

Supporting Information for

Intrinsic reactivity of a uranium metallacyclopropene toward unsaturated organic molecules

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1. Figures

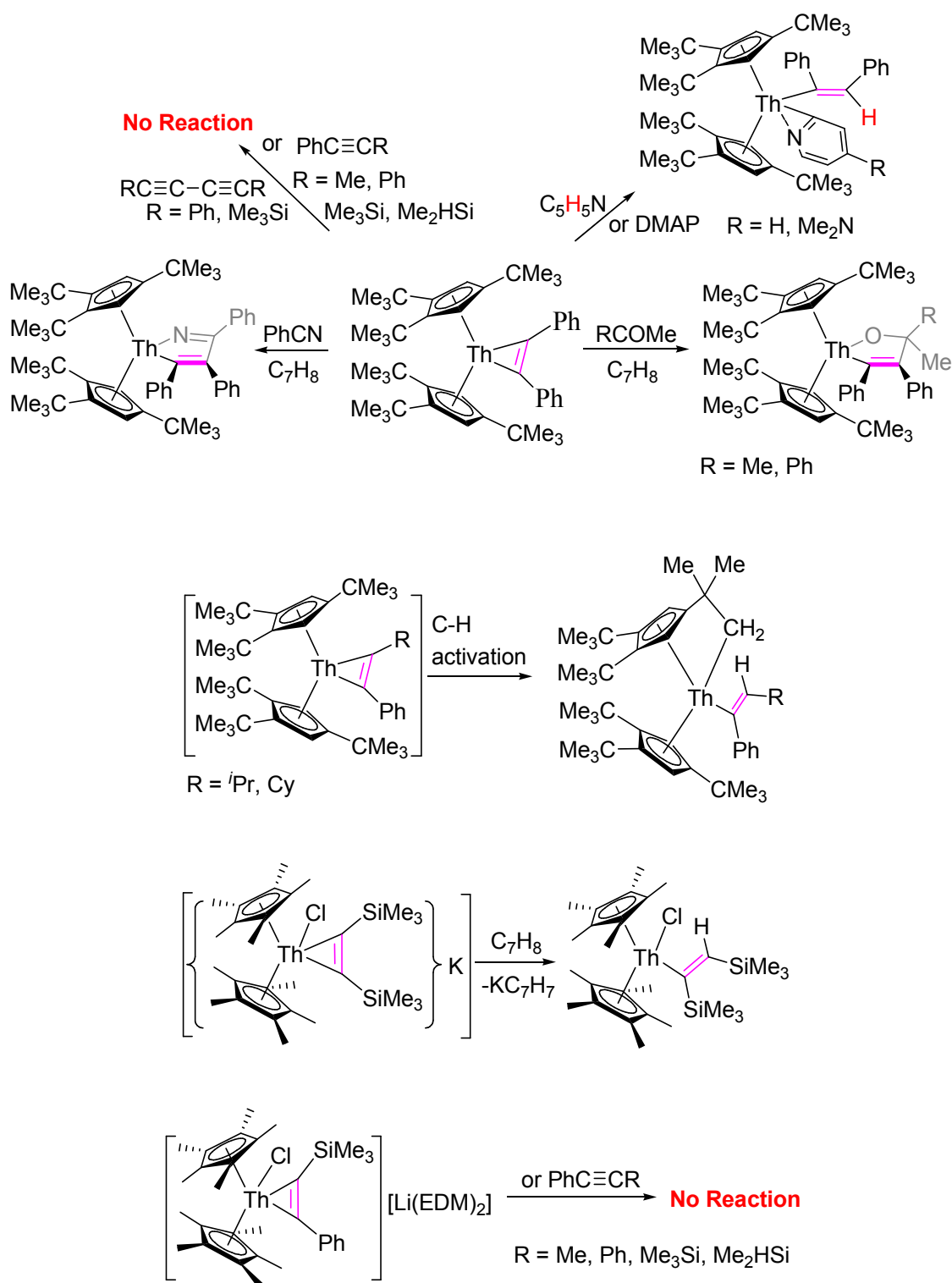


Figure S1. Selected reactivity of thorium metallacycloprenes.

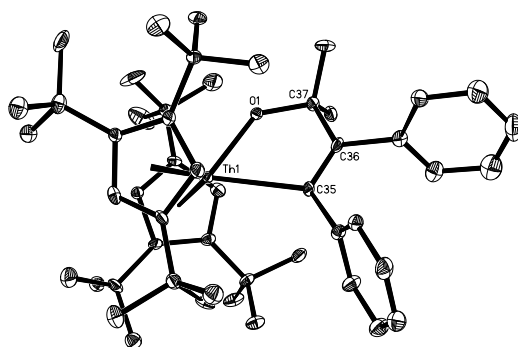


Figure S2. Molecular structure of **15** (thermal ellipsoids drawn at the 35% probability level). Selected bond lengths (Å) and angles (°): Th-C(Cp) (av.) 2.880(14), Th-C(Cp) (range) 2.795(13) to 3.001(14), Th-Cp (cent) (av.) 2.619(12), Th-O(1) 2.087(8), Th-C(35) 2.603(11), Cp(cent)-Th-Cp(cent) 131.9(4), O(1)-Th-C(35) 66.7(4).

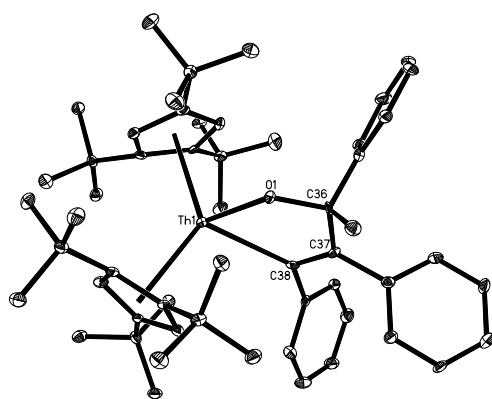


Figure S3. Molecular structure of **16** (thermal ellipsoids drawn at the 35% probability level). Selected bond lengths (Å) and angles (°): Th-C(Cp) (av.) 2.910(6), Th-C(Cp) (range) 2.815(5) to 3.050(6), Th-Cp (cent) (av.) 2.646(5), Th-O(1) 2.121(4), Th-C(38) 2.624(6), Cp(cent)-Th-Cp(cent) 129.3(2), O(1)-Th-C(38) 66.8(2).

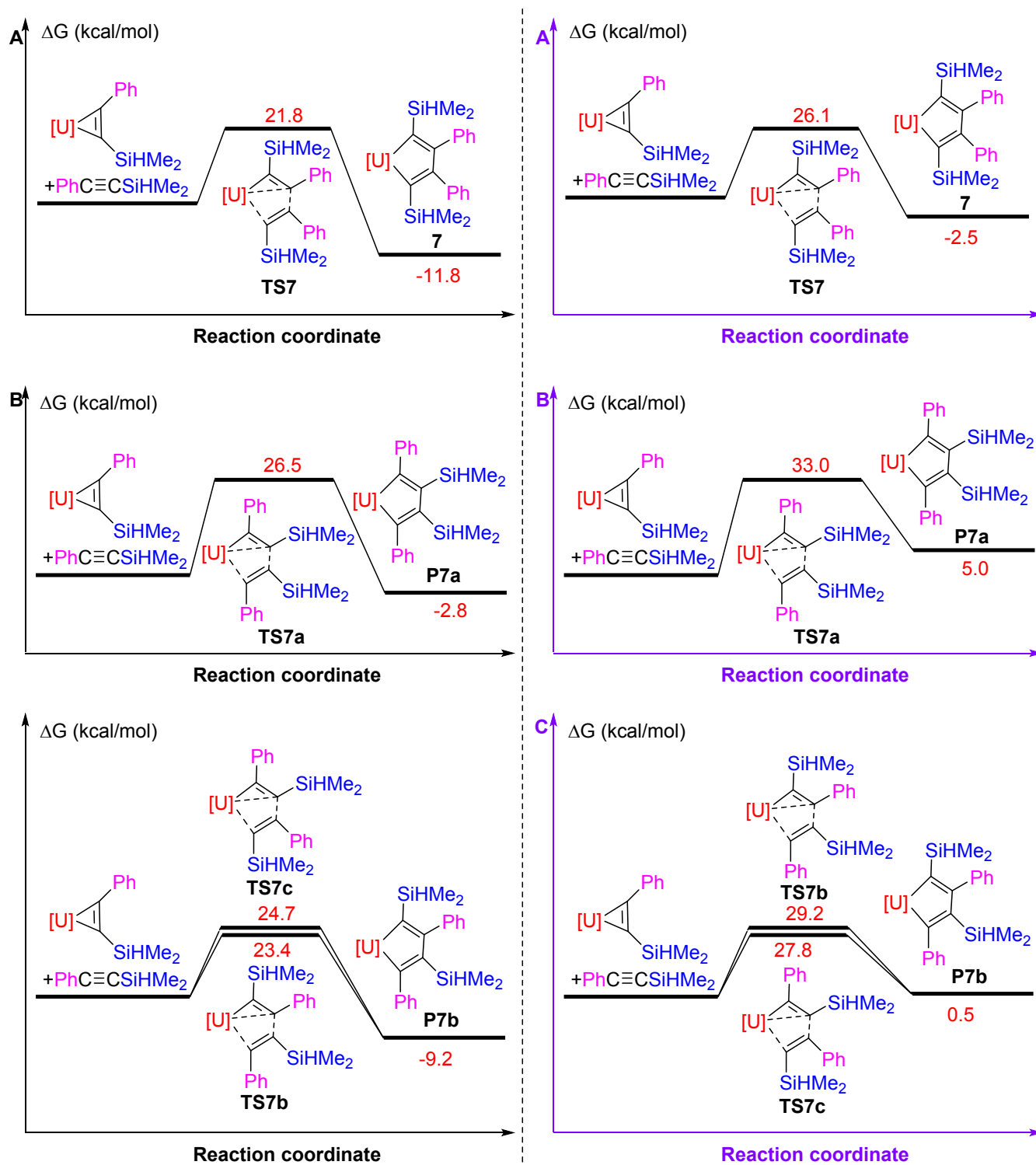
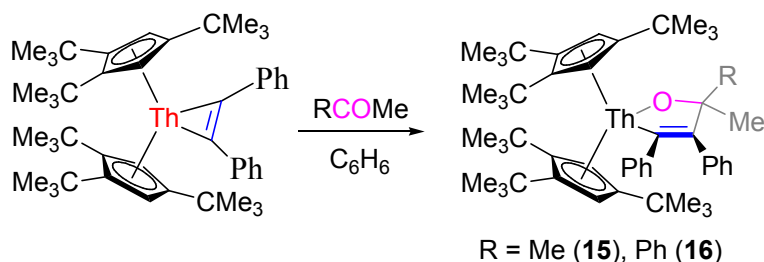


Figure S4. Free energy profile (kcal/mol) for the reaction of $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{SiHMe}_2)] + \text{PhC}\equiv\text{CSiHMe}_2$ (U was treated with ECP80MWB (left) and ECP60MWB (right)). [U] = $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}$.

2. Additional experiments



Scheme S1

Preparation of $[\eta^5\text{-}1,2,4\text{-(Me}_3\text{C)}_3\text{C}_5\text{H}_2]_2\text{Th[OCMe}_2\text{(C}_2\text{Ph}_2)]$ (15) Method A. A toluene solution (5 mL) of acetone (15 mg, 0.25 mmol) was added to a toluene (10 mL) solution of $[\eta^5\text{-}1,2,4\text{-(Me}_3\text{C)}_3\text{C}_5\text{H}_2]_2\text{Th}(\eta^2\text{-C}_2\text{Ph}_2)$ (220 mg, 0.25 mmol) with stirring at room temperature. After the solution was stirred at room temperature overnight, the solvent was removed. The residue was extracted with benzene (10 mL \times 3) and filtered. The volume of the filtrate was reduced to 5 mL, yellow crystals of **15** were isolated when this solution was kept at room temperature for one week. Yield: 182 mg (78%) (Found: C, 65.46; H, 8.03. $\text{C}_{51}\text{H}_{74}\text{OTh}$ requires C, 65.50; H, 7.98%). M.p.: 118-120 °C. ^1H NMR (C_6D_6): δ 7.07 (m, 8H, phenyl), 6.95 (s, 2H, ring CH), 6.84 (t, $J = 7.2$ Hz, 1H, phenyl), 6.72 (t, $J = 6.9$ Hz, 1H, phenyl), 6.64 (bs, 2H, ring CH), 1.62 (s, 36H, $\text{C}(\text{CH}_3)_3$), 1.26 (s, 18H, $\text{C}(\text{CH}_3)_3$), 1.23 (s, 6H, $\text{C}(\text{CH}_3)_2$) ppm. $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6): δ 208.0 (ThCPh), 170.8 (CPh), 154.9 (phenyl C), 143.9 (phenyl C), 142.7 (phenyl C), 142.5 (phenyl C), 142.1 (phenyl C), 130.0 (phenyl C), 127.4 (phenyl C), 127.2 (phenyl C), 127.1 (ring C), 125.3 (ring C), 122.2 (ring C), 117.8 (ring C), 117.4 (ring C), 91.6 (OCMe_2), 34.8 ($\text{C}(\text{CH}_3)_3$), 34.6 ($\text{C}(\text{CH}_3)_3$), 33.0 ($\text{C}(\text{CH}_3)_3$), 31.9 ($\text{C}(\text{CH}_3)_3$), 31.4 ($\text{C}(\text{CH}_3)_3$), 31.0 ($\text{C}(\text{CH}_3)_3$) ppm; two carbons overlapped. IR (KBr, cm^{-1}): 2958 (s), 1593 (m), 1479 (s), 1390 (s), 1361 (s), 1238 (s), 1155 (s), 958 (s), 889 (s), 812 (s).

