9284	0.9896	1.0392	1.0022
C	32	-	H	34	1.1021	0.9897	0.948	1.0098	1.05	1.0287
C	32	-	H	35	1.103	1.0019	0.9411	1.0059	1.0531	1.0193
C	36	-	H	37	1.1014	0.9498	0.9356	0.9997	1.0504	1.0113
C	36	-	H	38	1.1021	1.0004	0.9436	1.0082	1.0552	1.0222
C	36	-	H	39	1.103	1.0027	0.9411	1.0061	1.0529	1.0204
C	40	-	H	41	1.1034	0.9921	0.9434	1.0081	1.0568	1.0208
C	40	-	H	42	1.1022	0.9893	0.9495	1.0127	1.0531	1.0315
C	40	-	H	43	1.1028	1.0083	0.9429	1.0087	1.0566	1.0217
C	44	-	H	45	1.0962	0.9143	0.9229	0.9668	0.9687	0.8989
C	44	-	H	46	1.0984	0.8563	0.9054	0.9455	0.9477	0.8792
C	44	-	C	47	1.5216	0.9136	1.0161	1.0574	1.012	1.1112
C	47	-	H	48	1.0991	1.0112	0.9237	0.9717	1.0024	0.9218
C	47	-	H	49	1.102	0.9751	0.9286	0.9697	0.9968	0.9318
C	47	-	C	50	1.5328	0.9389	1.0043	1.0427	0.9167	1.1233
C	50	-	H	51	1.0992	1.0194	0.9239	0.9714	1.001	0.9234
C	50	-	H	52	1.1012	0.9285	0.9174	0.9605	0.9898	0.9153
C	50	-	C	53	1.5153	0.9051	1.0193	1.0607	1.0182	1.1134
C	53	-	H	54	1.0939	0.8748	0.9143	0.9573	0.9575	0.8841
C	53	-	H	55	1.1024	0.9218	0.9207	0.9606	0.9627	0.9008
C	56	-	C	57	1.5372	0.9133	1.0073	1.0464	0.9185	1.1328
C	56	-	C	58	1.5369	0.9149	1.0078	1.0465	0.9183	1.133

C	56	-	C	59	1.5427	0.9185	1.0035	1.0422	0.9117	1.1294
C	57	-	H	60	1.1007	0.9846	0.9451	0.9909	1.028	0.9711
C	57	-	H	61	1.099	0.8505	0.9283	0.9696	1.0064	0.9517
C	57	-	H	62	1.1052	0.9887	0.9373	0.9822	1.0179	0.9652

Table S14. (NN^{DMP})UI_2(THF)							BOND-ORDERS (THRESHOLD = 0.200)			
Atom	**No.**		**Atom**	**No.**	**DIST. [A]**	**MAYER**	**G-J**	**N-M (1)**	**N-M (2)**	**N-M (3) (*)**
U	1 -	I		2	3.0304	0.8442	1.0297	1.3925	1.455	1.4947
U	1	-	I	3	3.0453	0.8467	1.0375	1.4059	1.4675	1.508
U	1	-	Fe	4	3.2003	0.3244	0.409	0.6518	0.3617	0.6007
U	1	-	O	7	2.5296	0.258	0.3498	0.4659	0.5777	0.4805
U	1	-	N	8	2.2288	0.6812	1.1122	1.4409	1.5758	1.4976
U	1	-	N	9	2.22	0.6715	1.1174	1.4449	1.579	1.5013
Fe	4	-	C	10	2.0972	0.4003	0.3392	0.4684	0.6214	0.4472
Fe	4	-	C	12	2.0716	0.3974	0.339	0.4683	0.6078	0.4462
Fe	4	-	C	14	2.0726	0.394	0.3336	0.4608	0.5946	0.4387
Fe	4	-	C	16	2.0993	0.3966	0.3358	0.4633	0.5996	0.4412
Fe	4	-	C	18	2.152	0.388	0.2403	0.3307	0.2811	0.3066
Fe	4	-	C	19	2.0972	0.384	0.3275	0.4522	0.5986	0.4312
