

Supporting Information for

Preparation of a Uranium Metallacyclocumulene and Its Reactivity toward Unsaturated Organic Molecules

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1. Crystal parameters

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

Compound	2	3	4	5	6·C ₆ H ₁₄
Formula	C ₄₂ H ₅₂ U	C ₃₆ H ₆₀ Si ₂ U	C ₄₉ H ₅₇ NSU	C ₅₅ H ₇₄ N ₂ U	C ₆₄ H ₈₂ N ₂ U
Fw	794.86	787.05	930.04	1001.19	1117.34
crystal system	tetragonal	monoclinic	monoclinic	triclinic	triclinic
space group	<i>I</i> -42 <i>d</i>	<i>C</i> 2/ <i>c</i>	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> (-1)	<i>P</i> (-1)
<i>a</i> (Å)	24.935(16)	10.817(9)	21.053(12)	10.680(11)	10.919(1)
<i>b</i> (Å)	24.935(16)	18.009(9)	11.026(6)	11.535(12)	14.294(1)
<i>c</i> (Å)	11.671(11)	19.810(12)	18.894(10)	20.41(3)	18.058(1)
α (deg)	90	90	90	100.04(2)	76.41(1)
β (deg)	90	106.86(2)	107.47(1)	92.65(2)	88.11(1)
γ (deg)	90	90	90	99.24(1)	86.40(1)
<i>V</i> (Å ³)	7256(12)	3790(4)	4184(4)	2437(5)	2733.7(2)
<i>Z</i>	8	4	4	2	2
<i>D</i> _{calc} (g/cm ³)	1.455	1.379	1.477	1.365	1.357
μ (Mo/K α) _{calc} (cm ⁻¹)	4.500	4.366	3.963	3.367	3.009
size (mm)	0.20 × 0.20 × 0.20	0.20 × 0.20 × 0.20	0.20 × 0.20 × 0.20	0.15 × 0.10 × 0.10	0.15 × 0.20 × 0.20
<i>F</i> (000)	3168	1584	1864	1020	1144
2 θ range (deg)	3.27 to 55.46	4.19 to 55.20	4.06 to 55.38	3.64 to 50.50	6.58 to 59.94
no. of reflns, collected	24779	11879	27389	12491	25416
no of obsd reflns	4218	4322	9648	8494	13062
no of variables	202	186	481	535	602
abs corr (<i>T</i> _{max} , <i>T</i> _{min})	0.75, 0.55	0.75, 0.51	0.75, 0.44	0.75, 0.56	1.00, 0.67
<i>R</i>	0.053	0.048	0.067	0.072	0.047
<i>R</i> _w	0.100	0.098	0.155	0.180	0.097
<i>R</i> _{all}	0.077	0.065	0.091	0.084	0.058
Gof	0.97	0.95	1.02	1.12	1.05
CCDC	1529308	1529313	1529307	1529309	1529312

Table S2. Crystal Data and Experimental Parameters for Compounds 7-10

Compound	7	8	9·2C₆H₆	10·0.5C₆H₁₄
Formula	C ₄₉ H ₆₂ N ₂ U	C ₅₄ H ₇₂ O ₂ U	C ₈₀ H ₈₄ O ₂ U	C ₇₂ H ₁₀₁ S ₂ U ₂
Fw	917.03	991.14	1315.50	1506.70
crystal system	triclinic	triclinic	triclinic	triclinic
space group	<i>P</i> (-1)	<i>P</i> (-1)	<i>P</i> (-1)	<i>P</i> (-1)
<i>a</i> (Å)	10.997(15)	10.426(7)	11.734(8)	11.959(13)
<i>b</i> (Å)	12.383(17)	11.296(8)	14.198(10)	14.189(15)
<i>c</i> (Å)	15.72(2)	22.085(16)	21.577(15)	20.45(2)
α (deg)	91.91(2)	94.73(1)	74.35(1)	104.94(2)
β (deg)	90.78(2)	102.02(1)	79.24(1)	96.01(2)
γ (deg)	97.89(2)	102.84(1)	86.69(1)	94.40(2)
<i>V</i> (Å ³)	2119(5)	2458(3)	3400(4)	3315(6)
<i>Z</i>	2	2	2	2
<i>D</i> _{calc} (g/cm ³)	1.437	1.339	1.285	1.509
μ (Mo/K α) _{calc} (cm ⁻¹)	3.864	3.339	2.431	4.980
size (mm)	0.10 × 0.10 × 0.10	0.20 × 0.20 × 0.20	0.20 × 0.20 × 0.20	0.20 × 0.20 × 0.15
<i>F</i> (000)	924	1008	1344	1498
2 θ range (deg)	3.32 to 55.61	3.73 to 50.50	2.98 to 55.01	3.15 to 55.73
no. of reflns, collected	13378	13040	22689	22161
no of obsd reflns	9523	8627	15351	15308
no of variables	483	526	794	710
abs corr (<i>T</i> _{max} , <i>T</i> _{min})	0.75, 0.44	0.75, 0.61	0.75, 0.61	0.75, 0.48
<i>R</i>	0.068	0.063	0.045	0.052
<i>R</i> _w	0.159	0.168	0.096	0.120
<i>R</i> _{all}	0.116	0.074	0.069	0.087
Gof	0.95	1.01	0.98	0.96
CCDC	1529306	1529311	1529310	1529314

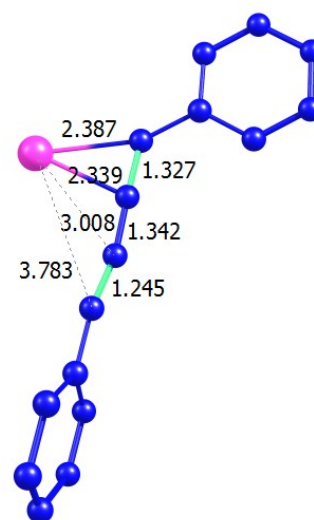
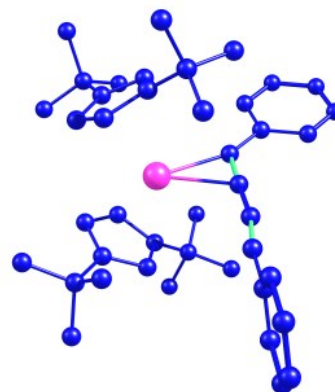
2. Computational details

Table S3. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for the isomerization of **2**, obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
2	C	16.647965	20.098854	11.000783	
	C	16.167171	21.401538	11.310215	
	H	15.287991	21.859080	10.870222	
	C	16.921833	21.957764	12.380417	
	C	17.945652	21.016127	12.674712	
	H	18.693772	21.112748	13.453224	
	C	17.773067	19.881024	11.837137	
	H	18.367649	18.977004	11.879525	
	C	15.902961	19.073808	10.150264	
	C	14.525690	18.834046	10.806539	
	H	14.640159	18.484998	11.839114	
	H	13.963860	18.073897	10.248548	
	H	13.926913	19.751091	10.825797	
	C	16.641507	17.730218	10.105644	
	H	17.635009	17.822419	9.655731	
	H	16.071680	17.009130	9.507565	
	H	16.762474	17.307358	11.109594	
	C	15.675722	19.577148	8.716831	
	H	15.151709	20.538928	8.710715	
	H	15.066951	18.861359	8.149832	
	H	16.625384	19.699591	8.183343	
	C	16.475620	23.124748	13.258207	
	C	15.907608	24.293990	12.440589	
	H	15.093315	23.974081	11.780898	
	H	16.677842	24.761910	11.821518	
	H	15.503806	25.059519	13.114960	
	C	17.610573	23.640780	14.151932	
	H	17.244235	24.457532	14.785835	
	H	18.448030	24.020587	13.560098	
	H	17.989428	22.856244	14.817281	
	C	15.351865	22.581730	14.170748	
	H	14.998849	23.368105	14.850523	
	H	15.709244	21.740992	14.776517	
	H	14.497235	22.232287	13.580327	
	C	19.179173	24.278546	10.660397	
	C	20.001754	23.596430	11.432387	
	C	21.043904	24.010819	12.356791	
	C	21.529115	25.334579	12.369603	
	H	21.106091	26.054406	11.673581	
	C	22.532593	25.717453	13.251634	
	H	22.896137	26.742114	13.243286	
	C	23.070341	24.791825	14.149827	
H	23.853098	25.093251	14.841184		
C	22.596272	23.479818	14.156054		
H	23.006117	22.755687	14.855763		
C	21.597856	23.092747	13.266345		
H	21.226497	22.072417	13.274014		
U	18.701290	21.911502	10.212095		
C	18.223169	24.278476	9.763674		
C	17.400641	23.596230	8.991737		