Method B. NMR Scale. A C_6D_6 (0.3 mL) solution of acetone (1.2 mg, 0.02 mmol) was slowly added to a J. Young NMR tube charged with $[\eta^5\text{-}1,2,4\text{-(Me}_3\text{C)}_3\text{C}_5\text{H}_2]_2\text{Th}(\eta^2\text{-C}_2\text{Ph}_2)$ (18 mg, 0.02 mmol) and C_6D_6 (0.2 mL). Resonances of **15** were observed by ^1H NMR spectroscopy (100% conversion).

Preparation of [η^5 -1,2,4-(Me₃C)₃C₅H₂]₂Th[OCPhMe(C₂Ph₂)] (16). Method A. This compound was prepared as colourless crystals from the reaction of [η^5 -1,2,4-(Me₃C)₃C₅H₂]₂Th(η^2 -C₂Ph₂) (220 mg, 0.25 mmol) and PhCOCH₃ (30 mg, 0.25 mmol) in toluene (15 mL) at room temperature and recrystallization from a benzene solution by a similar procedure as that in the synthesis of **15**. Yield: 204 mg (82%) (Found: C, 67.51; H, 7.65. C₅₆H₇₆OTh requires C, 67.45; H, 7.68.). M.p.: 180-182 °C. ¹H NMR (C₆D₆): δ 8.13 (d, J = 7.5 Hz, 2H, phenyl), 7.35 (m, 4H, phenyl), 7.15 (m, 6H, phenyl), 6.79 (m, 5H, phenyl, ring CH), 6.58 (s, 1H, ring CH), 6.40 (s, 1H, ring CH), 1.96 (s, 3H, CH₃), 1.75 (s, 9H, C(CH₃)₃), 1.61 (s, 9H, C(CH₃)₃), 1.60 (s, 9H, C(CH₃)₃), 1.46 (s, 9H, C(CH₃)₃), 1.23 (s, 9H, C(CH₃)₃), 1.06 (s, 9H, C(CH₃)₃) ppm. ¹³C{¹H} NMR (C₆D₆): δ 213.7 (ThCPh), 168.4 (CPh), 147.0 (phenyl C), 143.9 (phenyl C), 143.4 (phenyl C), 141.9 (phenyl C), 137.8 (phenyl C), 130.7 (phenyl C), 129.3 (phenyl C), 129.1 (phenyl C), 128.5 (phenyl C), 127.3 (phenyl C), 127.0 (phenyl C), 125.6 (phenyl C), 125.4 (ring C), 122.5 (ring C), 119.5 (ring C), 118.1 (ring C), 116.4 (ring C), 94.5 (CO), 34.9 (C(CH₃)₃), 34.7 (C(CH₃)₃), 33.6 (C(CH₃)₃), 32.8 (C(CH₃)₃), 32.0 (CH₃), 30.9 (C(CH₃)₃), 29.8 (C(CH₃)₃) ppm. IR (KBr, cm⁻¹): 2958 (s), 1595 (m), 1479 (s), 1460 (s), 1390 (s), 1361 (s), 1236 (s), 1211 (s), 1093 (s), 1064 (s), 908 (s), 812 (s).

Method B. NMR Scale. A C₆D₆ (0.3 mL) solution of PhCOCH₃ (2.4 mg, 0.02 mmol) was slowly added to a J. Young NMR tube charged with [η^5 -1,2,4-(Me₃C)₃C₅H₂]₂Th(η^2 -C₂Ph₂) (18 mg, 0.02 mmol) and C₆D₆ (0.2 mL). Resonances of **16** were observed by ¹H NMR spectroscopy (100% conversion).

3. Crystal parameters

Table S1. Crystal Data and Experimental Parameters for Compounds 2-4 and 6-8

Compound	2	3	4	2(6)·C ₆ H ₆	7	8
Formula	C ₃₃ H ₅₃ NSi ₂ U	C ₃₅ H ₅₈ N ₂ Si ₂ U	C ₄₉ H ₆₃ NSi ₂ U	C ₈₂ H ₉₈ U ₂	C ₄₀ H ₅₄ Si ₂ U	C ₄₂ H ₅₈ Si ₂ U
Fw	757.97	801.04	960.21	1559.66	829.04	857.09
crystal system	triclinic	orthorhombic	monoclinic	triclinic	triclinic	monoclinic
space group	<i>P</i> (-1)	<i>Pbca</i>	<i>P2</i> ₁ / <i>n</i>	<i>P</i> (-1)	<i>P</i> (-1)	<i>C2/c</i>
<i>a</i> (Å)	9.946(9)	19.17(2)	9.716(5)	11.201(15)	10.010(7)	20.461(13)
<i>b</i> (Å)	10.905(10)	19.61(3)	21.054(10)	15.69(2)	11.707(11)	12.778(9)
<i>c</i> (Å)	17.123(16)	20.30(3)	21.626(9)	19.70(3)	17.678(12)	15.797(14)
α (deg)	78.45(1)	90	90	88.63(2)	83.00(2)	90
β (deg)	81.55(1)	90	90.34(1)	81.50(3)	76.37(1)	108.45(1)
γ (deg)	68.88(1)	90	90	89.31(2)	65.07(1)	90
<i>V</i> (Å ³)	1692(3)	7631(18)	4424(4)	3423(8)	1825(2)	3918(5)
<i>Z</i>	2	8	4	2	2	4
<i>D</i> _{calc} (g/cm ³)	1.488	1.394	1.442	1.513	1.508	1.453
μ (Mo/K α) _{calc} (cm ⁻¹)	4.889	4.340	3.756	4.769	4.538	4.231
size (mm)	0.20 × 0.20 × 0.20	0.20 × 0.10 × 0.10	0.35 × 0.10 × 0.10	0.20 × 0.20 × 0.15	0.20 × 0.20 × 0.20	0.20 × 0.20 × 0.10
<i>F</i> (000)	756	3216	1936	1548	828	1720
2 θ range (deg)	4.06 to 55.81	3.59 to 54.80	2.70 to 50.50	3.30 to 50.50	3.84 to 55.55	3.82 to 55.33
no. of reflns, collected	11415	47262	19859	18455	12571	12473
no of obsd reflns	7806	8433	7874	12239	8419	4520
no of variables	350	374	498	781	408	212
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	0.75, 0.57	0.75, 0.44	0.75, 0.52	0.75, 0.50	0.75, 0.52	0.75, 0.59
<i>R</i>	0.064	0.043	0.067	0.045	0.073	0.056
<i>R</i> _w	0.169	0.093	0.155	0.101	0.168	0.127
<i>R</i> _{all}	0.071	0.082	0.090	0.072	0.106	0.068
Gof	1.01	1.01	0.98	0.96	0.95	1.01
CCDC	1496478	1496489	1496486	1496480	1496479	1496477

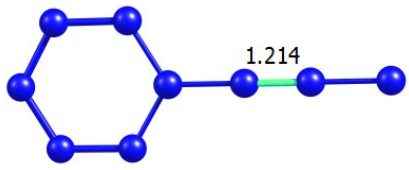
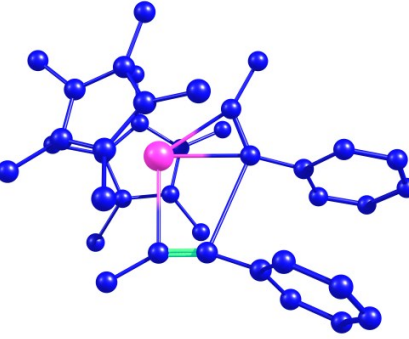
Table S2. Crystal Data and Experimental Parameters for Compounds 11-16

Compound	11·0.5C ₆ H ₆	12	13·C ₆ H ₆	14	15	16
Formula	C ₄₄ H ₆₆ N ₃ U	C ₃₄ H ₃₈ O ₂ U	C ₅₈ H ₇₄ O ₄ U ₂	C ₃₄ H ₅₈ OSi ₂ U	C ₅₁ H ₇₄ OTh	C ₅₆ H ₇₆ OTh
Fw	875.02	716.67	1311.23	777.01	935.14	997.20
crystal system	triclinic	monoclinic	triclinic	triclinic	triclinic	monoclinic
space group	<i>P</i> (-1)	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> (-1)	<i>P</i> (-1)	<i>P</i> (-1)	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	10.564(10)	9.525(4)	9.666(10)	9.785(8)	10.578(8)	11.624(4)
<i>b</i> (Å)	13.462(12)	18.419(8)	11.556(12)	10.877(9)	11.855(8)	19.697(7)
<i>c</i> (Å)	15.492(15)	16.332(7)	12.665(13)	17.182(14)	20.884(15)	20.839(8)
α (deg)	75.61(2)	90	69.07(1)	79.24(1)	77.73(1)	90
β (deg)	76.10(2)	92.40(1)	86.75(1)	76.81(1)	82.30(1)	97.45(1)
γ (deg)	74.44(1)	90	74.08(1)	78.00(2)	68.24(1)	90
<i>V</i> (Å ³)	2020(3)	2863(2)	1269(2)	1723(2)	2372(3)	4731(3)
<i>Z</i>	2	4	1	2	2	4
<i>D</i> _{calc} (g/cm ³)	1.439	1.663	1.716	1.498	1.309	1.400
μ (Mo/K α) _{calc} (cm ⁻¹)	4.050	5.698	6.417	4.803	3.175	3.190
size (mm)	0.20 × 0.20 × 0.20	0.20 × 0.15 × 0.10	0.30 × 0.10 × 0.10	0.20 × 0.15 × 0.15	0.15 × 0.15 × 0.15	0.15 × 0.15 × 0.15
<i>F</i> (000)	886	1400	638	780	956	2040
2 θ range (deg)	3.20 to 50.50	3.33 to 50.48	3.45 to 51.05	3.87 to 50.50	3.76 to 55.77	2.86 to 55.09
no. of reflns, collected	11284	15998	6469	9009	10970	31993
no of obsd reflns	7259	5172	4629	6274	10970	10878
no of variables	486	342	314	359	499	542
abs corr (<i>T</i> _{max} , <i>T</i> _{min})	0.75, 0.50	0.75, 0.59	0.75, 0.40	0.75, 0.45	0.75, 0.63	0.75, 0.55
<i>R</i>	0.060	0.044	0.050	0.078	0.087	0.052
<i>R</i> _w	0.162	0.089	0.125	0.205	0.224	0.094
<i>R</i> _{all}	0.069	0.075	0.064	0.087	0.099	0.090
Gof	1.01	1.03	1.08	1.03	1.04	0.96
CCDC	1496484	1496485	1496483	1496481	1496488	1496490

4. Computational details

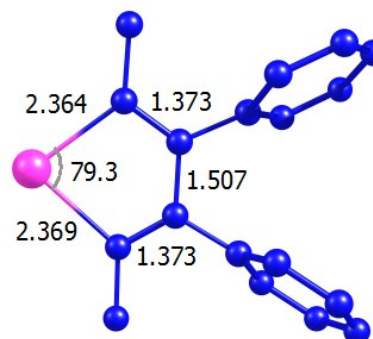
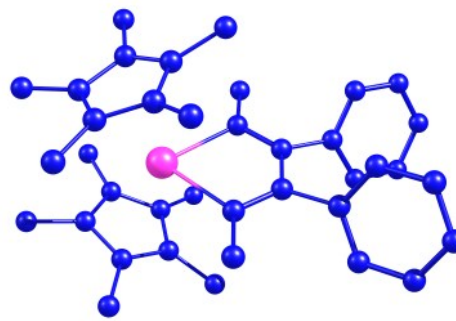
Table S3. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{Me})]+\text{PhC}\equiv\text{CMe}$, obtained with B3PW91-PCM method.

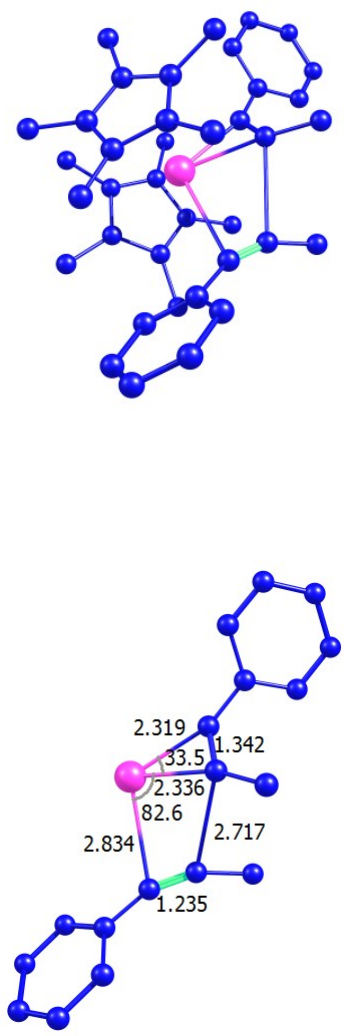
Species	Cartesian coordinates				
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{Me})]$	C	-2.399506	1.866968	-1.261602	
	C	-1.049553	2.220925	-1.563231	
	C	-0.516663	1.227839	-2.433328	
	C	-1.526477	0.242936	-2.637771	
	C	-2.698334	0.651103	-1.929427	
	C	-3.350450	2.727367	-0.479100	
	H	-3.656387	3.606658	-1.063600	
	H	-2.904962	3.112729	0.447471	
	H	-4.262572	2.189408	-0.206109	
	C	-0.382612	3.504170	-1.155574	
	H	0.706716	3.434891	-1.225919	
	H	-0.626744	3.792200	-0.125620	
	H	-0.698683	4.339234	-1.798027	
	C	0.812221	1.293431	-3.127811	
	H	0.730196	1.841960	-4.077625	
	H	1.208046	0.299861	-3.358224	
	H	1.564083	1.802210	-2.517805	
	C	-1.433600	-0.945219	-3.553294	
	H	-1.847787	-0.719996	-4.546724	
	H	-1.990403	-1.810841	-3.172854	
	H	-0.396271	-1.261133	-3.704938	
	C	-4.036629	-0.023496	-2.015224	
	H	-4.691182	0.251640	-1.182437	
	H	-3.953558	-1.116187	-2.021395	
	H	-4.560324	0.257946	-2.940320	
	C	-2.725484	-0.637566	1.916561	
	C	-1.560203	-0.210571	2.625200	
	C	-0.553283	-1.206150	2.464490	
	C	-1.078877	-2.226546	1.622202	
	C	-2.422908	-1.876471	1.292753	
	C	-4.068735	0.030178	1.977767	
	H	-4.699965	-0.229692	1.122275	
	H	-3.989911	1.122263	2.008104	
	H	-4.616316	-0.272470	2.882137	
	C	-1.465772	1.002448	3.507719	
	H	-1.807600	0.783352	4.529616	
	H	-2.084182	1.830838	3.141704	
	H	-0.436780	1.369780	3.588073	
	C	0.767981	-1.250822	3.173973	
	H	0.674313	-1.761481	4.143764	
H	1.162206	-0.248915	3.372282		
H	1.521731	-1.788996	2.591718		
C	-0.398805	-3.516963	1.260461		
H	0.685197	-3.398342	1.168228		
H	-0.765762	-3.920594	0.309435		
H	-0.581325	-4.289994	2.021359		
C	-3.369528	-2.746354	0.514712		
H	-3.695973	-3.608551	1.113030		
H	-2.913654	-3.157489	-0.395685		
H	-4.270486	-2.204028	0.213922		
C	1.420374	0.585100	0.320789		
C	1.436668	-0.638210	-0.260581		
U	-0.769317	-0.027485	-0.002364		
C	2.564223	-1.505573	-0.606463		
C	2.585834	-2.211979	-1.825298		