Fe	4	-	C	21	2.0753	0.3887	0.3343	0.4619	0.603	0.4402
Fe	4	-	C	23	2.0721	0.388	0.3363	0.4645	0.604	0.4426
Fe	4	-	C	25	2.0938	0.388	0.333	0.4596	0.6109	0.4386
Fe	4	-	C	27	2.1439	0.388	0.2483	0.3418	0.2969	0.3172
Si	5	-	N	8	1.7751	0.8492	0.8	0.8713	1.3118	0.8106
Si	5	-	C	28	1.889	0.8271	0.8854	0.9413	1.6424	0.8959
Si	5	-	C	32	1.8744	0.8655	0.9159	0.9729	1.6621	0.9252
Si	5	-	C	33	1.8923	0.803	0.8453	0.8806	1.0452	0.7779
Si	6	-	N	9	1.7722	0.8572	0.8012	0.8706	1.3078	0.8093
Si	6	-	C	11	1.8829	0.8363	0.8972	0.9533	1.6486	0.9068
Si	6	-	C	30	1.8733	0.8605	0.9192	0.977	1.6665	0.9294
Si	6	-	C	40	1.8992	0.7929	0.8315	0.8662	1.031	0.7649
O	7	-	C	22	1.4776	0.7669	0.9031	1.0158	0.9594	1.0925
O	7	-	C	29	1.4676	0.7732	0.9108	1.0245	0.9676	1.1019
N	8	-	C	18	1.403	1.0633	1.1073	1.1938	1.1704	1.2775
N	9	-	C	27	1.4028	1.068	1.0988	1.1826	1.1562	1.2661
C	10	-	C	12	1.425	1.1114	1.2745	1.3159	1.2385	1.3935
C	10	-	C	18	1.4452	1.0767	1.1771	1.209	1.2112	1.2393
C	10	-	H	50	1.0868	1.0458	0.9224	0.9644	0.9872	0.9086
C	11	-	H	51	1.103	1.0138	0.9376	1.0067	1.0618	1.0146
C	11	-	H	52	1.1021	0.9734	0.9381	1.0052	1.0594	1.014
C	11	-	H	53	1.1017	0.9923	0.9437	1.008	1.0551	1.0222
C	12	-	C	14	1.4324	1.0766	1.2421	1.2829	1.2146	1.3541
C	12	-	H	54	1.0874	1.0854	0.9224	0.97	0.9907	0.9082
C	13	-	C	15	1.5331	0.9409	1.0048	1.0434	0.9159	1.1245
C	13	-	C	22	1.5229	0.907	1.0149	1.0562	1.0106	1.1101
C	13	-	H	55	1.0988	1.0167	0.9247	0.9725	1.0029	0.9243
C	13	-	H	56	1.1009	0.9445	0.921	0.9644	0.9938	0.9205
C	14	-	C	16	1.4221	1.1087	1.2783	1.3182	1.251	1.3907
C	14	-	H	57	1.0871	1.0916	0.9213	0.9689	0.9886	0.9051
C	15	-	C	29	1.5164	0.9076	1.0179	1.059	1.0137	1.1128
C	15	-	H	58	1.1021	0.9699	0.9262	0.9679	0.9952	0.9289
C	15	-	H	59	1.0992	1.012	0.924	0.9716	1.0018	0.923
C	16	-	C	18	1.4455	1.0738	1.1746	1.2053	1.2081	1.232
C	16	-	H	60	1.085	1.0228	0.9107	0.9548	0.9756	0.8871
H	17	-	C	38	1.0898	0.9187	0.9114	0.9482	0.9588	0.8897
C	19	-	C	21	1.4233	1.1142	1.2784	1.3195	1.2448	1.3959
C	19	-	C	27	1.4448	1.0812	1.1797	1.212	1.2128	1.2419
C	19	-	H	62	1.0865	1.04	0.9195	0.962	0.9839	0.902
H	20	-	C	45	1.092	0.9934	0.9252	0.9645	0.9757	0.9066