	C	16.358381	24.010481	8.067393	
	C	15.872956	25.334156	8.054584	
	H	16.295866	26.054067	8.750587	
	C	14.869389	25.716840	7.172566	
	H	14.505654	26.741434	7.180911	
	C	14.331790	24.791114	6.274388	
	H	13.548977	25.092410	5.583038	
	C	14.806077	23.479182	6.268154	
	H	14.396341	22.754988	5.568447	
	C	15.804566	23.092298	7.157851	
	H	16.176113	22.072035	7.150253	
	C	20.754465	20.098601	9.423436	
	C	21.235454	21.401233	9.114090	
	H	22.114693	21.858610	9.554134	
	C	20.480916	21.957632	8.043880	
	C	19.457024	21.016123	7.749445	
	H	18.708954	21.112915	6.970905	
	C	19.629394	19.880965	8.586985	
	H	19.034674	18.977041	8.544492	
	C	21.499290	19.073414	10.273933	
	C	22.876598	18.833563	9.617767	
	H	22.762184	18.484422	8.585218	
	H	23.438373	18.073454	10.175865	
	H	23.475397	19.750593	9.598464	
	C	20.760602	17.729898	10.318355	
	H	19.767074	17.822134	10.768210	
	H	21.330315	17.008687	10.916394	
	H	20.639666	17.307162	9.314349	
	C	21.726444	19.576607	11.707432	
	H	22.250543	20.538340	11.713678	
	H	22.335098	18.860715	12.274428	
	H	20.776737	19.699091	12.240834	
	C	20.927342	23.124592	7.166163	
	C	21.495352	24.293757	7.983894	
	H	22.309686	23.973796	8.643509	
	H	20.725123	24.761552	8.603063	
	H	21.899102	25.059385	7.309605	
	C	19.792555	23.640751	6.272294	
	H	20.159070	24.457446	5.638419	
	H	18.955077	24.020672	6.864022	
	H	19.413677	22.856251	5.606914	
	C	22.051155	22.581498	6.253747	
	H	22.404366	23.367878	5.574079	
	H	21.693759	21.740848	5.647868	
	H	22.905655	22.231911	6.844271	
TS2	C	16.985870	20.052514	11.212086	
	C	16.793334	21.342571	11.794900	
	H	16.036656	22.056093	11.488006	
	C	17.675026	21.511003	12.896177	
	C	18.485650	20.344798	12.936224	
	H	19.249583	20.128486	13.674770	
	C	18.046652	19.446814	11.926353	
	H	18.441155	18.453322	11.757816	
	C	16.099889	19.410449	10.147822	
	C	14.654642	19.367497	10.683614	
	H	14.604890	18.812044	11.627073	
	H	13.992526	18.874901	9.960162	
	H	14.265350	20.375293	10.864751	

C	16.552472	17.974456	9.850960
H	17.579593	17.947758	9.467825
H	15.902735	17.524946	9.090768
H	16.505477	17.344749	10.746648
C	16.115667	20.211759	8.834177
H	15.868506	21.267340	8.993503
H	15.386214	19.802068	8.124217
H	17.098359	20.156914	8.344822
C	17.567676	22.569256	13.987212
C	17.047181	23.908657	13.446915
H	16.061242	23.801018	12.980295
H	17.731651	24.334304	12.707600
H	16.943385	24.626364	14.269829
C	18.911401	22.796663	14.692793
H	18.794015	23.534826	15.495479
H	19.667831	23.171502	13.996602
H	19.288372	21.874525	15.150420
C	16.553734	22.035803	15.024995
H	16.430363	22.756711	15.843578
H	16.891416	21.085627	15.454715
H	15.572230	21.869035	14.566467
C	19.132173	23.830634	10.488469
C	20.179853	23.587994	11.265834
C	21.106558	24.541806	11.885966
C	20.998955	25.927859	11.660127
H	20.202519	26.290587	11.014651
C	21.890101	26.820440	12.245460
H	21.790564	27.886804	12.056523
C	22.910505	26.350431	13.076689
H	23.606422	27.048529	13.535418
C	23.030528	24.981417	13.315575
H	23.820427	24.608611	13.963401
C	22.139022	24.089115	12.724418
H	22.228253	23.023133	12.910952
U	19.270472	21.496927	10.561296
C	18.089645	24.124191	9.695531
C	17.107653	24.138520	8.930713
C	15.997677	24.392097	8.092865
C	14.719520	24.645195	8.642649
H	14.601319	24.654332	9.722572
C	13.628926	24.887444	7.815972
H	12.656124	25.082361	8.261200
C	13.773725	24.886041	6.426905
H	12.917766	25.076872	5.785282
C	15.031018	24.638772	5.871323
H	15.157570	24.638083	4.791239
C	16.130114	24.392284	6.685311
H	17.105269	24.202834	6.245673
C	21.543705	19.801228	10.509768
C	21.926012	21.015886	9.869249
H	22.683518	21.700187	10.231231
C	21.233050	21.151870	8.635225
C	20.364811	20.028460	8.539364
H	19.700980	19.802538	7.710539
C	20.559117	19.205184	9.678452
H	20.069609	18.254599	9.852735
C	22.284803	19.147111	11.671783
C	23.624105	18.613662	11.116289



	H	23.453280	17.882452	10.317977	
	H	24.202168	18.124655	11.911072	
	H	24.231624	19.426759	10.703574	
	C	21.506501	17.963475	12.261499	
	H	20.551964	18.279303	12.694065	
	H	22.093275	17.491334	13.058545	
	H	21.304511	17.195622	11.505964	
	C	22.590544	20.152849	12.791262	
	H	23.191456	20.991059	12.422588	
	H	23.159000	19.668177	13.594735	
	H	21.670754	20.558171	13.229593	
	C	21.521353	22.157742	7.526582	
	C	22.256716	23.394306	8.060819	
	H	23.230999	23.129934	8.487563	
	H	21.674669	23.906826	8.833770	
	H	22.438657	24.103208	7.244114	
	C	20.228909	22.607477	6.826046	
	H	20.464696	23.282862	5.994332	
	H	19.566596	23.149399	7.511666	
	H	19.674667	21.757976	6.409527	
	C	22.425064	21.457692	6.488548	
	H	22.676764	22.147425	5.672592	
	H	21.926440	20.583351	6.054674	
	H	23.359808	21.118265	6.949329	
P2	C	17.952989	19.242629	12.430877	
	C	17.072848	20.355530	12.301432	
	H	16.158868	20.357595	11.715969	
	C	17.488319	21.408620	13.158913	
	C	18.702734	20.974879	13.757368	
	H	19.279554	21.525682	14.491202	
	C	18.975666	19.644620	13.325000	
	H	19.796138	19.029741	13.675134	
	C	17.681397	17.853085	11.864821	
	C	16.371545	17.328736	12.490839	
	H	16.449254	17.289556	13.583230	
	H	16.151879	16.316919	12.126828	
	H	15.521580	17.971642	12.237411	
	C	18.804857	16.872168	12.222219	
	H	19.770385	17.192107	11.817512	
	H	18.582868	15.879223	11.813687	
	H	18.910789	16.769511	13.308184	
	C	17.508949	17.900652	10.336800	
	H	16.692549	18.573038	10.046851	
	H	17.273827	16.905180	9.940233	
	H	18.427410	18.244428	9.845889	
	C	16.624797	22.590916	13.583732	
	C	15.782184	23.136079	12.421572	
	H	15.126222	22.365649	11.998839	
	H	16.412598	23.532059	11.619805	
	H	15.138584	23.950174	12.776955	
	C	17.456368	23.730988	14.185113	
	H	16.793925	24.539775	14.516945	
	H	18.159161	24.143822	13.456927	
	H	18.025446	23.396837	15.060617	
	C	15.665844	22.063876	14.676266	
	H	15.015571	22.872860	15.033166	
	H	16.224364	21.671632	15.534077	
	H	15.029518	21.258939	14.290783	