	C 3.651901 -1.699901 0.270118 C 3.650369 -3.040841 -2.167708 C 4.706045 -2.549350 -0.060376 C 4.717245 -3.218216 -1.284570 H 1.748281 -2.097131 -2.510101 H 3.657086 -1.184148 1.226825 H 3.642467 -3.561663 -3.122895 H 5.527304 -2.684730 0.640365 H 5.543165 -3.875438 -1.545121 C 2.567427 1.461631 0.729252 H 2.680832 1.455043 1.823411 H 3.531446 1.149993 0.299902 H 2.393280 2.510051 0.453406	
PhC≡CMe	C 2.605992 0.000579 -0.000946 C 1.392015 0.000160 -0.001847 C -0.035932 0.000073 -0.001397 C -0.752142 1.211087 -0.000817 H -0.205158 2.149562 -0.001239 C -2.143595 1.206738 0.000554 H -2.683551 2.150218 0.001158 C -2.844394 -0.000132 0.001312 H -3.931280 -0.000211 0.002595 C -2.143418 -1.206898 0.000542 H -2.683239 -2.150457 0.001161 C -0.751963 -1.211045 -0.000827 H -0.204843 -2.149442 -0.001231 C 4.062043 -0.000215 0.001640 H 4.458917 -0.876638 -0.524698 H 4.460006 0.894518 -0.491865 H 4.457503 -0.019625 1.024841	
TS6a	C 0.754857 -2.428696 -1.402799 C 1.902431 -1.776121 -1.939407 C 2.902429 -1.733983 -0.930188 C 2.363176 -2.340160 0.242269 C 1.046226 -2.790158 -0.058366 C -0.439082 -2.855576 -2.209534 H -0.142457 -3.550965 -3.007862 H -0.954555 -2.016169 -2.692206 H -1.170379 -3.380013 -1.588776 C 2.129134 -1.474686 -3.392929 H 2.629843 -2.320516 -3.888093 H 2.767690 -0.598331 -3.551594 H 1.189494 -1.306616 -3.928350 C 4.340344 -1.385210 -1.181100 H 4.914256 -1.308432 -0.254907 H 4.465168 -0.442913 -1.727407 H 4.819118 -2.165219 -1.791504 C 3.098914 -2.639045 1.517599 H 4.007212 -2.038062 1.616114 H 3.406097 -3.693999 1.561715 H 2.482781 -2.452565 2.405108 C 0.217524 -3.673996 0.826405 H -0.855325 -3.511786 0.694321 H 0.439390 -3.508751 1.884686 H 0.422498 -4.734256 0.615161 C 2.608096 2.260945 -0.112545 C 3.024910 1.487110 1.008052 C 1.991767 1.531964 1.984933 C 0.933575 2.334273 1.468690 C 1.319063 2.791777 0.176180 C 3.485682 2.616036 -1.280011 H 4.327511 3.245938 -0.959402 H 2.943006 3.179785 -2.044723	

	H 3.924012 1.736675 -1.768694 C 4.427653 1.023998 1.271551 H 4.968274 1.774315 1.868661 H 4.996498 0.882335 0.349087 H 4.465926 0.088266 1.838530 C 2.141238 1.031673 3.392383 H 2.854647 1.657164 3.949556 H 2.519240 0.003859 3.437894 H 1.194961 1.056730 3.937237 C -0.286479 2.789369 2.215347 H -0.521500 2.122427 3.049510 H -1.173575 2.825731 1.574280 H -0.144430 3.798623 2.629936 C 0.588236 3.847860 -0.601328 H 0.713549 4.831494 -0.126085 H -0.487881 3.656422 -0.663015 H 0.961092 3.940161 -1.625460 C -0.422374 -0.625014 1.799516 C -1.356651 -0.569506 0.844309 C -1.464402 1.005974 -1.595494 C -0.327936 1.067141 -2.092769 H -0.706156 -0.247171 3.893678 H 0.347946 -1.612823 3.575560 C -2.765699 -0.934258 1.000727 C -3.342312 -2.005543 0.294182 H -2.744305 -2.525734 -0.447592 C -4.651772 -2.415034 0.536149 H -5.059726 -3.260857 -0.013671 C -5.441886 -1.741167 1.467185 H -6.466592 -2.054733 1.651047 C -4.899568 -0.655816 2.157330 H -5.503501 -0.117369 2.884937 C -3.581875 -0.264947 1.934907 H -3.164136 0.569970 2.492065 C -2.874156 1.167360 -1.413082 C -3.773535 0.291199 -2.046175 H -3.387475 -0.564920 -2.590258 C -5.143122 0.524531 -1.982861 H -5.826994 -0.161141 -2.475815 C -5.638496 1.628413 -1.289058 H -6.709444 1.806991 -1.241960 C -4.754244 2.500778 -0.652491 H -5.133592 3.362460 -0.109504 C -3.384244 2.272624 -0.708367 H -2.697786 2.954396 -0.216407 H 0.382180 0.900648 -4.082110 H 0.331124 2.555152 -3.451632 C -0.553067 -1.099453 3.217588 H -1.414041 -1.769939 3.352694 C 0.557604 1.514506 -3.192267 H 1.620985 1.449956 -2.948406 U 0.825607 -0.005647 -0.010941	
P6a	C 0.989122 -2.384710 -1.441667 C 2.152117 -1.739571 -1.947507 C 3.161455 -1.792004 -0.941494 C 2.612706 -2.457410 0.193144 C 1.273244 -2.828974 -0.116628 C -0.258598 -2.714696 -2.207386 H -0.234765 -3.755926 -2.561066 H -0.379093 -2.073901 -3.085579 H -1.157725 -2.600510 -1.592976 C 2.350851 -1.211867 -3.339870 H 2.864866 -1.948931 -3.973715	

H	2.965240	-0.302969	-3.357440
H	1.400576	-0.973837	-3.826759
C	4.600222	-1.416985	-1.150381
H	5.142322	-1.316475	-0.206243
H	4.713898	-0.475500	-1.700419
H	5.119963	-2.187655	-1.738077
C	3.353710	-2.819379	1.449555
H	4.175534	-2.125432	1.656288
H	3.795385	-3.823491	1.377645
H	2.699576	-2.825605	2.329102
C	0.384345	-3.718813	0.703012
H	-0.667085	-3.421714	0.640268
H	0.662636	-3.715889	1.761193
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C	3.484692	2.648529	-1.281558
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H	2.843318	2.684955	-2.169938
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H	5.192380	1.898866	1.875201
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H	2.836586	1.708307	4.130495
H	2.962328	0.078843	3.475013
H	1.381139	0.734963	3.908643
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H	-0.326738	1.990189	3.200886
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H	-0.088373	3.671598	2.712965
C	0.554569	3.671737	-0.546045
H	0.681152	4.703489	-0.186215
H	-0.511827	3.433138	-0.487768
H	0.833565	3.666525	-1.603991
C	-0.649323	-0.526567	1.388115
C	-1.768287	-0.263431	0.637378
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H	-0.840084	-0.391603	3.536516
H	0.185052	-1.709553	3.001394
C	-3.127498	-0.647899	1.148053
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H	-3.482173	-2.122289	-0.382445
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H	-5.666783	-2.842252	0.516904
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H	-6.592342	-1.769242	2.562721
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H	-5.294539	0.023314	3.700718
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H	-3.008607	-0.542855	-2.951985
C	-4.738114	0.736642	-3.027785
H	-5.124485	0.279188	-3.935813
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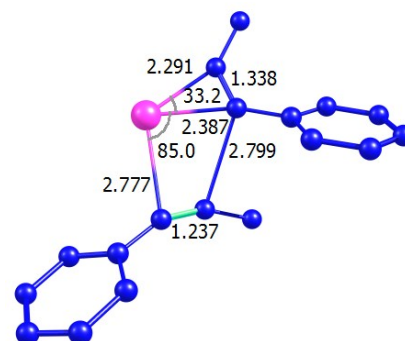
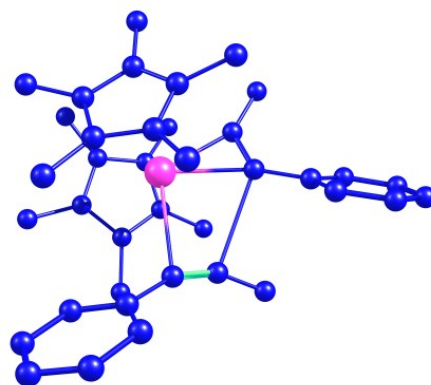


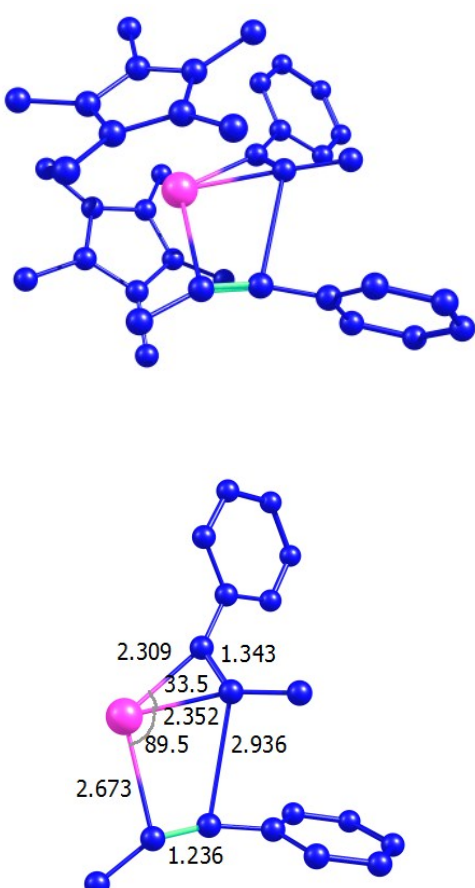
	C -4.925710 2.356829 -1.255531 H -5.457735 3.174486 -0.774696 C -3.739162 1.883307 -0.699558 H -3.356699 2.333040 0.213545 H -0.633260 0.452931 -3.580217 H -1.337699 1.938767 -2.949611 C -0.731661 -1.158267 2.755727 H -1.578669 -1.847241 2.876658 C -0.530938 1.210459 -2.789505 H 0.421766 1.720151 -2.984209 U 1.221468 -0.045079 0.025388	
TS6b	C -0.760176 -1.271296 2.524919 C -1.666939 -1.753728 1.543007 C -0.933816 -2.559405 0.622251 C 0.422507 -2.590409 1.054222 C 0.535365 -1.778383 2.215465 C -1.165963 -0.634114 3.821435 H -0.305998 -0.237843 4.367119 H -1.646877 -1.377466 4.475140 H -1.886350 0.181829 3.694290 C -3.160620 -1.646950 1.648992 H -3.540422 -2.354205 2.401909 H -3.664653 -1.877099 0.707124 H -3.491686 -0.649953 1.961154 C -1.514455 -3.392255 -0.484687 H -0.860148 -3.421842 -1.362294 H -2.485197 -3.008095 -0.811450 H -1.671375 -4.431924 -0.161831 C 1.490594 -3.493088 0.511357 H 2.469355 -3.005927 0.458961 H 1.245648 -3.840932 -0.495642 H 1.599375 -4.386016 1.144562 C 1.750629 -1.664963 3.091821 H 2.633773 -2.083186 2.600272 H 1.614654 -2.220141 4.031316 H 1.986614 -0.630598 3.368652 C 0.342856 2.257413 1.837445 C -0.918098 2.523517 1.224535 C -0.686779 2.791639 -0.155922 C 0.711621 2.665006 -0.396966 C 1.347909 2.347414 0.836427 C 0.621947 2.234606 3.312752 H 1.394703 1.508335 3.587966 H -0.269801 2.005957 3.900633 H 0.987273 3.217866 3.645395 C -2.220716 2.668509 1.963002 H -2.725962 1.714988 2.169820 H -2.929009 3.290280 1.404363 H -2.067335 3.157755 2.932107 C -1.663680 3.354833 -1.152223 H -2.623133 3.600017 -0.685721 H -1.873086 2.681403 -1.991513 H -1.272953 4.288319 -1.578060 C 1.413027 3.048637 -1.667984 H 2.300525 2.433530 -1.847574 H 1.747027 4.096518 -1.631827 H 0.756398 2.956090 -2.539113 C 2.822042 2.388824 1.107667 H 3.110344 3.372973 1.507605 H 3.410685 2.212603 0.204834 H 3.132815 1.641169 1.845174 C -1.999896 0.007747 -1.882410 C -0.994879 0.080896 -2.596275	