C	21	-	C	23	1.4337	1.0815	1.2429	1.2839	1.2126	1.3568
C	21	-	H	63	1.0874	1.088	0.9223	0.9696	0.9905	0.9081
C	22	-	H	64	1.0957	0.8749	0.9128	0.9534	0.9555	0.8866
C	22	-	H	65	1.0981	0.8945	0.921	0.9636	0.9656	0.8972
C	23	-	C	25	1.4245	1.1115	1.2754	1.316	1.2396	1.3932
C	23	-	H	66	1.0875	1.0909	0.9217	0.9692	0.9899	0.9069
H	24	-	C	35	1.091	1.0478	0.9262	0.9719	0.9852	0.9111
C	25	-	C	27	1.4461	1.0806	1.1778	1.2097	1.2102	1.2407
C	25	-	H	67	1.0876	1.036	0.9113	0.9563	0.9801	0.8919
H	26	-	C	36	1.091	1.0447	0.9266	0.9725	0.9849	0.9101
C	28	-	H	68	1.1024	0.9964	0.9452	1.0109	1.0581	1.0252
C	28	-	H	69	1.1033	1.0047	0.9387	1.0075	1.061	1.017
C	28	-	H	70	1.1024	0.9829	0.9453	1.0106	1.0571	1.0255
C	29	-	H	71	1.0954	0.9123	0.9219	0.9653	0.9672	0.8967
C	29	-	H	72	1.1014	0.8659	0.906	0.9453	0.9481	0.8833
C	30	-	H	73	1.1002	0.9246	0.9357	0.9988	1.0473	1.0124

C	30	-	H	74	1.1014	0.9248	0.9319	1.0008	1.0616	1.0044
C	30	-	H	75	1.103	1.0194	0.937	1.0055	1.0591	1.0146
H	31	-	C	37	1.0909	1.0441	0.9246	0.971	0.984	0.9083
C	32	-	H	61	1.101	0.911	0.9326	0.9982	1.0544	1.0055
C	32	-	H	76	1.1014	0.9135	0.9301	0.9939	1.0473	1.0039
C	32	-	H	77	1.1027	1.0141	0.9357	1.0042	1.0596	1.0119
C	33	-	C	34	1.4041	1.2751	1.4112	1.4627	1.3987	1.5418

Table S15. (NN^{TMS})UI_2(THF) BOND-ORDERS (THRESHOLD = 0.200)

Atom	No.		Atom	No.	DIST. [A]	MAYER	G-J	N-M (1)	N-M (2)	N-M (3) (*)
U	1	-	I	2	3.0281	1.248	1.0304	1.4042	1.5014	1.4876
U	1	-	I	3	3.0508	1.1933	1.0021	1.3685	1.4693	1.4541
U	1	-	Fe	4	3.2168	0.3191	0.3517	0.5597	0.1686	0.5113
U	1	-	O	7	2.5373	0.2629	0.3665	0.4904	0.649	0.4997
U	1	-	N	8	2.2231	0.6791	1.0551	1.3753	1.5975	1.4202
U	1	-	N	9	2.2224	0.682	1.0586	1.3797	1.6012	1.4246
Fe	4	-	C	10	2.0978	0.4037	0.3394	0.465	0.6181	0.4448
Fe	4	-	C	12	2.072	0.3961	0.3382	0.4637	0.604	0.4428
Fe	4	-	C	14	2.0708	0.3942	0.339	0.4648	0.6019	0.4436
Fe	4	-	C	16	2.0938	0.4002	0.3411	0.4672	0.6166	0.4467
Fe	4	-	C	18	2.1557	0.3949	0.2461	0.3361	0.2873	0.312
Fe	4	-	C	19	2.0994	0.401	0.3388	0.4642	0.6162	0.444
Fe	4	-	C	21	2.0718	0.3968	0.3387	0.4644	0.6049	0.4435
Fe	4	-	C	23	2.0696	0.3924	0.3392	0.4651	0.6023	0.4439
Fe	4	-	C	25	2.0929	0.3983	0.3415	0.4677	0.6173	0.4472