C	18.993323	23.493874	10.670307
C	19.964686	23.472306	11.625011
C	20.701654	24.582248	12.232684
C	20.920899	25.795472	11.549787
H	20.512936	25.920333	10.550948
C	21.648872	26.827340	12.135420
H	21.813456	27.750112	11.583481
C	22.159154	26.686831	13.427453
H	22.722025	27.496501	13.885403
C	21.940252	25.498937	14.126013
H	22.329009	25.380210	15.134835
C	21.233246	24.457810	13.530146
H	21.070395	23.531278	14.073887
U	19.473043	21.276768	11.160443
C	18.334757	24.524822	10.004130
C	17.708388	25.366325	9.366727
C	17.014392	26.389442	8.664642
C	16.916547	27.689533	9.202033
H	17.378339	27.896702	10.163151
C	16.237770	28.689915	8.514706
H	16.169287	29.685988	8.944991
C	15.651395	28.421519	7.276312
H	15.125073	29.206684	6.739674
C	15.744053	27.139943	6.730506
H	15.289355	26.924604	5.766688
C	16.412621	26.131320	7.416323
H	16.481340	25.132359	6.994958
C	22.130724	20.314639	10.985751
C	22.056606	21.494257	10.190065
H	22.588209	22.416036	10.392356
C	21.246997	21.252395	9.044922
C	20.767320	19.919822	9.171356
H	20.148965	19.394508	8.449817
C	21.312332	19.348528	10.349728
H	21.168754	18.324836	10.671464
C	23.066413	20.093866	12.169054
C	24.514871	20.310295	11.684096
H	24.757456	19.630144	10.859557
H	25.223111	20.123738	12.501469
H	24.669201	21.336086	11.332112
C	22.948666	18.661927	12.707366
H	21.931959	18.439792	13.050081
H	23.625051	18.524180	13.559154
H	23.218562	17.922845	11.944116
C	22.773568	21.085213	13.305515
H	22.831907	22.122069	12.959305
H	23.497088	20.960268	14.121433
H	21.771693	20.923280	13.723828
C	21.114041	22.118026	7.796746
C	21.597968	23.551584	8.048203
H	22.656687	23.571375	8.331404
H	21.019799	24.034818	8.841111
H	21.488123	24.148234	7.134756
C	19.660959	22.155679	7.294672
H	19.597828	22.716078	6.353512
H	19.006372	22.653821	8.019474
H	19.273370	21.147854	7.100641
C	21.999185	21.488899	6.699034

	H	21.958223	22.091753	5.782670	
	H	21.667717	20.473430	6.453564	
	H	23.044613	21.432373	7.023626	

Table S4. Frequencies of the stationary points optimized for the isomerization of **2**, obtained with B3PW91-PCM method.

Species	Frequencies (cm ⁻¹)										
2	16	20	24	27	35	38	42	49	52	53	57
	59	70	91	91	93	101	106	124	131	140	142
	160	169	178	183	186	187	200	219	229	231	231
	232	237	240	241	251	259	263	287	288	292	293
	299	303	303	304	331	334	343	347	348	356	357
	364	366	387	390	394	415	417	418	421	449	450
	462	473	479	480	500	501	506	514	541	555	557
	586	588	605	608	623	630	631	656	663	679	681
	703	704	759	770	774	778	804	818	820	825	826
	831	836	839	843	843	857	857	927	933	933	936
	937	938	944	947	951	954	957	957	958	959	968
	968	968	970	977	977	1000	1000	1015	1015	1045	1046
	1047	1051	1051	1057	1057	1058	1060	1060	1075	1079	1080
	1110	1110	1111	1112	1188	1188	1197	1201	1203	1206	1211
	1212	1217	1235	1235	1237	1238	1245	1246	1272	1272	1284
	1285	1334	1335	1335	1335	1366	1375	1380	1393	1398	1401
	1403	1411	1411	1412	1412	1417	1419	1423	1424	1441	1442
	1446	1446	1478	1480	1489	1489	1498	1500	1502	1502	1506
	1506	1507	1508	1511	1511	1511	1513	1521	1522	1523	1524
	1524	1524	1525	1527	1530	1533	1535	1540	1543	1544	1551
	1551	1635	1635	1660	1662	1694	1974	3045	3045	3047	3047
	3050	3050	3056	3056	3060	3060	3061	3062	3118	3118	3120
	3120	3123	3123	3123	3123	3126	3127	3129	3129	3134	3134
	3138	3138	3139	3139	3146	3149	3157	3157	3167	3167	3195
	3195	3203	3203	3213	3213	3221	3221	3229	3229	3242	3242
	3246	3246	3265	3266							
	TS2	-64	16	18	24	25	31	35	38	45	51
58		67	72	78	86	87	92	107	109	125	142
144		171	181	190	193	201	207	223	228	238	242
246		248	249	253	257	260	272	274	289	295	296
298		302	306	328	330	344	345	347	352	358	363
366		368	386	391	397	409	417	419	422	428	446
449		464	467	469	482	498	500	504	508	526	558
561		577	612	612	621	630	632	666	671	684	690
701		706	711	759	775	779	782	827	828	830	833
835		839	841	844	845	859	861	905	934	936	939
943		944	944	946	952	954	955	957	959	959	966
966		968	972	975	978	987	990	1000	1007	1016	1047
1050		1051	1054	1055	1055	1058	1061	1067	1070	1082	1089
1109		1111	1115	1118	1187	1188	1199	1202	1204	1208	1214
1217		1225	1234	1236	1241	1243	1245	1246	1272	1273	1287
1288		1329	1333	1339	1341	1342	1372	1376	1397	1398	1402
1404		1411	1413	1415	1416	1419	1421	1425	1425	1444	1445
1451		1453	1482	1485	1487	1489	1501	1502	1502	1504	1506
1507		1508	1510	1511	1511	1513	1514	1521	1523	1523	1523
1524		1525	1530	1533	1535	1537	1541	1542	1547	1551	1562
1616		1622	1638	1658	1661	1808	2162	3045	3045	3047	3047
3048		3051	3053	3054	3054	3058	3059	3060	3113	3120	3120
3121		3121	3122	3123	3124	3126	3127	3127	3128	3131	3133
3133		3134	3136	3138	3138	3142	3146	3146	3149	3156	3191
3193		3199	3200	3209	3214	3218	3219	3225	3230	3230	3242
3244		3259	3261	3270							

P2	11	18	20	23	33	34	51	56	60	64	71
	74	78	82	84	85	101	106	107	117	138	141
	147	172	186	195	197	200	206	218	226	230	230
	241	244	250	252	253	271	271	291	293	294	296
	299	304	330	334	337	344	348	352	354	358	361
	363	381	385	399	408	412	414	421	428	432	448
	450	467	482	484	484	501	503	505	553	557	559
	574	609	614	615	627	632	661	665	687	691	695
	704	710	742	771	773	778	781	825	828	831	835
	840	843	846	855	857	859	867	929	933	937	938
	941	942	946	946	951	954	955	956	958	959	967
	967	970	970	973	976	997	999	1011	1014	1015	1049
	1050	1051	1053	1055	1056	1060	1060	1063	1064	1077	1081
	1110	1111	1115	1116	1187	1189	1202	1204	1204	1207	1213
	1215	1219	1236	1240	1240	1243	1245	1247	1272	1273	1287
	1288	1326	1334	1334	1336	1342	1372	1373	1396	1400	1403
	1404	1410	1413	1415	1417	1418	1420	1423	1423	1444	1445
	1446	1448	1478	1484	1487	1488	1501	1501	1502	1503	1507
	1507	1508	1509	1511	1512	1512	1513	1522	1522	1523	1523
	1524	1526	1527	1533	1535	1538	1538	1541	1546	1551	1558
	1575	1585	1632	1634	1660	1667	2240	3044	3045	3047	3049
	3049	3050	3054	3057	3057	3059	3060	3062	3117	3117	3118
	3120	3121	3122	3123	3124	3125	3127	3130	3131	3131	3132
	3134	3137	3137	3138	3144	3145	3156	3157	3158	3170	3189
	3195	3197	3203	3211	3215	3219	3222	3225	3226	3227	3234
	3245	3259	3261	3265							