	C 2.120412 -0.348759 -0.775399 C 1.261191 -1.020443 -1.557576 C -4.037467 0.758140 -0.650347 H -3.472864 1.557510 -0.186601 C -5.398239 0.621895 -0.390318 H -5.886433 1.322778 0.281890 C -6.131873 -0.404919 -0.983272 H -7.193203 -0.510385 -0.775588 C -5.493145 -1.295866 -1.848166 H -6.056410 -2.096601 -2.320407 C -4.135503 -1.162782 -2.119159 H -3.642917 -1.847222 -2.803422 C -3.385434 -0.129248 -1.520902 C -0.214640 0.365333 -3.807017 H -0.024361 -0.554281 -4.368336 H 0.747345 0.830964 -3.585536 H -0.793872 1.041966 -4.448339 C 3.582515 -0.308182 -0.851646 C 4.396316 -0.638727 0.248473 H 3.922930 -0.914398 1.186618 C 5.785811 -0.616898 0.155713 H 6.385680 -0.891249 1.020981 C 6.409949 -0.230088 -1.031105 H 7.494508 -0.200551 -1.099207 C 5.622521 0.123567 -2.127577 H 6.093174 0.430922 -3.059209 C 4.232991 0.075231 -2.042444 H 3.632081 0.344206 -2.908182 C 1.558868 -1.987552 -2.668870 H 1.972207 -1.483058 -3.552368 H 2.321455 -2.712771 -2.353963 H 0.676226 -2.549596 -2.999410 U 0.011950 0.029692 0.114112	
P6b	C -0.654901 -1.280624 2.802736 C -1.597805 -1.737568 1.838107 C -0.901940 -2.522582 0.878290 C 0.474885 -2.560039 1.250365 C 0.626824 -1.788718 2.438957 C -1.003202 -0.634185 4.112377 H -0.131723 -0.177717 4.589282 H -1.401213 -1.381304 4.815010 H -1.771810 0.141307 4.014317 C -3.085075 -1.559673 1.939890 H -3.511383 -2.270902 2.662488 H -3.586167 -1.721459 0.982235 H -3.361727 -0.556746 2.286337 C -1.504521 -3.372796 -0.199737 H -0.888322 -3.382307 -1.105075 H -2.501697 -3.027017 -0.482124 H -1.599313 -4.414864 0.140665 C 1.482563 -3.470212 0.604307 H 2.460297 -3.416558 1.090991 H 1.633920 -3.247784 -0.457574 H 1.147263 -4.514377 0.673865 C 1.870110 -1.649468 3.274094 H 2.723241 -2.163525 2.821880 H 1.723022 -2.089835 4.269358 H 2.169389 -0.605461 3.435362 C 0.388731 2.372395 2.006005 C -0.835644 2.624921 1.320182 C -0.539841 2.795232 -0.063191 C 0.869395 2.645073 -0.229965 C 1.441326 2.389742 1.046502	<p>A 3D ball-and-stick model of a complex organic molecule. The structure features a central pink atom (likely a metal or a specific non-carbon atom) coordinated to several nitrogen atoms (blue) and carbon atoms (grey). The molecule has a highly branched, cage-like structure with multiple rings and a complex spatial arrangement. Hydrogen atoms are shown as small white spheres.</p>

	C 0.579151 2.384567 3.495487 H 1.339346 1.670887 3.833943 H -0.347706 2.159442 4.029571 H 0.912798 3.377574 3.831482 C -2.166340 2.828342 1.992275 H -2.537425 1.932884 2.508944 H -2.937786 3.130662 1.277861 H -2.103325 3.621641 2.748673 C -1.450998 3.298828 -1.148292 H -2.480783 3.422302 -0.802232 H -1.478616 2.635141 -2.019504 H -1.110753 4.283230 -1.498961 C 1.601509 2.952423 -1.501809 H 2.625997 2.572990 -1.484552 H 1.653969 4.039779 -1.662212 H 1.102398 2.519166 -2.375110 C 2.905711 2.330940 1.373257 H 3.266098 3.312612 1.714082 H 3.508911 2.039938 0.509584 H 3.126103 1.619571 2.178323 C -1.382180 -0.291085 -1.455734 C -0.564875 -0.484997 -2.544205 C 1.598225 -0.363743 -1.259458 C 0.915837 -0.670175 -2.413151 C -3.609457 0.623053 -0.780482 H -3.079505 1.358217 -0.182198 C -5.001358 0.608894 -0.780577 H -5.547854 1.341479 -0.190564 C -5.694062 -0.348324 -1.522715 H -6.780860 -0.369524 -1.518880 C -4.970326 -1.287250 -2.258973 H -5.493863 -2.050866 -2.830292 C -3.577400 -1.258623 -2.268714 H -3.035279 -2.011628 -2.833919 C -2.851450 -0.291864 -1.538057 C -1.090395 -0.476556 -3.970601 H -1.087917 -1.472581 -4.433396 H -0.468574 0.162895 -4.609076 H -2.113642 -0.097602 -4.010393 C 3.067842 -0.355124 -1.175866 C 3.729078 -0.863196 -0.040148 H 3.133087 -1.317301 0.745546 C 5.113430 -0.805395 0.096221 H 5.584535 -1.221351 0.984214 C 5.893933 -0.208306 -0.894124 H 6.974298 -0.153367 -0.787581 C 5.264921 0.327838 -2.018572 H 5.855806 0.809246 -2.794924 C 3.880847 0.253412 -2.157982 H 3.411344 0.691493 -3.034321 C 1.600399 -1.265546 -3.632906 H 1.674394 -0.558436 -4.469834 H 2.612362 -1.598246 -3.393063 H 1.039467 -2.130745 -4.007047 U -0.004273 0.086959 0.465703	
TS6c	C 1.761479 -1.038783 2.275110 C 1.747560 0.378768 2.171052 C 0.430711 0.830644 2.482599 C -0.363341 -0.309950 2.788432 C 0.451860 -1.466937 2.641149 C 3.007541 -1.875369 2.305479 H 2.781791 -2.944295 2.284650 H 3.570379 -1.683797 3.231410	

H	3.690158	-1.661565	1.475080
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H	3.514428	1.276079	2.999361
H	2.734245	2.263600	1.760556
H	3.681392	0.849815	1.298120
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H	-1.053026	2.398201	2.626456
H	0.511391	2.941968	2.002104
H	0.314559	2.591488	3.717987
C	-1.750354	-0.273467	3.360358
H	-2.276593	-1.221768	3.219159
H	-2.367103	0.506123	2.903925
H	-1.717508	-0.077666	4.442407
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C	1.189603	-1.001171	-2.571494
C	-0.050594	-1.693714	-2.468559
C	0.115841	-2.764797	-1.545624
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H	4.172150	-2.243516	-1.484935
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H	0.924687	0.962623	-3.495309
H	1.260429	-0.357038	-4.618450
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H	-2.187587	-1.545870	-2.788598
H	-1.291060	-2.227230	-4.152022
H	-1.219925	-0.495709	-3.830449
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H	-0.469377	-4.802224	-1.891758
H	-1.826341	-3.685830	-1.717893
H	-0.923400	-4.204672	-0.293317
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C	-0.743163	1.882607	-1.463503
C	-2.216841	0.009424	0.003478
C	-2.012827	-1.288905	0.255259
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C	4.034531	3.094169	-1.052993
H	4.999748	2.709092	-1.371824
C	3.943457	4.357273	-0.469939
H	4.835385	4.961517	-0.328349
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H	2.610469	5.828616	0.375046
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H	0.579018	4.459352	0.037130
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C	-1.939540	2.100597	-2.280917
H	-2.705872	2.637397	-1.715589
H	-2.383642	1.167499	-2.631220
H	-1.657256	2.707687	-3.151218
C	-3.477884	0.753095	0.034003
C	-3.588019	1.988994	0.701145



	H	-2.704094	2.403430	1.178738	
	C	-4.792555	2.686427	0.747715	
	H	-4.846475	3.632867	1.281591	
	C	-5.923835	2.184106	0.101463	
	H	-6.861813	2.733060	0.127277	
	C	-5.833636	0.971190	-0.582097	
	H	-6.705441	0.569817	-1.094627	
	C	-4.633567	0.263389	-0.608208	
	H	-4.578206	-0.680807	-1.144329	
	C	-3.002884	-2.342606	0.657412	
	H	-3.885228	-1.911036	1.152304	
	H	-3.373266	-2.886430	-0.221860	
	H	-2.569779	-3.100856	1.320901	
	U	0.119141	-0.481336	0.025336	
TS6	C	2.672223	-1.034865	-1.730426	
	C	1.678011	-2.015350	-1.993590	
	C	0.570750	-1.366093	-2.614274	
	C	0.895566	0.013352	-2.756304	
	C	2.182459	0.222995	-2.187831	
	C	4.095785	-1.336251	-1.364894	
	H	4.636559	-0.440385	-1.050150	
	H	4.631789	-1.745877	-2.234628	
	H	4.186989	-2.079738	-0.565258	
	C	1.905932	-3.497167	-1.906888	
	H	2.547989	-3.833366	-2.734652	
	H	0.973184	-4.063392	-1.983131	
	H	2.408775	-3.801996	-0.981303	
	C	-0.638758	-2.045807	-3.188680	
	H	-1.518645	-1.395526	-3.163048	
	H	-0.894476	-2.957880	-2.638843	
	H	-0.477314	-2.333831	-4.237923	
	C	0.117173	1.022738	-3.548302	
	H	0.127356	2.016490	-3.090178	
	H	-0.930155	0.729605	-3.656750	
	H	0.533733	1.121145	-4.561734	
	C	2.984847	1.491315	-2.266387	
	H	2.360129	2.340253	-2.558469	
	H	3.783447	1.408702	-3.018034	
	H	3.471321	1.750628	-1.318261	
	C	2.604680	0.114581	1.877346	
	C	2.096012	-1.159830	2.263802	
	C	0.775325	-0.972416	2.762247	
	C	0.463206	0.414584	2.663315	
	C	1.599472	1.086768	2.130688	
	C	4.039277	0.434406	1.573348	
	H	4.150196	1.179300	0.777230	
	H	4.605290	-0.453031	1.279523	
	H	4.534136	0.852895	2.462744	
	C	2.905737	-2.425459	2.320242	
	H	3.310041	-2.724391	1.344640	
	H	2.319158	-3.267056	2.701592	
	H	3.767387	-2.310727	2.992176	
	C	-0.062621	-1.968139	3.513795	
	H	0.328428	-2.985909	3.427732	
	H	-1.105601	-1.987181	3.177537	
	H	-0.076656	-1.723619	4.585404	
	C	-0.767205	1.062312	3.227694	
	H	-0.997892	2.006036	2.725615	
	H	-0.645922	1.277744	4.300028	
	H	-1.645501	0.414649	3.132490	
	C	1.818141	2.568877	2.074342	
	H	2.432522	2.897887	2.926159	
	H	0.878393	3.123771	2.109094	
					

	H	2.341596	2.880726	1.163773	
	C	-2.016034	-1.903322	0.277685	
	C	-0.964208	-2.538035	0.414144	
	C	-0.563207	1.683978	-0.215992	
	C	-1.411842	0.784291	-0.738807	
	C	-4.154721	-1.974085	-0.920370	
	H	-3.664017	-2.523777	-1.717858	
	C	-5.516700	-1.698931	-0.988430	
	H	-6.090625	-2.037002	-1.847213	
	C	-6.143333	-0.991554	0.038271	
	H	-7.206763	-0.775251	-0.018955	
	C	-5.400502	-0.564779	1.140982	
	H	-5.884928	-0.018213	1.945780	
	C	-4.038589	-0.835609	1.216530	
	H	-3.459694	-0.500272	2.070999	
	C	-3.397419	-1.540623	0.183064	
	C	-0.189756	-3.758709	0.710314	
	H	0.876106	-3.571164	0.861663	
	H	-0.290984	-4.467874	-0.117750	
	H	-0.582795	-4.236703	1.614482	
	C	-0.713985	3.138603	-0.146711	
	C	0.251057	4.018611	-0.672754	
	H	1.143126	3.604527	-1.134730	
	C	0.086352	5.399926	-0.606930	
	H	0.846554	6.051907	-1.032272	
	C	-1.035899	5.950289	0.014326	
	H	-1.157182	7.028775	0.078097	
	C	-1.998230	5.096964	0.555293	
	H	-2.879323	5.509459	1.042707	
	C	-1.845743	3.714851	0.466279	
	H	-2.607730	3.059668	0.881736	
	C	-2.697153	1.056448	-1.461497	
	H	-3.551152	1.026388	-0.773511	
	H	-2.694691	2.054777	-1.922720	
	H	-2.912301	0.316108	-2.241247	
	U	0.512155	-0.348337	-0.000491	
6	C	2.858180	-1.027699	-1.703509	
	C	1.783362	-1.940263	-1.907576	
	C	0.733343	-1.244862	-2.567889	
	C	1.152286	0.103130	-2.768706	
	C	2.463090	0.238095	-2.227792	
	C	4.245678	-1.411226	-1.277391	
	H	4.823663	-0.551759	-0.927086	
	H	4.800294	-1.846125	-2.122044	
	H	4.248109	-2.162717	-0.480412	
	C	1.838306	-3.412240	-1.616099	
	H	2.405246	-3.946059	-2.392453	
	H	0.841143	-3.859257	-1.577787	
	H	2.333779	-3.629471	-0.662093	
	C	-0.509826	-1.835392	-3.163464	
	H	-1.369601	-1.166455	-3.053455	
	H	-0.772460	-2.792324	-2.704573	
	H	-0.373360	-2.015739	-4.240142	
	C	0.412105	1.094356	-3.622959	
	H	0.918158	2.063222	-3.659444	
	H	-0.612752	1.269930	-3.278389	
	H	0.349456	0.730439	-4.658416	
	C	3.354760	1.443249	-2.338216	
	H	2.786871	2.372496	-2.449558	
	H	4.016590	1.367920	-3.212715	
	H	4.003576	1.561883	-1.462504	
	C	2.770067	0.177579	1.973313	
	C	2.153074	-1.067827	2.286941	