Fe	4	-	C	27	2.1563	0.3937	0.2458	0.3355	0.2865	0.3115
Si	5	-	N	8	1.7806	0.8469	0.7998	0.8721	1.3612	0.8123
Si	5	-	C	28	1.8876	0.8389	0.888	0.9454	1.6643	0.8952
Si	5	-	C	32	1.8927	0.826	0.8769	0.9333	1.6546	0.8837
Si	5	-	C	36	1.8774	0.8554	0.9077	0.966	1.6765	0.9142
Si	6	-	N	9	1.7822	0.8449	0.7986	0.8706	1.3586	0.8108
Si	6	-	C	40	1.888	0.8387	0.8873	0.9447	1.6636	0.8945
Si	6	-	C	44	1.8923	0.8263	0.8778	0.9342	1.655	0.8845
Si	6	-	C	48	1.8771	0.8548	0.9083	0.9666	1.6767	0.9148
O	7	-	C	52	1.4712	0.7681	0.9027	1.0136	0.9582	1.0892
O	7	-	C	61	1.4737	0.7658	0.9026	1.013	0.957	1.0887
N	8	-	C	18	1.3993	1.0709	1.1053	1.1909	1.1621	1.282
N	9	-	C	27	1.3995	1.0718	1.105	1.1904	1.1621	1.2812
C	10	-	H	11	1.0867	1.0445	0.9232	0.9646	0.9877	0.9108
C	10	-	C	12	1.4245	1.1116	1.2742	1.3159	1.2349	1.3952
C	10	-	C	18	1.4457	1.0765	1.1767	1.2083	1.2106	1.2393
C	12	-	H	13	1.0874	1.0837	0.9237	0.9705	0.9918	0.9108
C	12	-	C	14	1.4329	1.0811	1.2446	1.2861	1.2131	1.3598
C	14	-	H	15	1.0874	1.0877	0.9229	0.9698	0.9905	0.9089
C	14	-	C	16	1.4241	1.1143	1.2726	1.3132	1.2355	1.3909
C	16	-	H	17	1.0869	1.0321	0.9133	0.9573	0.9813	0.8947
C	16	-	C	18	1.4468	1.0769	1.1734	1.2043	1.2067	1.2345
C	19	-	H	20	1.0866	1.0421	0.9229	0.964	0.9869	0.9101
C	19	-	C	21	1.4245	1.1125	1.2741	1.3157	1.235	1.3948
C	19	-	C	27	1.445	1.0794	1.1767	1.2083	1.2107	1.239
C	21	-	H	22	1.0874	1.0841	0.9236	0.9705	0.9918	0.9108
C	21	-	C	23	1.4329	1.0831	1.2443	1.2858	1.2126	1.3596
C	23	-	H	24	1.0874	1.0881	0.9229	0.9698	0.9905	0.9089
C	23	-	C	25	1.4241	1.1118	1.2724	1.3131	1.2352	1.3908
C	25	-	H	26	1.087	1.0321	0.9137	0.9577	0.9817	0.8951
C	25	-	C	27	1.4468	1.0753	1.1732	1.2041	1.2066	1.2342
C	28	-	H	29	1.1021	0.9962	0.9449	1.01	1.0564	1.0254
C	28	-	H	30	1.1018	0.9654	0.9399	1.006	1.0567	1.0181
C	28	-	H	31	1.1038	1.0136	0.9408	1.0084	1.0582	1.021
C	32	-	H	33	1.1023	0.988	0.9488	1.0129	1.0549	1.0314
C	32	-	H	34	1.1031	0.9992	0.9459	1.0117	1.0586	1.0265
C	32	-	H	35	1.1038	1.0076	0.9423	1.0095	1.0586	1.0226
C	36	-	H	37	1.1013	0.9138	0.9327	0.9992	1.0555	1.0068
C	36	-	H	38	1.1007	0.9255	0.9358	0.9998	1.0498	1.0124
C	36	-	H	39	1.1037	1.0187	0.9386	1.0056	1.0558	1.0177
C	40	-	H	41	1.1018	0.9637	0.9399	1.0059	1.0566	1.018