Table S5. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for the isomerization of **2**, obtained with B3PW91-PCM method

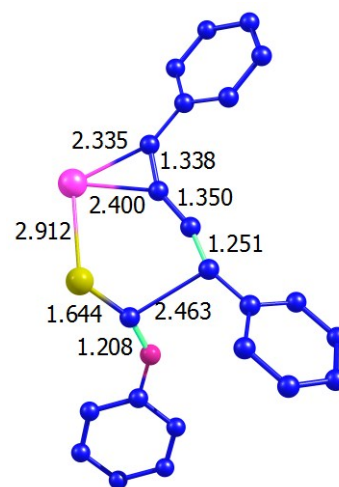
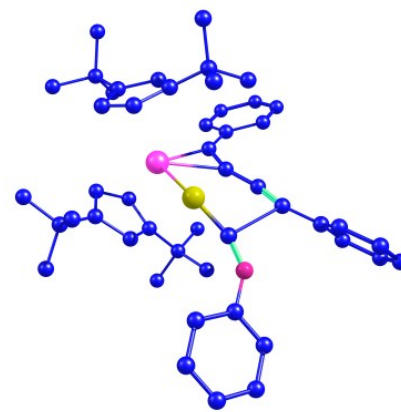
species	E	H	G (sol)
2	-2107.417494(0.0)	-2107.36972(0.0)	-2107.474980(0.0)
TS2	-2107.38487(20.5)	-2107.33769(20.1)	-2107.441980(20.7)
P2	-2107.393357(15.1)	-2107.34591(14.9)	-2107.451320(14.8)

Table S6. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for **2**+ PhNCS, obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
2	C	16.647965	20.098854	11.000783	
	C	16.167171	21.401538	11.310215	
	H	15.287991	21.859080	10.870222	
	C	16.921833	21.957764	12.380417	
	C	17.945652	21.016127	12.674712	
	H	18.693772	21.112748	13.453224	
	C	17.773067	19.881024	11.837137	
	H	18.367649	18.977004	11.879525	
	C	15.902961	19.073808	10.150264	
	C	14.525690	18.834046	10.806539	
	H	14.640159	18.484998	11.839114	
	H	13.963860	18.073897	10.248548	
	H	13.926913	19.751091	10.825797	
	C	16.641507	17.730218	10.105644	
	H	17.635009	17.822419	9.655731	
	H	16.071680	17.009130	9.507565	
	H	16.762474	17.307358	11.109594	
	C	15.675722	19.577148	8.716831	
	H	15.151709	20.538928	8.710715	
	H	15.066951	18.861359	8.149832	
	H	16.625384	19.699591	8.183343	
	C	16.475620	23.124748	13.258207	
	C	15.907608	24.293990	12.440589	
	H	15.093315	23.974081	11.780898	
	H	16.677842	24.761910	11.821518	
	H	15.503806	25.059519	13.114960	
	C	17.610573	23.640780	14.151932	
	H	17.244235	24.457532	14.785835	
	H	18.448030	24.020587	13.560098	
	H	17.989428	22.856244	14.817281	
	C	15.351865	22.581730	14.170748	
	H	14.998849	23.368105	14.850523	
	H	15.709244	21.740992	14.776517	
	H	14.497235	22.232287	13.580327	
	C	19.179173	24.278546	10.660397	
	C	20.001754	23.596430	11.432387	
	C	21.043904	24.010819	12.356791	
	C	21.529115	25.334579	12.369603	
	H	21.106091	26.054406	11.673581	
	C	22.532593	25.717453	13.251634	
H	22.896137	26.742114	13.243286		
C	23.070341	24.791825	14.149827		
H	23.853098	25.093251	14.841184		
C	22.596272	23.479818	14.156054		
H	23.006117	22.755687	14.855763		
C	21.597856	23.092747	13.266345		
H	21.226497	22.072417	13.274014		
U	18.701290	21.911502	10.212095		
C	18.223169	24.278476	9.763674		
C	17.400641	23.596230	8.991737		
C	16.358381	24.010481	8.067393		
C	15.872956	25.334156	8.054584		
H	16.295866	26.054067	8.750587		

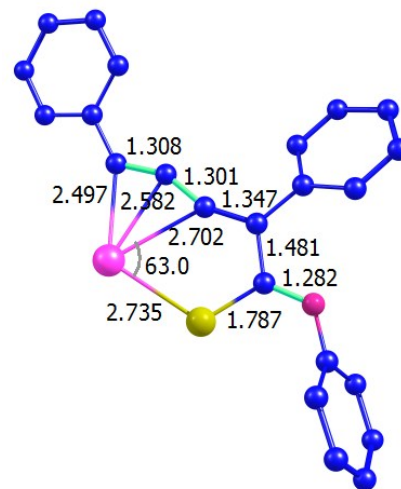
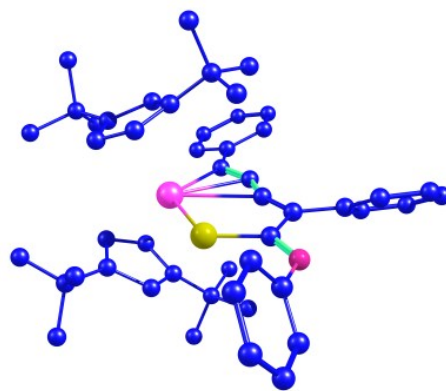
	C	14.869389	25.716840	7.172566	
	H	14.505654	26.741434	7.180911	
	C	14.331790	24.791114	6.274388	
	H	13.548977	25.092410	5.583038	
	C	14.806077	23.479182	6.268154	
	H	14.396341	22.754988	5.568447	
	C	15.804566	23.092298	7.157851	
	H	16.176113	22.072035	7.150253	
	C	20.754465	20.098601	9.423436	
	C	21.235454	21.401233	9.114090	
	H	22.114693	21.858610	9.554134	
	C	20.480916	21.957632	8.043880	
	C	19.457024	21.016123	7.749445	
	H	18.708954	21.112915	6.970905	
	C	19.629394	19.880965	8.586985	
	H	19.034674	18.977041	8.544492	
	C	21.499290	19.073414	10.273933	
	C	22.876598	18.833563	9.617767	
	H	22.762184	18.484422	8.585218	
	H	23.438373	18.073454	10.175865	
	H	23.475397	19.750593	9.598464	
	C	20.760602	17.729898	10.318355	
	H	19.767074	17.822134	10.768210	
	H	21.330315	17.008687	10.916394	
	H	20.639666	17.307162	9.314349	
	C	21.726444	19.576607	11.707432	
	H	22.250543	20.538340	11.713678	
	H	22.335098	18.860715	12.274428	
	H	20.776737	19.699091	12.240834	
	C	20.927342	23.124592	7.166163	
	C	21.495352	24.293757	7.983894	
	H	22.309686	23.973796	8.643509	
	H	20.725123	24.761552	8.603063	
	H	21.899102	25.059385	7.309605	
	C	19.792555	23.640751	6.272294	
	H	20.159070	24.457446	5.638419	
	H	18.955077	24.020672	6.864022	
	H	19.413677	22.856251	5.606914	
	C	22.051155	22.581498	6.253747	
	H	22.404366	23.367878	5.574079	
	H	21.693759	21.740848	5.647868	
	H	22.905655	22.231911	6.844271	
PhNCS	C	3.223564	-0.157964	0.000078	
	C	2.671463	1.123540	0.000039	
	C	1.290846	1.295916	-0.000026	
	C	0.456977	0.170211	-0.000054	
	C	1.004509	-1.121731	-0.000018	
	C	2.386710	-1.275395	0.000047	
	H	4.302282	-0.286301	0.000130	
	H	3.318320	1.996434	0.000060	
	H	0.847617	2.286745	-0.000059	
	H	0.343858	-1.983224	-0.000050	
	H	2.811281	-2.275567	0.000073	
	N	-0.907795	0.343445	-0.000139	
	C	-2.071320	0.098944	-0.000199	
	S	-3.643481	-0.137983	0.000077	