C	0.816242	-0.806436	2.703873
C	0.602719	0.600974	2.643518
C	1.804895	1.207466	2.182449
C	4.226219	0.421811	1.700093
H	4.393062	1.138917	0.886999
H	4.757243	-0.497600	1.441408
H	4.718909	0.838982	2.589946
C	2.814318	-2.416615	2.324748
H	3.754694	-2.430537	1.765453
H	2.174519	-3.207410	1.913957
H	3.051754	-2.710838	3.356882
C	-0.118486	-1.795936	3.335351
H	0.070534	-2.818586	2.995772
H	-1.165938	-1.565271	3.119023
H	-0.001671	-1.793422	4.429306
C	-0.613138	1.310702	3.161652
H	-0.684336	2.328984	2.770958
H	-0.584337	1.378344	4.259208
H	-1.538246	0.789404	2.892714
C	2.076155	2.681729	2.082655
H	2.494107	3.070407	3.022784
H	1.168957	3.253333	1.866039
H	2.803885	2.913622	1.295948
C	-2.157760	-0.723133	-0.080752
C	-1.069906	-1.536840	0.114667
C	-0.908782	1.466238	-0.222638
C	-2.081874	0.755537	-0.326997
C	-4.086788	-2.000037	-1.117775
H	-3.514399	-2.070470	-2.039667
C	-5.351463	-2.583193	-1.041751
H	-5.757809	-3.103197	-1.906266
C	-6.092967	-2.501124	0.136533
H	-7.078312	-2.956395	0.197075
C	-5.558764	-1.831295	1.237245
H	-6.126539	-1.763258	2.162355
C	-4.295762	-1.245678	1.156141
H	-3.886170	-0.723915	2.018579
C	-3.539469	-1.317579	-0.022614
C	-1.254395	-3.015409	0.357730
H	-0.327533	-3.497234	0.689986
H	-1.569706	-3.535337	-0.558263
H	-2.027345	-3.228987	1.108887
C	-0.859371	2.936256	-0.260236
C	0.100236	3.619261	-1.033493
H	0.765384	3.040018	-1.667397
C	0.205447	5.007803	-1.018211
H	0.951265	5.497076	-1.641078
C	-0.635306	5.769706	-0.206218
H	-0.550065	6.853168	-0.186416
C	-1.583348	5.118943	0.584292
H	-2.243298	5.696191	1.228424
C	-1.695339	3.730733	0.555243
H	-2.435073	3.241006	1.183051
C	-3.394024	1.404132	-0.730901
H	-4.119463	1.423408	0.092483
H	-3.240266	2.429838	-1.072464
H	-3.871250	0.836016	-1.538533
U	0.836988	-0.145053	0.000747

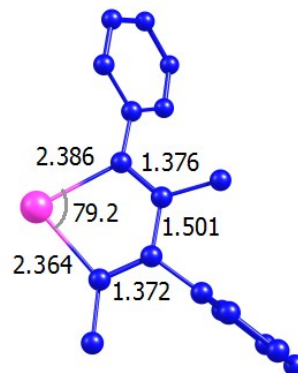
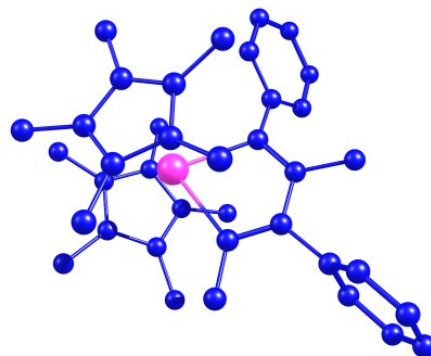


Table S4. Frequencies of the stationary points optimized for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(Me)}]+\text{PhC}\equiv\text{CMe}$, obtained with B3PW91-PCM method.

Species	Frequencies (cm ⁻¹)									
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{Th}[\eta^2\text{-C(Ph)=C(Me)}]$	16	21	29	38	42	58	64	85	87	94
	97	102	105	113	118	121	124	128	134	138
	140	147	151	156	158	162	174	179	186	188
	191	218	269	279	283	285	288	291	293	295
	295	297	309	344	364	371	389	391	417	450
	521	547	548	549	550	555	558	563	601	602
	625	629	630	632	635	675	712	770	817	819
	823	823	838	854	919	967	973	973	974	975
	979	990	1011	1025	1044	1046	1050	1052	1055	1058
	1059	1060	1061	1063	1063	1090	1092	1093	1094	1104
	1117	1128	1130	1185	1189	1190	1191	1193	1203	1243
	1329	1369	1406	1422	1422	1424	1425	1431	1434	1436
	1436	1437	1441	1450	1450	1455	1457	1475	1475	1484
	1487	1489	1493	1493	1494	1496	1498	1501	1502	1504
	1505	1508	1509	1509	1511	1513	1518	1522	1526	1529
	1530	1533	1535	1539	1542	1557	1558	1586	1630	1660
	3011	3032	3034	3034	3035	3035	3035	3036	3037	3038
	3039	3073	3083	3084	3087	3090	3091	3094	3100	3101
	3104	3111	3118	3126	3131	3139	3141	3142	3143	3144
	3145	3149	3153	3182	3188	3199	3210	3218		
PhC≡CMe	25	91	95	248	295	395	404	410	521	547
	633	705	716	772	856	929	973	998	1000	1015
	1057	1060	1063	1111	1191	1209	1310	1337	1373	1433
	1489	1494	1494	1544	1637	1670	2353	3047	3116	3122
	3197	3205	3216	3223	3228					
TS6a	-69	16	25	32	40	45	59	71	76	81
	87	90	94	103	103	109	113	116	119	122
	125	126	131	134	135	145	156	159	163	171
	175	177	184	187	188	192	199	205	218	226
	234	245	262	266	266	272	277	283	288	290
	290	296	300	313	353	364	372	380	387	397
	407	414	429	471	523	527	536	547	548	548
	550	553	554	567	606	608	624	629	630	631
	632	634	653	697	711	729	767	775	816	817
	819	826	828	846	853	913	927	960	968	969
	970	976	978	979	984	985	998	1011	1015	1023
	1026	1044	1045	1047	1049	1053	1055	1056	1060	1061
	1061	1063	1063	1064	1090	1091	1091	1092	1102	1109
	1114	1127	1128	1184	1190	1191	1191	1192	1193	1203
	1209	1238	1276	1327	1338	1370	1374	1407	1413	1418
	1421	1423	1424	1427	1430	1432	1434	1435	1440	1454
	1456	1457	1458	1476	1477	1479	1483	1488	1488	1489
	1492	1493	1498	1498	1499	1503	1504	1506	1507	1509
	1512	1513	1514	1516	1518	1521	1525	1529	1530	1532
	1533	1536	1538	1546	1547	1555	1557	1624	1631	1637
	1661	1665	2133	3021	3029	3029	3032	3033	3033	3034
	3036	3037	3038	3041	3061	3086	3090	3092	3094	3096
	3096	3097	3100	3106	3107	3111	3119	3134	3137	3139
3147	3148	3148	3149	3151	3155	3158	3161	3163	3182	
3189	3200	3204	3209	3213	3221	3226	3230	3234		
P6a	16	18	27	30	41	50	51	60	70	77
	81	85	97	100	102	109	112	118	122	123
	128	132	136	143	149	153	161	165	167	172
	174	175	176	186	201	209	214	220	227	245
	270	271	274	276	278	281	288	291	292	294
	299	306	322	332	365	374	381	391	401	412
	415	479	502	546	548	548	549	550	554	555

	574	603	603	610	625	627	630	633	635	635
	673	703	715	717	736	781	788	817	818	823
	824	845	858	862	927	927	968	970	971	971
	973	975	976	993	994	998	1013	1015	1016	1043
	1047	1048	1050	1051	1056	1057	1059	1060	1061	1062
	1063	1064	1083	1091	1092	1093	1093	1109	1110	1128
	1129	1138	1142	1187	1187	1189	1191	1193	1194	1208
	1209	1250	1283	1336	1339	1370	1371	1413	1415	1421
	1421	1422	1424	1431	1432	1434	1435	1436	1441	1451
	1452	1456	1458	1473	1473	1480	1485	1489	1489	1491
	1491	1492	1494	1497	1499	1501	1501	1504	1505	1506
	1507	1510	1511	1513	1514	1519	1519	1522	1529	1530
	1534	1537	1537	1542	1544	1546	1553	1555	1567	1643
	1643	1667	1667	3020	3022	3035	3035	3035	3036	3036
	3036	3037	3037	3040	3040	3077	3079	3091	3092	3094
	3094	3096	3097	3100	3100	3109	3111	3112	3112	3130
	3130	3142	3143	3147	3148	3149	3150	3150	3151	3187
	3187	3193	3194	3203	3204	3209	3209	3219	3219	
TS6b	-90	21	26	31	41	42	49	58	64	74
	80	89	97	100	104	108	110	114	123	130
	133	137	141	143	150	156	162	164	167	172
	178	180	186	188	190	192	201	210	216	223
	232	264	266	272	275	277	283	284	286	289
	292	300	308	320	353	365	372	379	382	386
	414	416	434	461	500	519	532	548	549	549
	549	552	557	574	607	609	621	624	629	630
	631	632	665	706	711	726	767	770	817	819
	825	826	832	853	859	916	931	966	967	970
	977	978	979	984	988	994	1002	1009	1012	1014
	1037	1046	1047	1052	1053	1055	1056	1059	1061	1062
	1062	1063	1065	1068	1087	1088	1090	1092	1094	1107
	1111	1123	1128	1185	1187	1189	1190	1192	1193	1204
	1210	1240	1275	1328	1339	1370	1375	1406	1419	1420
	1421	1423	1424	1424	1430	1432	1435	1436	1441	1452
	1454	1456	1457	1473	1478	1484	1484	1487	1489	1490
	1491	1492	1497	1497	1501	1503	1505	1507	1510	1510
	1512	1514	1517	1518	1521	1522	1527	1528	1529	1531
	1532	1534	1538	1544	1549	1552	1554	1620	1630	1635
	1660	1664	2189	3028	3029	3029	3030	3031	3032	3034
	3035	3036	3037	3049	3061	3093	3094	3096	3096	3098
	3099	3100	3104	3105	3107	3108	3113	3125	3135	3138
	3143	3145	3147	3153	3155	3158	3162	3164	3173	3183
	3190	3201	3202	3209	3213	3220	3221	3229	3262	
P6b	16	35	42	44	53	56	64	69	74	81
	83	86	89	97	102	106	111	115	121	130
	132	140	146	152	157	160	162	166	168	176
	184	190	192	194	198	202	206	226	265	268
	269	273	274	278	285	287	295	298	300	301
	304	330	365	373	385	395	402	409	426	427
	430	469	537	543	548	549	550	550	556	559
	564	603	604	607	620	623	630	631	632	633
	637	689	715	719	759	771	816	817	820	826
	828	858	864	867	879	924	930	969	970	972
	977	980	980	991	994	1003	1005	1013	1013	1032
	1047	1048	1052	1052	1054	1056	1058	1062	1063	1064
	1065	1065	1067	1089	1090	1092	1093	1107	1113	1118
	1126	1127	1185	1186	1189	1190	1191	1194	1208	1218
	1224	1258	1272	1334	1341	1370	1372	1412	1421	1421
	1422	1424	1425	1430	1433	1434	1436	1439	1441	1451
	1452	1458	1460	1473	1474	1482	1482	1487	1489	1490
	1491	1491	1492	1495	1499	1500	1502	1503	1505	1506
	1508	1509	1513	1515	1517	1523	1523	1527	1529	1529
	1531	1532	1534	1543	1544	1545	1556	1557	1588	1629

	1629	1660	1661	3032	3032	3033	3034	3035	3036	3038
	3041	3042	3044	3046	3049	3089	3090	3093	3094	3095
	3098	3098	3106	3107	3109	3110	3114	3139	3142	3148
	3149	3151	3153	3155	3156	3160	3161	3163	3164	3187
	3187	3194	3194	3212	3212	3219	3219	3229	3231	
TS6c	-122	14	23	29	37	43	45	55	59	74
	76	82	84	87	93	99	101	107	110	113
	117	126	133	138	141	147	149	155	159	166
	171	176	181	183	191	194	198	201	212	231
	239	247	262	267	274	280	282	283	285	289
	302	309	309	313	361	363	373	378	381	388
	414	417	428	460	492	519	527	546	547	548
	549	555	559	571	606	610	622	623	625	628
	631	636	668	705	712	726	766	774	820	821
	823	825	828	856	856	919	927	967	968	972
	976	979	982	982	984	991	1000	1011	1014	1025
	1033	1047	1048	1050	1052	1055	1057	1058	1058	1060
	1061	1062	1063	1066	1089	1091	1092	1094	1101	1109
	1110	1125	1129	1185	1187	1190	1190	1191	1194	1202
	1209	1239	1270	1327	1337	1368	1374	1408	1415	1421
	1423	1424	1425	1429	1431	1434	1435	1439	1443	1450
	1455	1456	1456	1472	1476	1479	1484	1487	1488	1490
	1490	1490	1492	1497	1497	1501	1503	1506	1508	1509
	1511	1513	1514	1517	1518	1520	1526	1527	1529	1530
	1532	1534	1537	1544	1549	1551	1553	1629	1630	1635
	1659	1664	2172	3023	3028	3030	3031	3032	3032	3033
	3034	3036	3036	3048	3058	3088	3096	3097	3100	3100
	3100	3102	3105	3107	3108	3109	3119	3126	3138	3140
	3144	3146	3150	3153	3154	3156	3156	3169	3179	3185
	3192	3200	3206	3208	3211	3219	3221	3228	3258	
TS6	-87	16	20	31	39	48	51	56	57	72
	78	83	96	97	100	106	116	118	121	128
	131	140	142	148	154	155	159	160	165	176
	179	181	185	187	193	208	213	216	222	234
	242	265	270	272	275	281	282	287	287	288
	297	301	303	322	347	360	376	378	379	385
	409	416	425	461	512	525	535	547	548	549
	549	552	555	568	607	609	622	626	630	631
	632	635	667	701	713	725	770	771	818	819
	824	827	839	855	855	918	932	966	968	969
	975	976	979	981	982	988	1003	1011	1015	1022
	1029	1044	1047	1050	1053	1054	1055	1056	1058	1060
	1061	1062	1062	1063	1091	1091	1092	1093	1096	1108
	1113	1127	1127	1184	1190	1190	1191	1192	1194	1204
	1210	1239	1282	1329	1339	1369	1374	1407	1417	1421
	1421	1422	1424	1426	1431	1433	1436	1437	1442	1453
	1453	1457	1459	1476	1476	1482	1484	1488	1490	1491
	1492	1494	1496	1498	1500	1504	1505	1505	1508	1509
	1510	1513	1513	1519	1522	1522	1524	1528	1529	1531
	1533	1536	1538	1546	1549	1551	1557	1614	1630	1636
	1660	1665	2178	3024	3029	3029	3030	3031	3031	3034
	3035	3036	3039	3041	3066	3088	3090	3093	3093	3097
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	3190	3202	3203	3210	3212	3219	3222	3230	3236	
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	76	82	88	92	96	102	107	118	122	125
	129	131	137	139	147	151	153	155	165	166
	174	181	185	185	187	193	216	226	233	234
	268	272	274	276	280	285	287	287	291	294
	297	307	319	368	373	388	390	399	412	421
	434	493	505	538	546	548	549	550	554	555
	559	603	605	605	624	625	627	631	632	634