C	40	-	H	42	1.102	0.9974	0.9451	1.0101	1.0562	1.0257
C	40	-	H	43	1.1039	1.0134	0.9407	1.0082	1.058	1.0209
C	44	-	H	45	1.1031	0.9986	0.9458	1.0115	1.0585	1.0261
C	44	-	H	46	1.1022	0.9879	0.9484	1.013	1.056	1.0307
C	44	-	H	47	1.1037	1.0094	0.9425	1.0096	1.0583	1.0229
C	48	-	H	49	1.1005	0.9285	0.9358	0.9999	1.0502	1.0124
C	48	-	H	50	1.1011	0.9113	0.933	0.9995	1.0559	1.0071
C	48	-	H	51	1.1037	1.0183	0.9386	1.0054	1.0554	1.0176
C	52	-	H	53	1.0953	0.9083	0.9205	0.9654	0.9669	0.8947
C	52	-	H	54	1.1004	0.8608	0.9059	0.9462	0.9487	0.8827
C	52	-	C	55	1.5173	0.9109	1.0178	1.0592	1.0141	1.1129
C	55	-	H	56	1.0991	1.0109	0.9234	0.9712	1.0016	0.9218
C	55	-	H	57	1.1023	0.9723	0.9271	0.9683	0.9954	0.93
C	55	-	C	58	1.5331	0.9405	1.0044	1.0428	0.9165	1.1235

C	58	-	H	59	1.0992	1.0207	0.9246	0.9721	1.002	0.9241
C	58	-	H	60	1.1011	0.9356	0.9178	0.9608	0.9904	0.9159
C	58	-	C	61	1.5204	0.9066	1.0167	1.0579	1.0123	1.1117
C	61	-	H	62	1.0959	0.8819	0.9117	0.9554	0.957	0.8841
C	61	-	H	63	1.1001	0.9159	0.922	0.9638	0.9665	0.9012

Table S16. (NN^{TBS})U(CH_2Ph)(OAr)						BOND-ORDERS (THRESHOLD = 0.200)				
Atom	**No.**		**Atom**	**No.**	**DIST. [A]**	**MAYER**	**G-J**	**N-M (1)**	**N-M (2)**	**N-M (3) (*)**
U	1	-	Fe	2	3.1975	0.2234	0.3719	0.6058	0.0043	0.544
U	1	-	O	5	2.1517	0.7149	1.0719	1.461	1.6832	1.4684
U	1	-	N	6	2.2778	0.6379	0.9606	1.2933	1.6652	1.3099
U	1	-	N	7	2.2725	0.6284	0.9573	1.289	1.6644	1.3064
U	1	-	C	38	2.4897	0.5514	0.7232	0.9509	1.3326	0.9495
Fe	2	-	C	8	2.1826	0.3845	0.2344	0.3193	0.2681	0.2963
Fe	2	-	C	9	2.1087	0.4176	0.3322	0.4544	0.5974	0.4342
Fe	2	-	C	11	2.067	0.4071	0.3422	0.4685	0.605	0.4473
Fe	2	-	C	13	2.068	0.3954	0.3375	0.462	0.6011	0.4412
Fe	2	-	C	15	2.0946	0.4085	0.3449	0.4718	0.625	0.4515
Fe	2	-	C	17	2.0688	0.3954	0.3358	0.4598	0.5986	0.4391
Fe	2	-	C	19	2.0669	0.3933	0.3414	0.4675	0.6071	0.4465
Fe	2	-	C	21	2.0947	0.404	0.337	0.4613	0.6176	0.4416
Fe	2	-	C	23	2.1632	0.3911	0.242	0.3299	0.2844	0.3065
Fe	2	-	C	24	2.0973	0.4055	0.3362	0.4599	0.6089	0.4399
Si	3	-	N	6	1.7772	0.8626	0.844	0.9187	1.4044	0.8643
Si	3	-	C	26	1.8851	0.8404	0.8966	0.9499	1.622	0.9022
Si	3	-	C	30	1.894	0.8318	0.89	0.9428	1.6288	0.897