Atom	X	Y	Z
C	10.254515	18.826032	10.022356
C	9.414201	19.968301	9.880843
H	8.491089	19.989585	9.312752
C	9.889923	21.025287	10.700562
C	11.102187	20.564154	11.279893
H	11.718445	21.114360	11.981432
C	11.314364	19.214773	10.878976
H	12.116993	18.578932	11.228873
C	9.917766	17.426045	9.517128
C	8.550393	17.019272	10.105946
H	8.572550	17.048385	11.201297
H	8.289858	15.998966	9.796315
H	7.751818	17.688394	9.767573
C	10.956335	16.400111	9.988259
H	11.958848	16.631424	9.614867
H	10.688843	15.400411	9.626108
H	11.004660	16.357442	11.082529
C	9.820395	17.388739	7.982740
H	9.067411	18.093430	7.613539
H	9.541709	16.385006	7.637042
H	10.778106	17.647775	7.514253
C	9.082343	22.244161	11.131481
C	8.210641	22.791790	9.993574
H	7.511486	22.036248	9.617305
H	8.817965	23.144072	9.155295
H	7.611657	23.636668	10.355765
C	9.972515	23.368493	11.675481
H	9.349774	24.206993	12.010626
H	10.662907	23.738498	10.913398
H	10.561731	23.036104	12.537964
C	8.151639	21.771017	12.272273
H	7.538668	22.606556	12.634555
H	8.731257	21.381899	13.117440
H	7.478228	20.976744	11.930250
C	11.474199	23.042648	8.175250
C	12.442322	22.925795	9.091858
C	13.257286	23.991840	9.683820
C	13.458631	25.218377	9.022003
H	12.986433	25.377387	8.055711
C	14.251219	26.214513	9.583708
H	14.400273	27.150297	9.049790
C	14.847623	26.019643	10.831705
H	15.462018	26.800764	11.272550
C	14.648153	24.816135	11.508520
H	15.102745	24.657556	12.483724
C	13.872007	23.811538	10.935154
H	13.717878	22.874469	11.462377
U	11.826594	20.717125	8.651364
C	10.676058	23.796701	7.390106
C	9.832298	24.157295	6.540043
C	9.054610	25.099072	5.802254
C	8.588009	26.278950	6.418619
H	8.832612	26.459978	7.461299
C	7.828935	27.197953	5.702647
H	7.478238	28.102535	6.193348
C	7.525007	26.967624	4.359003
H	6.936542	27.690899	3.800387
C	7.979712	25.803673	3.737704



	H	7.747001	25.617566	2.692216	
	C	8.726784	24.871829	4.451416	
	H	9.075602	23.963874	3.968734	
	C	14.395521	19.543171	8.706710	
	C	14.516351	20.727972	7.927626	
	H	15.134539	21.580107	8.186720	
	C	13.837300	20.563640	6.686194	
	C	13.199218	19.295857	6.747980	
	H	12.616303	18.837712	5.956201	
	C	13.543858	18.672807	7.979037	
	H	13.258179	17.670471	8.272674	
	C	15.253142	19.203607	9.922880	
	C	16.732367	19.257514	9.482520	
	H	16.921440	18.562155	8.656772	
	H	17.388426	18.982786	10.318464	
	H	17.013260	20.262121	9.148842	
	C	14.969537	17.784267	10.431936	
	H	13.929771	17.659442	10.749726	
	H	15.609128	17.560835	11.294001	
	H	15.178330	17.035123	9.659448	
	C	15.052581	20.209997	11.066159	
	H	15.286275	21.229690	10.742672	
	H	15.710757	19.967723	11.910343	
	H	14.019240	20.197714	11.431517	
	C	14.089323	21.406172	5.436369	
	C	13.844990	22.903740	5.666547	
	H	14.399936	23.275863	6.534798	
	H	12.783902	23.111773	5.830194	
	H	14.173654	23.474620	4.788570	
	C	13.236924	20.934966	4.250731	
	H	13.468448	21.539977	3.365675	
	H	12.166982	21.037662	4.456226	
	H	13.442291	19.888109	3.997107	
	C	15.575550	21.204186	5.061314	
	H	15.809959	21.745461	4.135539	
	H	15.801250	20.143131	4.902700	
	H	16.239980	21.576639	5.848824	
	C	6.442575	21.700701	5.958237	
	C	5.339162	22.558633	5.899408	
	H	5.501941	23.629078	5.976555	
	C	4.062525	22.026239	5.743915	
	H	3.205023	22.692153	5.699950	
	C	3.883490	20.645977	5.642237	
	H	2.885645	20.233852	5.519148	
	C	4.988764	19.794135	5.696754	
	H	4.852980	18.718887	5.614843	
	C	6.269934	20.312967	5.854866	
	H	7.136669	19.659110	5.893237	
	N	7.710414	22.260670	6.111826	
	C	8.856473	21.912485	6.269240	
	S	10.107138	20.845485	6.305071	
4	C	10.159081	19.137757	10.440585	
	C	9.260149	20.236497	10.323530	
	H	8.272455	20.180343	9.883410	
	C	9.801800	21.383114	10.960738	
	C	11.098956	21.013617	11.406990	
	H	11.780745	21.643871	11.964618	
	C	11.313159	19.641409	11.093967	

H	12.184070	19.065892	11.378993
C	9.789442	17.682047	10.161875
C	8.566537	17.338151	11.040433
H	8.786883	17.500223	12.101883
H	8.288313	16.285293	10.905617
H	7.698192	17.951275	10.777112
C	10.925856	16.728447	10.549735
H	11.827824	16.900255	9.954983
H	10.614092	15.690628	10.383628
H	11.191602	16.830163	11.608529
C	9.410138	17.453350	8.689862
H	8.577911	18.094186	8.381790
H	9.109145	16.409825	8.533011
H	10.252588	17.661059	8.019104
C	9.004405	22.618821	11.366656
C	8.049532	23.081498	10.256791
H	7.360233	22.285786	9.954227
H	8.594741	23.407800	9.366240
H	7.444018	23.924672	10.611481
C	9.910717	23.786272	11.777597
H	9.297213	24.632038	12.110668
H	10.534453	24.127584	10.946626
H	10.569851	23.513839	12.609899
C	8.160165	22.209717	12.595928
H	7.570674	23.063922	12.952946
H	8.799771	21.868599	13.418227
H	7.467592	21.397974	12.346865
C	11.440723	23.489457	8.305732
C	12.361097	23.206646	9.191195
C	13.336640	24.069168	9.836563
C	13.633364	25.341113	9.301526
H	13.124220	25.662952	8.396898
C	14.565673	26.171110	9.911307
H	14.784623	27.144347	9.479418
C	15.215583	25.760192	11.078045
H	15.941689	26.412025	11.556693
C	14.926838	24.510434	11.625924
H	15.424132	24.186298	12.536454
C	14.003041	23.671799	11.008392
H	13.780509	22.701351	11.437754
U	11.430198	20.940083	8.711690
C	10.469983	23.159285	7.504893
C	9.488453	23.335552	6.598997
C	9.176871	24.673181	6.045754
C	9.334967	25.816570	6.847572
H	9.642641	25.700918	7.883376
C	9.085779	27.087285	6.339419
H	9.204263	27.956159	6.982104
C	8.678758	27.244910	5.013910
H	8.483917	28.237154	4.614895
C	8.521870	26.118811	4.206384
H	8.210027	26.230194	3.170847
C	8.762686	24.844514	4.713970
H	8.633632	23.975944	4.079768
C	13.985000	19.671426	8.544718
C	14.063023	20.857194	7.758150
H	14.740691	21.680909	7.949820
C	13.247009	20.727577	6.598839