678	693	717	717	738	773	790	816	818	824
825	859	861	867	924	925	956	970	972	972
973	978	979	985	992	996	1001	1012	1015	1045
1046	1047	1050	1052	1054	1055	1057	1058	1060	1061
1062	1065	1066	1091	1092	1093	1093	1107	1109	1126
1127	1128	1185	1188	1188	1191	1192	1193	1197	1208
1209	1241	1288	1332	1335	1368	1370	1410	1420	1420
1421	1423	1424	1430	1431	1434	1435	1436	1441	1451
1453	1458	1459	1473	1473	1480	1484	1486	1489	1490
1490	1493	1494	1497	1498	1502	1503	1503	1504	1505
1507	1509	1511	1512	1515	1515	1519	1522	1527	1531
1531	1533	1536	1539	1542	1544	1554	1556	1580	1629
1641	1660	1666	3024	3034	3034	3035	3035	3036	3037
3038	3040	3040	3041	3053	3082	3092	3093	3096	3099
3101	3104	3106	3107	3107	3108	3109	3111	3135	3137
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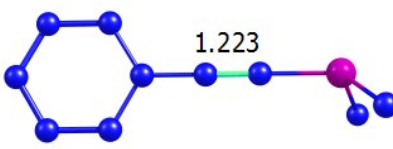
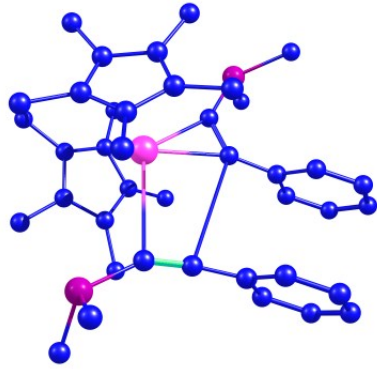
Table S5. The energies, enthalpies and free energies (in au at 298.15 K) and corresponding relative values (in kcal/mol) for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(Me)}]+\text{PhC}\equiv\text{CMe}$, obtained with B3PW91-PCM method.^a

Species	E	H	G
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{Th}[\eta^2\text{-C(Ph)=C(Me)}]$	-1604.064320	-1604.026306	-1604.115010
PhC≡CMe	-347.441314	-347.432004	-347.461470
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{Th}[\eta^2\text{-C(Ph)=C(Me)}]+\text{PhC}\equiv\text{CM}$	-1951.505634(0.0)	-1951.458310(0.0)	-1951.576480(0.0)
TS6a	-1951.482636(14.4)	-1951.436469(13.7)	-1951.540010(22.9)
P6a	-1951.543040(-23.5)	-1951.497021(-24.3)	-1951.600630(-15.2)
TS6b	-1951.482431(14.6)	-1951.436420(13.7)	-1951.539000(23.5)
P6b	-1951.546489(-25.6)	-1951.501197(-26.9)	-1951.602590(-16.4)
TS6c	-1951.484503(13.3)	-1951.438010(12.7)	-1951.541650(21.9)
TS6	-1951.485628(12.6)	-1951.439674(11.7)	-1951.542540(21.3)
6	-1951.547522(-26.3)	-1951.501468(-27.1)	-1951.604630(-17.7)

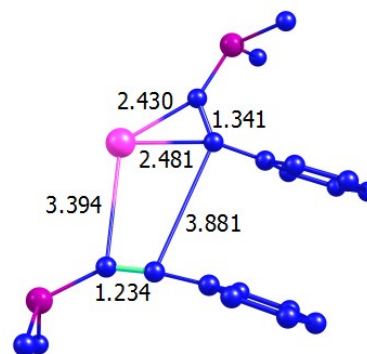
^a The U was treated with ECP60MWB, in which 60 electrons are in the core region and the corresponding optimized segmented ((14s13p10d8f6g)/[10s9p5d4f3g]) basis set is applied for the valence shells of U.

Table S6. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$, obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{SiHMe}_2)]$	C	-0.700084	-2.952584	-1.986830	
	C	-1.427616	-1.748235	-2.210540	
	C	-0.532380	-0.794151	-2.794208	
	C	0.743144	-1.413839	-2.936238	
	C	0.645675	-2.739825	-2.423427	
	C	-1.276488	-4.272782	-1.560148	
	H	-0.552262	-4.886363	-1.012055	
	H	-1.591535	-4.862827	-2.432887	
	H	-2.158845	-4.153872	-0.922883	
	C	-2.909401	-1.561889	-2.036211	
	H	-3.448345	-1.790276	-2.966818	
	H	-3.170888	-0.531531	-1.767761	
	H	-3.319740	-2.219054	-1.262022	
	C	-0.920687	0.547143	-3.348035	
	H	-0.079607	1.247102	-3.339599	
	H	-1.739766	1.008510	-2.784498	
	H	-1.262247	0.461613	-4.390012	
	C	1.928602	-0.813017	-3.630682	
	H	2.868391	-1.274467	-3.313437	
	H	2.016441	0.258284	-3.427506	
	H	1.850420	-0.939076	-4.720197	
	C	1.714025	-3.796183	-2.482550	
	H	2.716757	-3.359192	-2.522120	
	H	1.602367	-4.424784	-3.377633	
	H	1.682218	-4.472411	-1.619402	
	C	0.148453	-2.582159	2.254540	
	C	-1.146763	-2.009213	2.085411	
	C	-1.029224	-0.597312	2.276900	
	C	0.333032	-0.301335	2.579049	
	C	1.067050	-1.525818	2.555709	
	C	0.470193	-4.050831	2.280774	
	H	1.485381	-4.259227	1.922882	
	H	-0.223017	-4.638580	1.669318	
	H	0.409886	-4.449757	3.303324	
	C	-2.434209	-2.765051	1.918767	
	H	-3.169088	-2.211927	1.322919	
	H	-2.903140	-2.964869	2.892965	
	H	-2.282110	-3.735286	1.435027	
	C	-2.172374	0.378890	2.299606	
	H	-2.991317	0.072756	1.638570	
	H	-1.863077	1.385746	1.998354	
	H	-2.598450	0.466709	3.309170	
	C	0.884456	1.026863	3.004233	
H	1.889814	1.193776	2.605435		
H	0.946521	1.093092	4.100126		
H	0.258668	1.857967	2.663948		
C	2.499193	-1.689371	2.979586		
H	2.580007	-1.772512	4.073470		
H	3.115293	-0.840631	2.668033		
H	2.953364	-2.591793	2.556686		
C	2.536032	-0.008805	-0.274928		
C	1.633508	0.985346	-0.358275		
C	4.002866	-0.024834	-0.237802		
C	4.712227	-1.180105	-0.612389		
H	4.148450	-2.054670	-0.930260		
C	6.104064	-1.221712	-0.586320		
H	6.624462	-2.125887	-0.894409		

	C 6.829616 -0.111802 -0.151777 H 7.915862 -0.144248 -0.118806 C 6.146309 1.037655 0.250087 H 6.701154 1.905027 0.601256 C 4.755584 1.081837 0.202485 H 4.233701 1.979187 0.524575 Si 1.670786 2.826813 -0.575539 H 2.346341 3.491586 0.594243 C 2.600225 3.365338 -2.138730 H 3.630792 2.993712 -2.134263 H 2.631694 4.459028 -2.219120 H 2.110913 2.978617 -3.040871 C -0.080464 3.546762 -0.634597 H -0.642232 3.158664 -1.492866 H -0.053253 4.639967 -0.720966 H -0.642697 3.299742 0.274043 U 0.379056 -1.090166 -0.133072	
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TS7	C 1.315590 0.210435 -2.746174 C 2.619869 0.221156 -2.156293 C 2.931586 -1.112837 -1.768621 C 1.816343 -1.945611 -2.097241 C 0.829004 -1.124951 -2.721152 C 0.660827 1.367382 -3.443791 H 0.779822 2.306590 -2.896371 H -0.413870 1.204996 -3.573562 H 1.088459 1.514965 -4.446038 C 3.601038 1.356560 -2.199126 H 4.256248 1.273915 -3.079260 H 4.252924 1.384269 -1.319187 H 3.101817 2.326777 -2.266323 C 4.296879 -1.608262 -1.391468 H 4.257958 -2.542577 -0.824954 H 4.861845 -0.879066 -0.801966 H 4.888684 -1.808451 -2.296984 C 1.809366 -3.445195 -2.036350 H 2.312328 -3.878244 -2.913761 H 0.792057 -3.842475 -2.013895 H 2.325058 -3.827463 -1.148914 C -0.419498 -1.623371 -3.381962 H -1.162160 -0.828662 -3.503771	

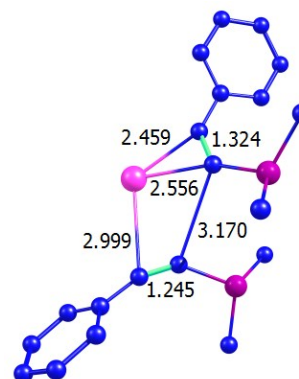
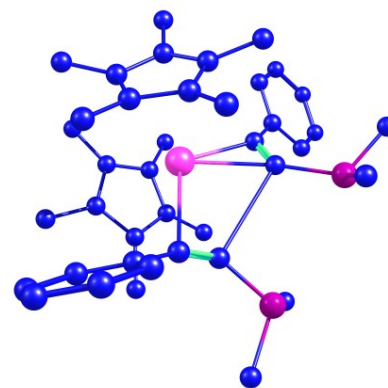
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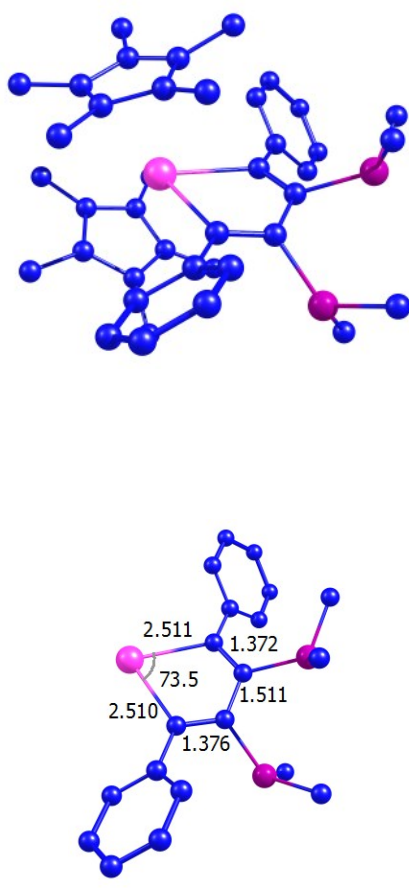


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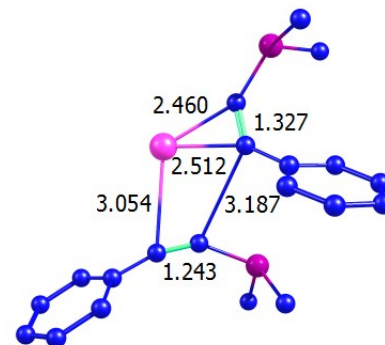
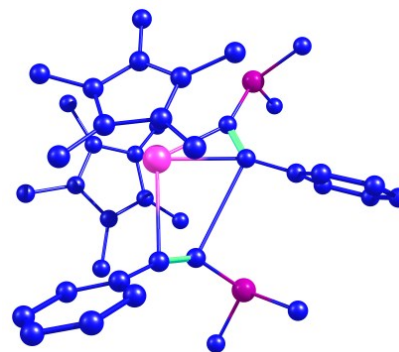
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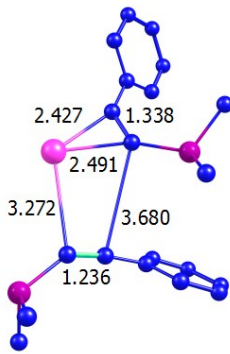
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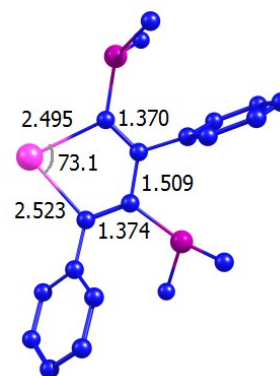
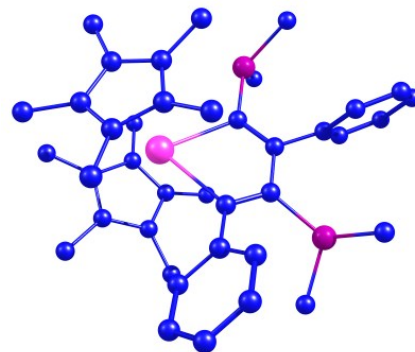
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H	1.057750	5.191572	0.381666
C	3.101315	1.102638	-0.399041