Si	3	-	C	34	1.9287	0.7532	0.7925	0.8192	0.8967	0.7147
Si	4	-	N	7	1.7724	0.8732	0.844	0.9193	1.4102	0.8655
Si	4	-	C	16	1.8955	0.8271	0.8787	0.9315	1.6205	0.8861
Si	4	-	C	32	1.9299	0.7353	0.7965	0.8237	0.8993	0.7185
Si	4	-	C	44	1.8841	0.8375	0.9019	0.9563	1.6334	0.9089
O	5	-	C	10	1.3579	0.9066	1.09	1.2006	1.2316	1.2653
N	6	-	C	8	1.4	1.0779	1.119	1.2082	1.178	1.3038
N	7	-	C	23	1.4009	1.0752	1.113	1.2031	1.1671	1.3004
C	8	-	C	9	1.4465	1.0792	1.1759	1.2059	1.2096	1.2339
C	8	-	C	15	1.447	1.0791	1.1735	1.2036	1.207	1.2341
C	9	-	C	11	1.4244	1.1088	1.2692	1.31	1.2353	1.386
C	9	-	H	51	1.0891	0.999	0.9107	0.95	0.9724	0.8895
C	10	-	C	12	1.4319	1.242	1.2894	1.3223	1.323	1.2988
C	10	-	C	27	1.4215	1.2851	1.3328	1.368	1.3709	1.3462
C	11	-	C	13	1.432	1.0826	1.2451	1.2865	1.2138	1.3602
C	11	-	H	52	1.0869	1.0897	0.9225	0.9697	0.9905	0.9083
C	12	-	C	14	1.395	1.2837	1.4353	1.4763	1.4643	1.5147
C	12	-	C	28	1.5414	0.9372	0.9641	0.9817	0.9831	0.9792
C	13	-	C	15	1.4242	1.1099	1.2712	1.3123	1.2312	1.3916
C	13	-	H	53	1.0873	1.0821	0.9238	0.9702	0.9912	0.911
C	14	-	C	18	1.3905	1.2196	1.4028	1.4573	1.411	1.5225
C	14	-	H	54	1.0867	0.9874	0.921	0.9607	0.9738	0.9041
C	15	-	H	55	1.0871	1.0513	0.9227	0.9647	0.9883	0.9094
C	16	-	H	56	1.1017	0.9702	0.9458	1.0084	1.0513	1.0254
C	16	-	H	57	1.1035	1.0037	0.9414	1.0071	1.055	1.02
C	16	-	H	58	1.1016	0.9937	0.9456	1.0096	1.0551	1.0244
C	17	-	C	19	1.4324	1.0877	1.2448	1.2868	1.2128	1.3611
C	17	-	C	24	1.4236	1.1139	1.2744	1.3158	1.2372	1.394
C	17	-	H	59	1.0871	1.0861	0.9229	0.9699	0.991	0.9096
C	18	-	C	22	1.3825	1.2596	1.4474	1.503	1.458	1.5691
C	18	-	H	60	1.09	1.0642	0.9261	0.9735	0.9881	0.9148
C	19	-	C	21	1.4249	1.1208	1.2698	1.3122	1.2294	1.3922
C	19	-	H	61	1.0872	1.084	0.9233	0.9702	0.9915	0.9107
C	20	-	C	32	1.5366	0.9138	1.0081	1.047	0.9198	1.1331
C	20	-	H	62	1.0998	0.9284	0.9482	0.9883	1.021	0.9752
C	20	-	H	63	1.1061	1.0079	0.939	0.9831	1.0178	0.9675
C	20	-	H	64	1.1015	0.9595	0.9479	0.9903	1.0246	0.9746
C	21	-	C	23	1.4468	1.0895	1.1744	1.2065	1.2076	1.2389
C	21	-	H	65	1.0868	1.0412	0.9225	0.9627	0.9864	0.9102
C	22	-	C	27	1.4025	1.2472	1.392	1.4324	1.4184	1.4709
C	22	-	H	66	1.0889	0.9743	0.9254	0.9622	0.9743	0.9101