C	12.574963	19.482592	6.726363
H	11.868947	19.064360	6.019677
C	13.021453	18.842671	7.913124
H	12.729592	17.849323	8.230081
C	15.016157	19.257034	9.593232
C	16.377294	19.162598	8.865875
H	16.328179	18.449846	8.034952
H	17.155862	18.824433	9.561605
H	16.682706	20.133476	8.461229
C	14.711873	17.875301	10.184843
H	13.755607	17.852811	10.714982
H	15.494000	17.598352	10.901476
H	14.687122	17.102910	9.407695
C	15.149911	20.280092	10.728320
H	15.375399	21.279256	10.342103
H	15.964520	19.992108	11.404417
H	14.231581	20.343105	11.322707
C	13.384985	21.554176	5.321516
C	13.712226	23.027225	5.603342
H	14.620764	23.136798	6.206167
H	12.893058	23.529424	6.125357
H	13.881874	23.555576	4.657399
C	12.135072	21.478258	4.435191
H	12.313635	22.018533	3.497607
H	11.267257	21.927309	4.925470
H	11.882397	20.444199	4.175917
C	14.569341	20.937666	4.540463
H	14.729025	21.481746	3.600600
H	14.376665	19.886459	4.297556
H	15.495956	20.985467	5.123892
C	6.935820	21.127139	5.036318
C	5.549168	21.161290	5.256713
H	5.131490	21.990943	5.820435
C	4.732938	20.144917	4.769692
H	3.663388	20.178187	4.963418
C	5.276816	19.097618	4.023842
H	4.635745	18.312115	3.632257
C	6.649836	19.075042	3.775814
H	7.083185	18.270394	3.186260
C	7.478029	20.074301	4.280164
H	8.545318	20.058590	4.081360
N	7.703087	22.204429	5.480569
C	8.737157	22.113470	6.232121
S	9.338073	20.606208	6.981521

Table S7. Frequencies of the stationary points optimized for 2+ PhNCS, obtained with B3PW91-PCM method.

Species	Frequencies (cm ⁻¹)										
2	16	20	24	27	35	38	42	49	52	53	57
	59	70	91	91	93	101	106	124	131	140	142
	160	169	178	183	186	187	200	219	229	231	231
	232	237	240	241	251	259	263	287	288	292	293
	299	303	303	304	331	334	343	347	348	356	357
	364	366	387	390	394	415	417	418	421	449	450
	462	473	479	480	500	501	506	514	541	555	557
	586	588	605	608	623	630	631	656	663	679	681
	703	704	759	770	774	778	804	818	820	825	826
	831	836	839	843	843	857	857	927	933	933	936
	937	938	944	947	951	954	957	957	958	959	968
	968	968	970	977	977	1000	1000	1015	1015	1045	1046
	1047	1051	1051	1057	1057	1058	1060	1060	1075	1079	1080
	1110	1110	1111	1112	1188	1188	1197	1201	1203	1206	1211
	1212	1217	1235	1235	1237	1238	1245	1246	1272	1272	1284
	1285	1334	1335	1335	1335	1366	1375	1380	1393	1398	1401
	1403	1411	1411	1412	1412	1417	1419	1423	1424	1441	1442
	1446	1446	1478	1480	1489	1489	1498	1500	1502	1502	1506
	1506	1507	1508	1511	1511	1511	1513	1521	1522	1523	1524
	1524	1524	1525	1527	1530	1533	1535	1540	1543	1544	1551
	1551	1635	1635	1660	1662	1694	1974	3045	3045	3047	3047
	3050	3050	3056	3056	3060	3060	3061	3062	3118	3118	3120
	3120	3123	3123	3123	3123	3126	3127	3129	3129	3134	3134
	3138	3138	3139	3139	3146	3149	3157	3157	3167	3167	3195
3195	3203	3203	3213	3213	3221	3221	3229	3229	3242	3242	
3246	3246	3265	3266								
PhNCS	34	60	248	362	394	415	435	479	506	627	698
	699	770	846	926	949	975	1003	1016	1059	1112	1192
	1203	1306	1342	1377	1499	1540	1645	1665	2226	3207	3216
	3226	3234	3238								
TS4	-274	10	16	22	22	25	27	29	33	39	47
	49	52	58	62	67	72	72	79	85	90	95
	101	107	111	116	132	139	145	151	158	172	178
	196	197	203	210	223	229	231	234	238	243	245
	247	254	256	268	270	277	293	295	298	300	308
	318	325	332	335	346	350	350	353	360	364	365
	368	370	387	394	409	413	415	418	419	422	447
	448	460	460	471	479	481	493	500	504	508	525
	534	548	559	561	575	601	606	610	623	627	630
	665	670	671	685	692	701	702	704	710	728	769
	771	774	776	778	826	829	829	834	839	841	844
	853	856	856	858	861	873	929	933	933	934	936
	939	944	946	947	953	954	956	956	958	959	967
	967	969	972	974	977	978	995	998	999	1004	1013
	1015	1017	1049	1050	1052	1052	1056	1057	1057	1059	1059
	1062	1064	1081	1082	1110	1110	1111	1112	1115	1186	1189
	1190	1198	1202	1202	1204	1207	1214	1214	1227	1235	1235
	1238	1239	1246	1247	1254	1272	1273	1285	1287	1319	1334
	1335	1335	1337	1342	1373	1374	1379	1395	1401	1403	1404
	1413	1413	1416	1417	1418	1420	1423	1424	1444	1445	1447
1449	1479	1480	1487	1488	1498	1501	1502	1503	1503	1506	
1507	1508	1510	1511	1511	1512	1513	1523	1523	1524	1524	

	1526	1526	1531	1532	1535	1537	1538	1538	1541	1545	1550
	1553	1590	1631	1636	1647	1659	1661	1662	1722	2004	2106
	3044	3045	3048	3049	3052	3054	3054	3056	3057	3061	3061
	3061	3119	3119	3121	3122	3122	3124	3125	3126	3126	3126
	3130	3130	3132	3135	3138	3139	3145	3146	3147	3148	3150
	3158	3163	3167	3190	3196	3197	3203	3205	3209	3212	3216
	3217	3222	3223	3225	3228	3229	3238	3238	3246	3247	3248
	3265	3275									
4	12	18	21	25	29	31	38	40	45	46	47
	51	53	63	70	72	75	82	91	93	97	104
	108	115	129	142	144	153	168	172	176	185	187
	195	205	218	224	229	233	238	243	244	247	249
	254	262	268	279	285	289	298	298	300	301	305
	314	334	337	343	349	352	355	357	363	365	370
	384	390	395	396	412	416	419	420	426	431	447
	449	459	474	479	482	499	500	513	521	547	558
	559	580	584	604	607	617	628	628	631	646	661
	664	669	678	683	689	704	705	706	770	774	776
	779	783	801	826	829	830	833	835	843	846	847
	851	859	861	864	869	916	929	932	935	937	939
	941	946	948	953	954	958	958	959	959	964	967
	967	968	971	971	981	987	997	1005	1012	1015	1015
	1047	1048	1050	1052	1054	1054	1056	1057	1058	1058	1060
	1076	1080	1084	1109	1112	1115	1116	1119	1142	1185	1190
	1190	1200	1202	1204	1208	1215	1216	1217	1233	1234	1234
	1238	1245	1246	1252	1273	1274	1285	1285	1299	1323	1332
	1333	1337	1340	1352	1374	1377	1378	1394	1398	1403	1406
	1413	1414	1415	1417	1421	1423	1424	1426	1446	1448	1449
	1451	1476	1479	1489	1490	1494	1500	1500	1502	1503	1505
	1506	1506	1507	1507	1509	1511	1514	1521	1523	1524	1525
	1526	1528	1530	1533	1533	1534	1535	1535	1539	1542	1545
	1550	1554	1634	1638	1639	1647	1660	1665	1671	1696	1995
	3046	3047	3049	3049	3052	3056	3058	3059	3060	3063	3063
	3064	3120	3121	3122	3124	3124	3126	3126	3127	3129	3130
	3130	3131	3134	3135	3139	3140	3145	3146	3149	3154	3157
	3157	3157	3160	3192	3195	3199	3200	3203	3207	3214	3214
	3216	3222	3222	3225	3228	3242	3253	3256	3256	3256	3266
	3271	3275									