	C 3.097221 1.907789 -1.554088 H 2.260716 1.831764 -2.243513 C 4.149547 2.777073 -1.835714 H 4.128995 3.365930 -2.750283 C 5.219017 2.902519 -0.947676 H 6.034968 3.588271 -1.161284 C 5.222814 2.141129 0.222025 H 6.044942 2.233870 0.928579 C 4.185413 1.250469 0.489036 H 4.201128 0.658303 1.399729 Si 3.434536 -2.448513 -0.098018 H 2.848583 -3.826580 -0.177492 C 4.572225 -2.246488 -1.601589 H 4.053599 -2.420988 -2.549120 H 5.402015 -2.962116 -1.536349 H 4.997949 -1.237065 -1.632387 C 4.566923 -2.410456 1.426948 H 5.221940 -1.532495 1.387189 H 5.206126 -3.302551 1.438494 H 4.021226 -2.378269 2.375163 U -0.344146 -0.649566 0.029562	
TS7c	C 0.240985 -3.206981 1.672222 C 1.261558 -2.314605 2.095819 C 0.634687 -1.214232 2.766294 C -0.769737 -1.438253 2.762220 C -1.020721 -2.657110 2.064397 C 0.466566 -4.621403 1.225909 H -0.420745 -5.049021 0.752831 H 0.707198 -5.256299 2.091749 H 1.301632 -4.716370 0.524122 C 2.728095 -2.633515 2.098763 H 2.980758 -3.285967 2.948150 H 3.343443 -1.735527 2.195783 H 3.047902 -3.156101 1.190519 C 1.360697 -0.119741 3.493543 H 0.703387 0.726109 3.710398 H 2.207409 0.268967 2.917099 H 1.759186 -0.480289 4.452912 C -1.800258 -0.622217 3.481840 H -2.740305 -0.563213 2.925160 H -1.461560 0.404686 3.641789 H -2.020824 -1.053383 4.469114 C -2.322422 -3.407311 2.026593 H -3.139423 -2.801430 2.427229 H -2.264704 -4.315186 2.643823 H -2.609390 -3.726211 1.017670 C -0.430077 -2.836410 -2.088557 C 0.924070 -2.413213 -2.255221 C 0.901132 -1.057371 -2.697076 C -0.459765 -0.639136 -2.792779 C -1.283772 -1.742173 -2.420987 C -0.911133 -4.248044 -1.915507 H -1.764132 -4.322788 -1.231288 H -0.125733 -4.910346 -1.543669 H -1.246445 -4.655331 -2.880507 C 2.138715 -3.296405 -2.200694 H 1.997092 -4.147282 -1.526976 H 3.031513 -2.759958 -1.861426 H 2.372752 -3.712301 -3.191848 C 2.085088 -0.302429 -3.226140 H 3.024679 -0.712134 -2.843347 H 2.063442 0.761388 -2.971140 H 2.128733 -0.376104 -4.322549	

	C	-0.960954	0.642499	-3.394202	
	H	-1.690474	1.149947	-2.752949	
	H	-1.451095	0.458113	-4.360654	
	H	-0.139814	1.340395	-3.585243	
	C	-2.762652	-1.847361	-2.645468	
	H	-2.966980	-2.314698	-3.621139	
	H	-3.247489	-0.868548	-2.639639	
	H	-3.260820	-2.456183	-1.884215	
	C	2.035164	2.008563	-0.235923	
	C	2.604185	0.920125	-0.100050	
	C	-2.288161	0.160129	0.145276	
	C	-1.452989	1.128811	0.539423	
	C	1.881300	4.323331	0.534815	
	H	2.401755	4.033896	1.442474	
	C	1.534205	5.651100	0.314696	
	H	1.779326	6.401611	1.061152	
	C	0.875809	6.018689	-0.859917	
	H	0.604783	7.057506	-1.028090	
	C	0.566922	5.052633	-1.818817	
	H	0.054133	5.336701	-2.733479	
	C	0.910142	3.722938	-1.607773	
	H	0.666905	2.969114	-2.347944	
	C	1.568748	3.341687	-0.425312	
	Si	4.295264	0.144564	-0.098873	
	H	4.179083	-1.320294	-0.327892	
	C	5.134552	0.491195	1.553055	
	H	5.283534	1.569926	1.678297	
	H	6.120536	0.011035	1.574259	
	H	4.565720	0.129093	2.414343	
	C	5.322567	0.916411	-1.477679	
	H	4.874593	0.766815	-2.464433	
	H	6.325035	0.470850	-1.487841	
	H	5.432910	1.994657	-1.315569	
	C	-3.730564	0.151905	-0.114689	
	C	-4.579539	-0.866960	0.351589	
	H	-4.154365	-1.675620	0.936884	
	C	-5.945127	-0.857419	0.077298	
	H	-6.576649	-1.652721	0.467803	
	C	-6.502514	0.154246	-0.705882	
	H	-7.565634	0.153223	-0.933216	
	C	-5.673710	1.161387	-1.202588	
	H	-6.089867	1.953538	-1.821710	
	C	-4.312776	1.163373	-0.905808	
	H	-3.675231	1.953479	-1.295861	
	Si	-1.789272	2.822836	1.232322	
	H	-1.525394	3.863233	0.184477	
	C	-3.554234	3.112230	1.873092	
	H	-4.304034	3.076555	1.077592	
	H	-3.616095	4.093870	2.361253	
	H	-3.827538	2.352694	2.615805	
	C	-0.652398	3.212484	2.701886	
	H	-1.000727	2.702381	3.608398	
	H	-0.652005	4.289194	2.911723	
	H	0.379945	2.901699	2.516425	
	U	-0.110088	-0.903422	0.018861	
P7b	C	-2.127122	-2.336836	-2.131087	
	C	-2.286215	-0.938795	-2.368726	
	C	-1.026781	-0.414147	-2.781760	
	C	-0.085958	-1.488432	-2.799003	
	C	-0.762731	-2.678022	-2.391505	
	C	-3.250181	-3.303852	-1.888895	
	H	-2.892636	-4.262531	-1.502912	
	H	-3.783445	-3.513774	-2.826981	

H	-3.995640	-2.919026	-1.183611
C	-3.592810	-0.196980	-2.347813
H	-4.100753	-0.274300	-3.320042
H	-3.460853	0.867214	-2.131767
H	-4.283454	-0.599994	-1.598147
C	-0.774263	0.959731	-3.326039
H	0.227835	1.321940	-3.073363
H	-1.492736	1.687844	-2.940519
H	-0.856177	0.961915	-4.422812
C	1.283863	-1.416871	-3.402470
H	1.936260	-2.215493	-3.038389
H	1.773402	-0.463039	-3.185454
H	1.227888	-1.515052	-4.496572
C	-0.187336	-4.066006	-2.421933
H	0.877095	-4.074554	-2.164183
H	-0.278726	-4.507306	-3.424662
H	-0.700653	-4.742880	-1.730256
C	-1.689223	-2.968285	1.824493
C	-2.407154	-1.775903	2.150229
C	-1.483003	-0.850822	2.718047
C	-0.192120	-1.467689	2.738685
C	-0.324363	-2.778664	2.198217
C	-2.300890	-4.281193	1.427324
H	-1.644123	-4.872969	0.779572
H	-3.253305	-4.153046	0.905396
H	-2.501956	-4.895448	2.316813
C	-3.901107	-1.627212	2.091718
H	-4.216802	-0.580872	2.032688
H	-4.371545	-2.051507	2.990103
H	-4.336579	-2.148182	1.231784
C	-1.800808	0.421132	3.450534
H	-2.858365	0.688382	3.373064
H	-1.213730	1.271306	3.088624
H	-1.577775	0.303060	4.520202
C	1.001195	-0.882763	3.432730
H	1.907344	-1.460961	3.238788
H	0.845114	-0.870272	4.521331
H	1.196392	0.147633	3.117108
C	0.728968	-3.849239	2.170019
H	0.679375	-4.471691	3.074814
H	1.738632	-3.434020	2.116907
H	0.610853	-4.524144	1.314425
C	-0.640480	1.416424	0.110549
C	0.630820	1.891875	0.320994
C	1.815444	0.972243	0.156133
C	1.737732	-0.390302	0.038252
C	-3.037695	2.040721	0.588419
H	-3.121011	1.175617	1.238879
C	-4.138230	2.874581	0.415849
H	-5.069491	2.649251	0.930891
C	-4.054696	3.991144	-0.418716
H	-4.917424	4.636198	-0.563480
C	-2.854186	4.255155	-1.078003
H	-2.776615	5.109439	-1.746902
C	-1.748628	3.427725	-0.888119
H	-0.826329	3.629331	-1.425369
C	-1.801202	2.306663	-0.031723
Si	0.974666	3.629165	1.073283
H	2.109925	3.405412	2.022817
C	-0.430007	4.292009	2.157896
H	-1.285383	4.653512	1.580419
H	-0.035336	5.132034	2.744623
H	-0.793399	3.538496	2.864718



C	1.507082	5.026901	-0.092678
H	2.373171	4.748983	-0.700100
H	1.784257	5.902863	0.507976
H	0.694988	5.330164	-0.763014
C	3.149815	1.654198	0.018394
C	3.478667	2.312861	-1.175897
H	2.742297	2.359155	-1.975064
C	4.737429	2.884177	-1.359750
H	4.974763	3.376085	-2.300288
C	5.690850	2.820407	-0.343367
H	6.672328	3.266298	-0.483920
C	5.372698	2.183463	0.856566
H	6.104300	2.138853	1.659989
C	4.115334	1.607376	1.033994
H	3.868135	1.123695	1.975157
Si	3.201494	-1.528507	-0.236385
H	2.592423	-2.841530	-0.663926
C	4.466669	-1.072680	-1.577193
H	4.001596	-0.795667	-2.527523
H	5.121831	-1.934479	-1.759998
H	5.092001	-0.233885	-1.253674
C	4.238620	-1.960476	1.297873
H	4.863883	-1.112388	1.597340
H	4.906221	-2.796931	1.054159
H	3.639694	-2.256617	2.164468
U	-0.652150	-1.101985	-0.041876

Table S7. Frequencies of the stationary points optimized for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$, obtained with B3PW91-PCM method.

Species	Frequencies (cm ⁻¹)										
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C}(\text{Ph})=\text{C}(\text{SiHMe}_2)]$	10	18	22	31	41	46	59	63	74	87	
	95	106	107	113	115	116	122	126	127	131	
	141	145	149	152	156	158	159	165	167	171	
	173	177	178	181	192	211	226	279	280	283	
	283	286	288	289	293	294	296	302	324	371	
	382	388	396	415	435	503	549	551	551	552	
	556	557	568	602	603	613	623	628	631	632	
	634	636	659	691	709	715	742	781	788	818	
	819	822	824	859	868	882	903	911	932	973	
	974	975	977	978	995	1012	1048	1051	1051	1052	
	1058	1058	1059	1059	1060	1062	1065	1093	1093	1095	
	1095	1107	1130	1130	1185	1191	1194	1195	1196	1199	
	1222	1303	1310	1329	1371	1422	1423	1424	1426	1433	
	1434	1436	1436	1437	1440	1446	1448	1452	1453	1469	
	1473	1481	1481	1485	1486	1488	1489	1492	1493	1494	
	1499	1500	1502	1502	1508	1508	1509	1511	1512	1513	
	1522	1522	1527	1529	1530	1533	1534	1542	1544	1549	
	1551	1604	1634	1660	2136	3034	3034	3036	3037	3037	
	3038	3038	3039	3040	3041	3049	3051	3094	3097	3098	
	3099	3099	3100	3100	3107	3114	3117	3128	3129	3130	
	3130	3131	3133	3134	3135	3136	3139	3143	3145	3149	
	3150	3185	3191	3201	3211	3218					
	PhC≡CSiHMe ₂	10	50	58	133	147	151	167	202	284	294
		346	409	411	544	565	606	630	633	668	704
		711	758	774	793	845	858	880	910	912	934
		976	1004	1015	1060	1112	1191	1209	1264	1313	1320
1339		1374	1477	1479	1483	1489	1490	1540	1637	1669	
2213		2265	3058	3058	3141	3142	3149	3150	3200	3209	
3219		3227	3231								
TS7	-59	21	30	36	36	43	48	51	53	61	
	62	68	71	78	79	82	87	88	93	103	
	107	111	115	125	127	130	133	138	141	144	
	145	149	151	152	155	157	158	162	165	168	
	169	176	177	181	182	185	189	196	217	223	
	243	267	271	273	278	280	280	282	286	290	
	291	293	314	326	357	370	373	382	386	387	
	401	405	410	428	526	544	547	547	549	550	
	551	552	556	560	591	609	610	612	623	628	
	630	632	632	634	639	644	651	670	684	697	
	704	709	722	764	766	771	780	787	791	819	
	821	822	826	838	850	853	856	878	879	910	
	912	916	923	925	934	962	970	971	973	974	
	981	982	1001	1009	1015	1048	1049	1050	1051	1056	
	1057	1059	1059	1060	1060	1061	1062	1091	1094	1094	
	1097	1105	1115	1128	1132	1184	1193	1193	1195	1196	
	1197	1202	1209	1216	1253	1303	1311	1313	1320	1328	
	1342	1371	1378	1419	1420	1422	1424	1428	1430	1432	
	1434	1434	1439	1450	1451	1453	1453	1474	1474	1475	
	1478	1480	1480	1481	1484	1487	1489	1490	1490	1490	
	1492	1494	1495	1496	1500	1503	1505	1506	1508	1509	
	1510	1514	1518	1521	1524	1525	1528	1529	1531	1533	
	1537	1540	1544	1552	1553	1615	1629	1637	1660	1666	
2164	2173	2251	3029	3032	3033	3034	3034	3035	3036		
3038	3039	3040	3049	3053	3059	3060	3100	3102	3103		
3105	3107	3108	3109	3114	3117	3122	3128	3134	3138		
3139	3140	3143	3146	3147	3149	3149	3151	3153	3156		
3159	3160	3161	3162	3165	3181	3188	3204	3207	3214		