C	23	-	C	24	1.4458	1.0847	1.1776	1.209	1.2105	1.2398
C	24	-	H	68	1.0867	1.0272	0.9164	0.957	0.9803	0.8988
C	25	-	C	40	1.3963	1.2374	1.4134	1.4672	1.4149	1.5371
C	25	-	C	42	1.3909	1.2901	1.4594	1.5125	1.4634	1.5819
C	25	-	H	69	1.0916	1.0454	0.9262	0.9704	0.9838	0.9111
C	26	-	H	70	1.1025	1.012	0.9419	1.0072	1.0549	1.0189
C	26	-	H	71	1.1011	0.9357	0.945	1.0049	1.0455	1.0226
C	26	-	H	72	1.0994	0.8957	0.9398	1.001	1.0492	1.0127
C	27	-	C	37	1.5464	0.946	0.9624	0.9806	0.9825	0.9801
C	28	-	C	29	1.539	0.8878	0.9858	1.017	1.0145	1.0695
C	28	-	C	36	1.5383	0.8868	0.9863	1.0177	1.0151	1.0703
C	28	-	C	41	1.5376	0.9134	1	1.0317	1.0272	1.0878
C	29	-	H	73	1.1018	0.9779	0.9459	0.9913	1.0282	0.9704
C	29	-	H	74	1.102	0.9741	0.944	0.989	1.0247	0.9701
C	29	-	H	75	1.0938	0.8235	0.9379	0.9754	1.0085	0.961
C	30	-	H	76	1.1021	0.9927	0.9448	1.0098	1.0576	1.0228
C	30	-	H	77	1.1022	0.9932	0.9471	1.0111	1.0547	1.0273
C	30	-	H	78	1.1032	1.0069	0.9418	1.0074	1.0557	1.02
C	31	-	C	37	1.5447	0.8916	0.9876	1.0176	1.0133	1.0714
C	31	-	H	79	1.1002	0.9418	0.9454	0.9893	1.0264	0.9693
C	31	-	H	80	1.1024	0.996	0.9455	0.9906	1.0261	0.9729

C	31	-	H	81	1.0987	0.9926	0.9451	0.9908	1.0284	0.9699
C	32	-	C	33	1.5409	0.916	1.0061	1.045	0.9149	1.1323
C	32	-	C	45	1.5399	0.914	1.0084	1.0476	0.9184	1.1347
C	33	-	H	82	1.1061	0.9929	0.9385	0.9829	1.0186	0.9675
C	33	-	H	83	1.1022	0.9861	0.9486	0.9936	1.0292	0.9773
C	33	-	H	84	1.1014	0.9858	0.9483	0.9934	1.0297	0.9762
C	34	-	C	35	1.5377	0.912	1.0082	1.0475	0.9185	1.1344
C	34	-	C	39	1.5364	0.9148	1.0073	1.0464	0.9197	1.1322
C	34	-	C	43	1.5399	0.9172	1.006	1.0448	0.914	1.1323
C	35	-	H	85	1.1064	0.9971	0.9403	0.984	1.0178	0.9703
C	35	-	H	86	1.0996	0.9216	0.9446	0.9859	1.0213	0.9696
C	35	-	H	87	1.1021	0.9935	0.9476	0.9933	1.0294	0.9754
C	36	-	H	88	1.0922	0.8142	0.937	0.9752	1.0094	0.9595
C	36	-	H	89	1.1019	0.9775	0.9445	0.99	1.0257	0.9711
C	36	-	H	90	1.1015	0.9843	0.9455	0.9923	1.0299	0.9702
C	37	-	C	46	1.5328	0.9132	0.9938	1.0227	1.0207	1.0721
C	37	-	C	49	1.5438	0.8896	0.9882	1.0185	1.0141	1.0725
C	38	-	C	47	1.4685	1.0739	1.1357	1.1927	1.1617	1.2716
C	38	-	H	91	1.1019	0.9323	0.9169	0.9684	1.0067	0.9634