Table S8. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for **2+PhNCS**, obtained with B3PW91-PCM method

species	E	H	G (sol)
2	-2107.417494(0.0)	-2107.36972(0.0)	-2107.474980(0.0)
PhNCS	-722.407403	-722.398896	-722.426730
2+PhNCS	-2829.824897(0.0)	-2829.768616(0.0)	-2829.901710(0.0)
TS4	-2829.781603(27.2)	-2829.72552(27.0)	-2829.848040(33.7)
4	-2829.866021(-25.8)	-2829.81032(-26.2)	-2829.931030(-18.4)

Table S9. The energies, zero-point (vibrational) energy (ZPE) and entropies (at 298 K) for **2+PhNCS**, obtained with B3PW91-PCM(+D3)/6-31G(d) method.

species	E ^a	ZPE ^b	S (sol) ^c	G ^d
2	-2108.401824	0.822061	243.163	-2107.637244(0.0)
PhNCS	-722.518593	0.101896	61.209	-722.436023
2+PhNCS	-2830.920417	0.923957	304.372	-2830.073267(0.0)
TS4	-2830.896865	0.925418	287.278	-2830.037885(22.2)
4	-2830.985653	0.928257	281.786	-2830.122403(-30.8)

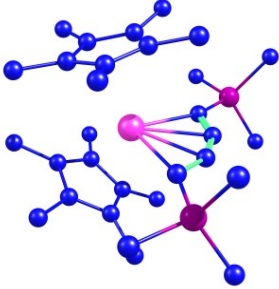
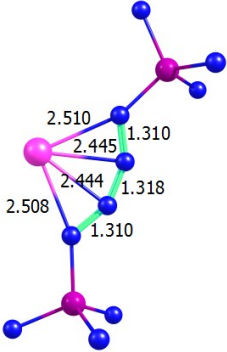
a. Values (in a.u.) calculated with B3PW91-PCM+D3/6-31G(d)+ECP60MWB method.

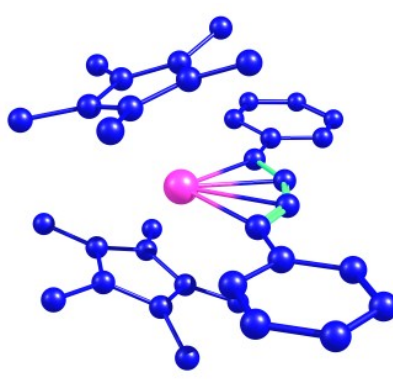
b. Values (in a.u.) calculated with B3PW91-PCM/6-31G(d)+ ECP60MWB method.

c. Values (in cal·mol⁻¹·K⁻¹) calculated with B3PW91-PCM/6-31G(d)+ ECP60MWB method.

d. Values (in a.u.) calculated with B3PW91-PCM/6-31G(d)+ ECP60MWB method, the values in parathesis are relative Gibbs free energies.

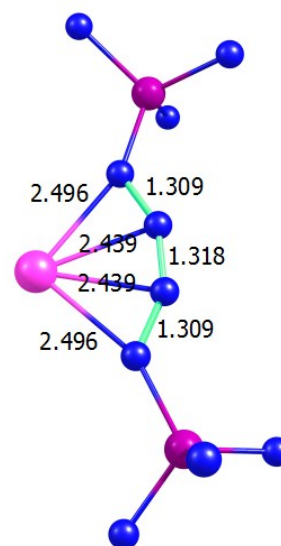
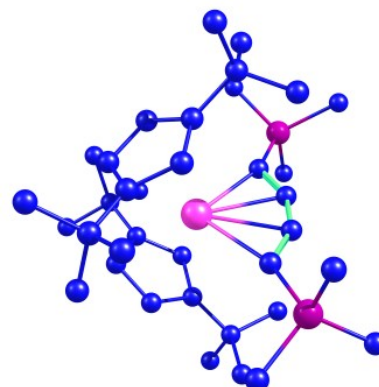
Table S10. The optimized Cartesian Coordinates (in Å) and structure (the hydrogen atoms omitted for clarity) of ($\eta^5\text{-C}_5\text{Me}_5$)₂U($\eta^2\text{-C}_4\text{TMS}_2$), ($\eta^5\text{-C}_5\text{Me}_5$)₂U($\eta^2\text{-C}_4\text{Ph}_2$) and [$\eta^5\text{-1,3-(Me}_3\text{C)}_2\text{C}_5\text{H}_3$]₂U[$\eta^4\text{-C}_4(\text{SiMe}_3)_2$] (**3**), obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
Cp* ₂ U(C ₄ TMS ₂)	C	5.279645	2.797718	12.903115	
	C	6.349673	3.698678	12.635168	
	C	6.424861	3.895294	11.227506	
	C	5.396043	3.120874	10.620876	
	C	4.694368	2.436076	11.654799	
	C	4.767015	2.429702	14.265619	
	H	4.092923	3.204964	14.657543	
	H	5.579977	2.311054	14.990116	
	H	4.207729	1.489451	14.248745	
	C	7.122889	4.475290	13.658368	
	H	8.128769	4.729704	13.308771	
	H	7.226907	3.919806	14.594120	
	H	6.616425	5.422969	13.895465	
	C	7.323747	4.894908	10.557127	
	H	7.309396	4.794967	9.468322	
	H	8.367593	4.807792	10.883243	
	H	7.007727	5.921985	10.788753	
	C	4.949554	3.172628	9.187511	
	H	4.737892	2.180180	8.771742	
	H	5.691955	3.648528	8.541993	
	H	4.021495	3.754960	9.094884	
	C	3.430824	1.652336	11.451398	
	H	2.558536	2.320225	11.390287	
	H	3.247735	0.954577	12.272632	
	H	3.450363	1.071069	10.522558	
	C	8.371541	-0.844929	10.312987	
	C	9.456877	-0.042521	10.759886	
	C	9.408339	1.194535	10.058461	
	C	8.304174	1.147807	9.155681	
	C	7.653652	-0.109104	9.327504	
	C	8.143556	-2.280829	10.683839	
	H	8.795705	-2.944194	10.096607	
	H	7.111219	-2.589303	10.492604	
	H	8.353619	-2.472957	11.741296	
	C	10.549848	-0.506015	11.676436	
	H	11.270899	-1.135919	11.135171	
	H	10.165572	-1.099174	12.512825	
	H	11.108943	0.333864	12.098833	
	C	10.441075	2.284062	10.102847	
	H	10.006877	3.273100	9.919448	
H	10.954535	2.326006	11.068278		
H	11.213211	2.130178	9.334689		
C	8.084602	2.114320	8.028230		
H	8.782350	1.901129	7.205035		
H	8.256881	3.153609	8.324656		
H	7.075335	2.050016	7.613884		
C	6.497536	-0.633663	8.522782		
H	6.012176	0.159255	7.944866		
H	5.729010	-1.094032	9.154190		
H	6.823819	-1.399847	7.805363		
C	10.999254	3.270636	14.193520		
H	11.740317	3.623172	14.921717		