	3216	3220	3223	3229	3238					
7	23	27	33	34	45	54	62	65	68	74
	78	79	84	90	91	94	95	99	103	108
	108	110	117	118	121	127	132	134	140	142
	144	148	150	154	158	159	163	169	172	174
	180	183	185	186	195	200	203	214	249	250
	264	277	279	281	285	285	286	288	289	293
	296	296	297	340	353	372	373	389	401	412
	416	441	481	545	548	549	550	552	555	556
	567	584	606	607	621	621	625	627	630	631
	633	640	642	643	655	680	682	707	715	719
	741	742	774	776	777	778	797	807	815	819
	820	825	826	859	864	867	875	917	917	926
	928	933	940	954	971	972	973	974	977	978
	993	994	1014	1015	1039	1046	1047	1052	1054	1055
	1056	1058	1060	1062	1062	1063	1072	1093	1095	1095
	1096	1108	1109	1130	1131	1187	1187	1191	1192	1196
	1198	1208	1209	1236	1267	1300	1301	1309	1310	1334
	1337	1369	1371	1421	1421	1423	1424	1431	1432	1435
	1435	1437	1440	1448	1448	1452	1454	1471	1471	1478
	1478	1480	1481	1485	1485	1486	1487	1488	1488	1490
	1492	1493	1494	1495	1501	1502	1505	1505	1506	1506
	1509	1510	1512	1517	1521	1523	1526	1527	1530	1533
	1535	1541	1541	1543	1549	1550	1563	1641	1641	1666
	1666	2132	2134	3036	3037	3039	3039	3040	3040	3040
	3041	3042	3043	3054	3055	3056	3059	3099	3103	3103
	3103	3106	3110	3111	3114	3115	3116	3132	3134	3135
3137	3137	3139	3148	3153	3154	3155	3156	3157	3161	
3161	3161	3161	3167	3168	3188	3189	3194	3195	3205	
3206	3210	3211	3220	3220						
TS7a	-29	21	29	30	40	41	46	52	55	60
	63	71	74	79	80	86	89	92	94	101
	107	108	116	118	129	130	137	144	146	147
	150	152	163	167	170	173	176	177	181	186
	189	193	194	197	199	203	210	213	217	225
	229	239	260	265	272	274	276	279	281	283
	287	296	300	306	335	353	367	372	375	385
	411	418	420	430	499	508	538	546	548	549
	550	552	555	563	600	609	610	613	620	621
	626	626	631	632	634	643	652	672	685	703
	710	714	716	751	752	767	777	785	788	818
	821	823	825	827	851	856	862	875	879	886
	903	909	915	927	929	966	966	975	977	978
	980	992	1003	1012	1014	1044	1047	1048	1050	1055
	1056	1057	1058	1058	1060	1060	1061	1090	1092	1093
	1095	1107	1113	1127	1128	1185	1191	1191	1192	1195
	1195	1200	1208	1215	1235	1306	1308	1312	1314	1330
	1338	1371	1374	1417	1420	1422	1423	1425	1429	1431
	1435	1436	1439	1449	1450	1453	1453	1473	1475	1475
	1477	1480	1481	1483	1483	1484	1486	1488	1490	1491
	1491	1492	1494	1497	1504	1505	1506	1508	1509	1510
	1513	1515	1518	1519	1522	1526	1529	1529	1531	1533
	1534	1540	1544	1549	1552	1631	1633	1659	1660	1667
	2085	2168	2249	3027	3030	3032	3034	3036	3037	3037
	3038	3039	3041	3052	3054	3055	3066	3088	3097	3097
	3104	3105	3105	3113	3114	3119	3120	3127	3130	3135
3137	3141	3149	3150	3150	3155	3157	3158	3160	3161	
3164	3165	3167	3168	3180	3187	3195	3203	3206	3211	
3217	3223	3230	3237	3261						
P7a	14	28	35	38	51	52	57	58	64	71
	75	77	81	90	94	94	98	103	106	110
	116	121	122	125	127	129	132	133	135	141
	144	145	151	153	160	163	166	172	174	180

	184	186	191	192	194	208	212	221	228	253
	260	263	267	272	275	281	282	284	287	288
	291	293	297	366	372	381	386	390	421	424
	430	451	492	501	545	547	550	551	551	552
	554	559	604	605	606	616	618	619	627	630
	630	634	638	641	645	662	682	693	694	713
	716	738	749	759	776	781	788	792	815	817
	823	825	854	859	864	870	872	901	906	912
	917	920	922	958	968	970	971	973	975	976
	991	994	1010	1011	1046	1046	1050	1051	1055	1056
	1056	1057	1061	1062	1062	1063	1068	1091	1092	1092
	1093	1110	1113	1128	1129	1185	1185	1188	1190	1194
	1194	1206	1208	1237	1238	1304	1307	1313	1317	1329
	1330	1370	1370	1418	1420	1422	1423	1431	1434	1434
	1435	1436	1440	1445	1446	1452	1453	1467	1469	1475
	1478	1480	1480	1481	1484	1485	1486	1487	1488	1488
	1489	1490	1493	1495	1498	1501	1503	1503	1503	1504
	1506	1509	1511	1513	1514	1515	1517	1527	1529	1531
	1533	1534	1538	1540	1543	1550	1551	1628	1628	1658
	1659	2180	2216	3034	3036	3039	3039	3040	3040	3043
	3043	3046	3046	3054	3054	3056	3056	3101	3102	3102
	3103	3104	3106	3113	3113	3117	3120	3128	3132	3133
	3137	3139	3141	3141	3144	3147	3149	3152	3152	3156
	3157	3159	3160	3163	3174	3188	3189	3194	3195	3209
	3212	3217	3219	3226	3228					
TS7b	-17	16	28	31	38	42	43	49	50	63
	69	73	74	81	83	87	88	93	102	105
	107	110	119	122	125	128	136	141	143	147
	148	152	154	157	157	162	164	167	170	174
	176	181	184	184	189	193	195	203	225	245
	250	261	266	268	274	279	280	284	287	292
	296	301	304	335	352	364	369	376	382	388
	400	412	418	427	507	519	543	548	549	551
	553	555	557	559	588	609	610	614	623	626
	629	632	632	633	638	638	642	665	687	703
	703	708	717	736	767	770	779	785	787	818
	820	826	829	830	846	858	862	873	878	895
	909	910	919	924	932	968	974	975	978	979
	981	992	1003	1010	1014	1048	1048	1053	1054	1054
	1057	1058	1060	1061	1061	1065	1074	1090	1092	1093
	1096	1106	1115	1126	1128	1185	1191	1192	1192	1194
	1195	1199	1212	1216	1239	1303	1308	1311	1317	1328
	1341	1369	1375	1419	1421	1423	1424	1429	1431	1432
	1432	1437	1441	1449	1450	1452	1453	1472	1473	1473
	1479	1480	1481	1483	1484	1487	1487	1488	1492	1493
	1493	1494	1497	1498	1503	1503	1505	1508	1512	1513
	1514	1517	1520	1521	1525	1527	1528	1531	1532	1533
	1536	1544	1546	1550	1552	1630	1633	1658	1658	1664
	2105	2173	2285	3030	3031	3032	3035	3036	3037	3039
	3045	3046	3050	3053	3054	3056	3058	3094	3105	3107
	3108	3109	3110	3111	3113	3119	3124	3131	3133	3133
	3135	3138	3143	3144	3146	3147	3150	3154	3156	3156
	3159	3165	3170	3170	3171	3187	3193	3204	3210	3212
	3216	3221	3225	3235	3248					
TS7c	-66	20	29	32	37	39	47	48	55	60
	63	63	71	77	80	83	85	91	94	101
	111	119	120	126	128	132	135	138	143	146
	147	148	152	156	160	169	170	172	177	180
	183	185	188	192	195	200	203	209	221	232
	235	263	264	269	272	273	277	281	282	286
	290	299	307	317	339	363	372	375	376	385
	407	411	418	430	510	543	547	548	550	551
	555	556	556	567	607	610	613	618	619	623

	627	627	632	633	635	644	655	673	681	699
	703	711	715	750	769	773	778	783	789	821
	823	824	825	837	854	859	863	872	876	894
	910	912	921	923	939	967	970	970	976	978
	983	990	1007	1011	1016	1049	1050	1053	1053	1056
	1058	1059	1060	1060	1061	1063	1066	1092	1094	1095
	1096	1107	1116	1129	1130	1184	1193	1193	1193	1195
	1197	1200	1211	1216	1250	1298	1307	1313	1321	1330
	1342	1370	1378	1420	1421	1424	1424	1430	1431	1433
	1435	1435	1440	1448	1450	1453	1455	1472	1473	1476
	1477	1478	1481	1483	1484	1485	1488	1489	1489	1491
	1491	1493	1493	1497	1503	1506	1506	1508	1508	1510
	1514	1515	1516	1518	1522	1527	1528	1529	1532	1535
	1537	1542	1545	1551	1555	1622	1632	1637	1659	1665
	2156	2176	2253	3026	3031	3033	3034	3037	3038	3038
	3039	3040	3041	3048	3053	3059	3060	3099	3101	3104
	3104	3105	3106	3109	3111	3115	3120	3123	3126	3138
	3140	3140	3141	3148	3148	3155	3156	3157	3158	3159
	3160	3161	3162	3162	3165	3184	3191	3202	3205	3215
	3215	3225	3233	3238	3250					
P7b	15	25	30	36	39	50	56	61	65	67
	72	75	75	80	86	91	96	98	104	105
	108	112	115	122	125	129	132	139	143	148
	150	151	154	158	161	163	166	173	176	181
	185	188	190	193	197	210	213	223	235	252
	260	262	270	279	281	283	287	288	292	293
	295	297	303	336	369	375	387	393	406	415
	426	449	468	519	548	550	551	552	553	556
	556	586	605	606	615	620	626	627	628	630
	631	637	641	642	658	678	681	693	707	715
	719	731	764	774	779	786	791	808	818	820
	822	825	841	862	863	873	874	903	914	915
	924	929	931	962	970	972	974	974	977	980
	994	995	1012	1014	1047	1048	1049	1053	1054	1054
	1057	1057	1058	1062	1064	1068	1075	1090	1092	1095
	1097	1106	1111	1127	1132	1186	1187	1190	1193	1194
	1197	1206	1212	1228	1265	1301	1304	1309	1314	1334
	1334	1369	1371	1418	1421	1423	1424	1431	1432	1433
	1435	1436	1439	1448	1449	1453	1454	1471	1471	1478
	1480	1481	1482	1483	1485	1486	1487	1489	1489	1489
	1491	1493	1494	1494	1498	1500	1501	1503	1504	1506
	1508	1509	1511	1512	1519	1525	1527	1528	1529	1530
	1533	1537	1538	1543	1549	1550	1552	1628	1639	1659
	1664	2126	2193	3037	3037	3038	3038	3039	3039	3041
	3042	3042	3045	3054	3055	3056	3056	3101	3101	3102
	3102	3104	3105	3111	3112	3115	3116	3132	3133	3134
	3135	3137	3139	3148	3149	3151	3152	3153	3154	3155
	3156	3162	3162	3166	3166	3188	3190	3195	3196	3205
	3213	3214	3220	3221	3225					

Table S8. The energies, enthalpies and free energies (in au at 298.15 K) and corresponding relative values (in kcal/mol) for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$, obtained with B3PW91-PCM method. ^a

Species	E	H	G(sol)
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]$	-1494.436371	-1494.394293	-1494.489590
$\text{PhC}\equiv\text{CSiHMe}_2$	-677.374363	-677.360999	-677.399020
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$	-2171.810734(0.0)	-2171.755292(0.0)	-2171.888610(0.0)
TS7	-2171.789522(13.3)	-2171.734585(13.0)	-2171.853810(21.8)
7	-2171.843723(-20.7)	-2171.789259(-21.3)	-2171.907400(-11.8)
TS7a	-2171.782767(17.5)	-2171.728041(17.1)	-2171.846310(26.5)
P7a	-2171.829591(-11.8)	-2171.775095(-12.4)	-2171.893080(-2.8)
TS7b	-2171.787738(14.4)	-2171.732997(14.0)	-2171.851280(23.4)
TS7c	-2171.785341(15.9)	-2171.73061(15.5)	-2171.849190(24.7)
P7b	-2171.839336(-17.9)	-2171.784842(-18.5)	-2171.903220(-9.2)

^a The U was treated with ECP80MWB, in which 80 electrons are in the core region and the corresponding optimized segmented ((7s6p5d)/[4s3p3d]) basis set is applied for the valence shells of U.

Table S9. The energies, enthalpies and free energies (in au at 298.15 K) and corresponding relative values (in kcal/mol) for $(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$, obtained with B3PW91-PCM method. ^a

Species	E	H	G(sol)
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]$	-1933.992864	-1933.950572	-1934.047250
$\text{PhC}\equiv\text{CSiHMe}_2$	-677.374363	-677.360999	-677.399020
$(\eta^5\text{-C}_5\text{Me}_5)_2\text{U}[\eta^2\text{-C(Ph)=C(SiHMe}_2)]+\text{PhC}\equiv\text{CSiHMe}_2$	-2611.367227(0.0)	-2611.311571(0.0)	-2611.446270(0.0)
TS7	-2611.339297(17.5)	-2611.284442(17.0)	-2611.404600(26.1)
7	-2611.385622(-11.5)	-2611.331040(-12.2)	-2611.450230(-2.5)
TS7a	-2611.329681(23.6)	-2611.275179(22.8)	-2611.393690(33.0)
P7a	-2611.373646(-4.0)	-2611.319125(-4.7)	-2611.438360(5.0)
TS7b	-2611.335459(19.9)	-2611.281022(19.2)	-2611.399710(29.2)
TS7c	-2611.337044(18.9)	-2611.282382(18.3)	-2611.402030(27.8)
P7b	-2611.381400(-8.9)	-2611.327201(-9.8)	-2611.445400(0.5)

^a The U was treated with ECP60MWB, in which 60 electrons are in the core region and the corresponding optimized segmented ((14s13p10d8f6g)/[10s9p5d4f3g]) basis set is applied for the valence shells of U.