C	38	-	H	92	1.1044	0.9324	0.9101	0.9619	1.0002	0.9571
C	39	-	H	93	1.1062	1.0016	0.9385	0.9824	1.0169	0.9666
C	39	-	H	94	1.1009	0.966	0.9461	0.9896	1.0254	0.9711
C	39	-	H	95	1.0994	0.8726	0.9442	0.9826	1.0143	0.9705
C	40	-	C	50	1.3962	1.2387	1.415	1.4689	1.4169	1.5386
C	40	-	H	96	1.0902	1.0536	0.9288	0.9756	0.9927	0.9204
C	41	-	H	97	1.1008	0.9866	0.9461	0.992	1.0294	0.9744
C	41	-	H	98	1.1007	0.9867	0.946	0.992	1.0294	0.9742
C	41	-	H	99	1.1009	0.9933	0.9437	0.9913	1.0302	0.9712
C	42	-	C	47	1.4127	1.2189	1.3254	1.3659	1.3648	1.3942
C	42	-	H 1	0	1.0904	0.9652	0.9264	0.9633	0.9781	0.9131
C	43	-	H 1	1	1.1016	0.9865	0.9484	0.9937	1.03	0.9766
C	43	-	H 1	2	1.1021	0.9839	0.9489	0.9937	1.029	0.978
C	43	-	H 1	3	1.1061	0.9929	0.9388	0.9833	1.019	0.9681
C	44	-	H 1	4	1.1007	0.9043	0.9421	1.0062	1.0552	1.0178
C	44	-	H 1	5	1.1021	1.0125	0.9408	1.0068	1.0565	1.0177
C	44	-	H 1	6	1.1009	0.9193	0.9423	1.0042	1.0497	1.0186
C	45	-	H 1	7	1.1014	0.9553	0.9453	0.9881	1.0244	0.971
C	45	-	H 1	8	1.1019	0.9918	0.9482	0.9937	1.03	0.976
C	45	-	H 1	9	1.1064	0.9988	0.9402	0.9842	1.0185	0.9702
C	46	-	H 1	10	1.1038	0.8639	0.9012	0.9382	0.9756	0.9143
C	46	-	H 1	11	1.1042	0.8508	0.8968	0.9326	0.9691	0.9107
C	46	-	H 1	12	1.1018	0.948	0.9367	0.9778	1.013	0.9544
C	47	-	C	48	1.412	1.2207	1.3274	1.3679	1.367	1.3955
C	48	-	C	50	1.3907	1.2887	1.46	1.513	1.4654	1.5815
C	48	-	H 1	13	1.0906	0.9422	0.9275	0.9621	0.9761	0.9151
C	49	-	H 1	14	1.1026	0.991	0.9455	0.9905	1.026	0.9732
C	49	-	H 1	15	1.0999	0.9395	0.9454	0.9896	1.0275	0.9686
C	49	-	H 1	16	1.0989	0.9943	0.9452	0.9912	1.0287	0.9706
C	50	-	H	67	1.0918	1.051	0.9273	0.9711	0.9843	0.9129

(*) Values from:

- Mayer bond-order analysis
- Gophinatan-Jug bond order analysis
- Nalewajski-Mrozek bond order analysis

a) N-M (1) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (3-index set)
b) N-M (2) - bond-orders calculated from two-electron valence indices based on partitioning of tr(Delta_P^2] (4-index set)
c) N-M (3) - bond-orders calculated from valence indices based on partitioning of tr(P*Delta_P]
A. Michalak, R.L. DeKock, T. Ziegler, J. Comp. Chem., subm. and original articles by Nalewajski et al.)