	H	10.408364	4.136822	13.875393	
	H	11.547942	2.899588	13.320276	
	C	11.013878	0.450345	15.426625	
	H	11.526901	0.028816	14.555700	
	H	10.418223	-0.348323	15.883913	
	H	11.779733	0.756228	16.150838	
	C	9.135623	2.588065	16.554622	
	H	9.916276	2.800037	17.296490	
	H	8.450030	1.852234	16.990645	
	H	8.576228	3.515109	16.389996	
	C	8.576963	1.358813	13.777516	
	C	7.721929	0.379993	13.941408	
	C	6.728266	-0.376453	13.520054	
	C	5.844105	-0.722407	12.617652	
	C	3.261475	-1.681946	13.986685	
	H	2.676794	-0.802109	13.696296	
	H	3.710349	-1.479744	14.966079	
	H	2.562530	-2.520011	14.103304	
	C	3.763531	-2.416927	11.037299	
	H	2.974469	-3.172959	11.135998	
	H	4.476001	-2.783931	10.289359	
	H	3.301600	-1.504101	10.644528	
	C	5.452884	-3.706655	13.268344	
	H	5.921113	-3.569547	14.250081	
	H	6.234528	-4.014002	12.564941	
	H	4.732396	-4.530393	13.350020	
	Si	9.920090	1.924480	14.963036	
	Si	4.590804	-2.117212	12.709073	
	U	7.155607	1.214469	11.714112	
Cp* ₂ U(C ₄ Ph ₂)	C	6.543237	13.855547	14.644952	
	C	7.592038	13.585839	15.567991	
	C	7.117422	13.895347	16.876523	
	C	5.773757	14.356945	16.762174	
	C	5.416607	14.318412	15.381729	
	C	6.674650	13.847718	13.150314	
	H	7.078953	14.806753	12.793904	
	H	5.713284	13.697555	12.650513	
	H	7.349093	13.060213	12.800441	
	C	8.994116	13.193735	15.200997	
	H	9.015807	12.488372	14.362739	
	H	9.516211	12.721656	16.038479	
	H	9.582565	14.072375	14.899935	
	C	7.945055	13.935627	18.129179	
	H	8.748366	13.193625	18.115949	
	H	7.344583	13.753453	19.027635	
	H	8.413694	14.922616	18.257304	
	C	4.995603	15.010129	17.868121	
	H	5.112989	14.492960	18.827089	
	H	3.926071	15.061082	17.648104	
	H	5.340133	16.042874	18.024303	
	C	4.144012	14.833637	14.770321	
	H	4.295231	15.826880	14.323973	
	H	3.344764	14.935367	15.510284	
	H	3.770758	14.184983	13.967877	
	C	4.502814	9.715488	17.703405	
	C	4.024548	10.949009	18.228924	
	C	3.181800	11.550493	17.250165	
	C	3.155191	10.692296	16.111152	

	C 3.967579 9.556503 16.393145 C 5.272340 8.671236 18.458318 H 5.925031 9.105506 19.220905 H 5.903174 8.070091 17.796035 H 4.586605 7.980223 18.970420 C 4.241290 11.440112 19.631807 H 3.500118 11.009966 20.320974 H 4.150548 12.528504 19.708638 H 5.227917 11.160753 20.017338 C 2.259338 12.714777 17.467824 H 2.145289 13.336779 16.573529 H 2.596347 13.360828 18.282686 H 1.252699 12.361505 17.735780 C 2.263427 10.873969 14.915796 H 2.623853 10.316443 14.046517 H 2.173445 11.926448 14.620384 H 1.243876 10.519878 15.128529 C 4.111819 8.330722 15.537926 H 5.110784 7.888605 15.619287 H 3.390031 7.556851 15.836733 H 3.938983 8.548845 14.479959 C 8.434249 10.556704 19.391573 H 7.605241 11.229362 19.592853 C 9.306784 10.197571 20.415088 H 9.153911 10.589075 21.417750 C 10.374895 9.338624 20.154891 H 11.057576 9.057683 20.952745 C 10.562602 8.841175 18.862520 H 11.393030 8.171175 18.653149 C 9.689969 9.197850 17.841312 H 9.833646 8.809625 16.836054 C 8.604536 10.064610 18.084967 C 7.680497 10.441944 17.028239 C 7.600800 10.078145 15.761995 C 6.990210 10.157455 14.606147 C 6.009057 10.656201 13.878674 C 5.619395 10.436976 12.495769 C 4.521379 11.123235 11.946210 H 3.974577 11.822303 12.572989 C 4.133734 10.918956 10.624816 H 3.282370 11.461554 10.221347 C 4.835813 10.021227 9.820127 H 4.533960 9.860286 8.788368 C 5.929812 9.330014 10.347721 H 6.481370 8.629009 9.725868 C 6.317088 9.534441 11.666742 H 7.167644 8.996961 12.078480 U 5.731391 11.647975 16.116951	
3	C 7.530638 -0.680483 4.795585 C 7.113921 0.583035 4.304663 H 6.375120 1.218251 4.776117 C 7.724113 0.846751 3.048164 C 8.590044 -0.250234 2.791910 H 9.192806 -0.390846 1.901967 C 8.479397 -1.179038 3.861498 H 8.970894 -2.143398 3.909077 C 6.886423 -1.465214 5.938493 C 6.319126 -2.775218 5.352820	

H	7.114084	-3.407095	4.941508
H	5.604250	-2.567964	4.548583
H	5.802325	-3.349599	6.132374
C	5.722636	-0.676881	6.555021
H	5.262874	-1.257269	7.363864
H	4.945525	-0.463934	5.812026
H	6.058385	0.275782	6.978682
C	7.881010	-1.822535	7.053378
H	8.730548	-2.393606	6.665463
H	7.390842	-2.435070	7.820999
H	8.268395	-0.922466	7.543758
C	7.241763	1.890438	2.045854
C	5.930785	1.350357	1.430490
H	6.095395	0.381152	0.945612
H	5.544171	2.049005	0.676895
H	5.160020	1.216488	2.197999
C	6.945069	3.244217	2.707706
H	6.218025	3.147279	3.521334
H	6.522381	3.936599	1.968835
H	7.852768	3.699112	3.115527
C	8.253325	2.100036	0.914280
H	9.205523	2.466373	1.308667
H	7.871567	2.837931	0.198049
H	8.442560	1.172151	0.362175
C	10.267794	3.303087	4.326942
C	10.937396	2.675113	3.393139
C	11.315169	5.005713	1.406588
H	10.312491	4.873687	0.984508
H	11.953446	5.437695	0.625550
H	11.240031	5.733860	2.222622
C	12.180976	2.158255	0.590795
H	11.221657	2.002352	0.085514
H	12.547874	1.179348	0.918119
H	12.888170	2.545514	-0.153472
C	13.747876	3.692159	2.757688
H	14.399879	4.142099	1.998275
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H	13.692212	4.383412	3.606248
Si	12.029514	3.369925	2.032340
U	9.884146	0.954958	4.863912
C	9.499028	3.303481	5.398103
C	8.830130	2.675910	6.332681
C	8.456231	5.003349	8.323006
H	9.457344	4.867006	8.747387
H	7.817555	5.436328	9.103159
H	8.536090	5.732568	7.508377
C	7.580181	2.158072	9.132525
H	8.540955	1.988343	9.630591
H	7.197453	1.184786	8.806643
H	6.883827	2.553783	9.882572
C	6.021379	3.700297	6.965571
H	5.369713	4.150527	7.725121
H	5.537916	2.781401	6.616007
H	6.080470	4.393405	6.118772
Si	7.737599	3.371069	7.692817
C	12.238250	-0.679422	4.932388
C	12.654312	0.584133	5.423784
H	13.392944	1.219806	4.952682



C	12.043675	0.847148	6.680221
C	11.178154	-0.250277	6.935867
H	10.575205	-0.391468	7.825567
C	11.289569	-1.178755	5.866095
H	10.798838	-2.143518	5.818265
C	12.883235	-1.463804	3.789779
C	13.459268	-2.768994	4.377758
H	12.668829	-3.403758	4.793301
H	14.175318	-2.555298	5.179262
H	13.976995	-3.342992	3.598529
C	14.040752	-0.671084	3.167199
H	14.499333	-1.250052	2.356694
H	14.820356	-0.454163	3.906425
H	13.698660	0.279781	2.744671
C	11.886866	-1.829778	2.679340
H	11.040951	-2.403081	3.071897
H	12.377407	-2.443107	1.912614
H	11.493952	-0.933373	2.186668
C	12.525094	1.890821	7.682977
C	13.836803	1.351880	8.297749
H	13.673392	0.382197	8.782079
H	14.222774	2.050506	9.051698
H	14.607592	1.219352	7.530029
C	12.820116	3.245241	7.021690
H	13.547112	3.149426	6.207882
H	13.242171	3.937812	7.760747
H	11.911810	3.699233	6.614211
C	11.513589	2.098642	8.814976
H	10.560823	2.464182	8.421215
H	11.894785	2.836535	9.531495
H	11.325643	1.170223	9.366626