

Supporting Information for

Preparation of a potassium chloride bridged thorium phosphinidide complex and its reactivity towards small organic molecules

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1. Figures

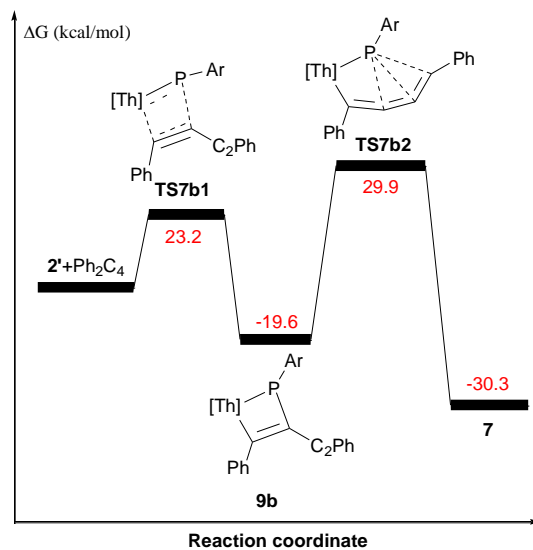


Figure S1. Energy profile (kcal/mol) for the reaction of $2 + \text{Ph}_2\text{C}_4$ (computed at $T = 298$ K). [Th] = $[\eta^5\text{-}1,3\text{-(Me}_3\text{C)}_2\text{C}_5\text{H}_3]_2\text{Th}$. Ar = 2,4,6- t -Pr $_3$ C $_6$ H $_2$.

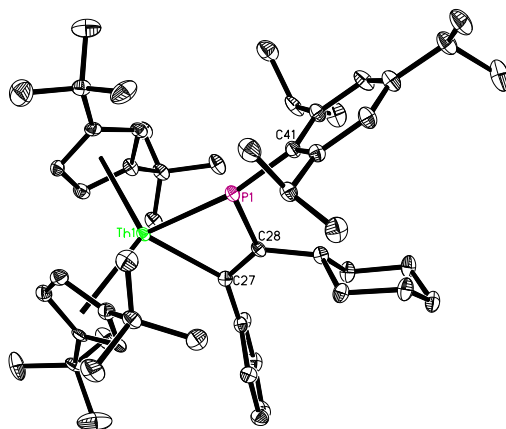


Figure S2 Molecular structure of **5a** (thermal ellipsoids drawn at the 35% probability level).

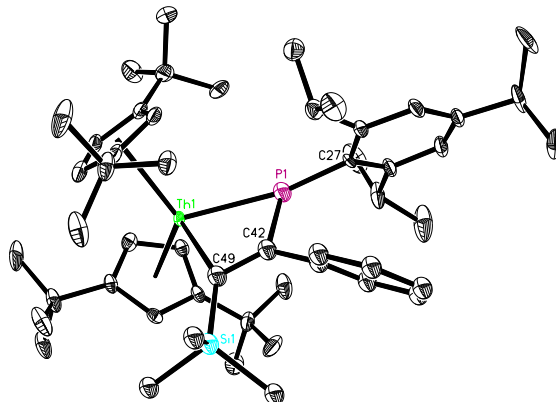


Figure S3 Molecular structure of **6b** (thermal ellipsoids drawn at the 35% probability level).

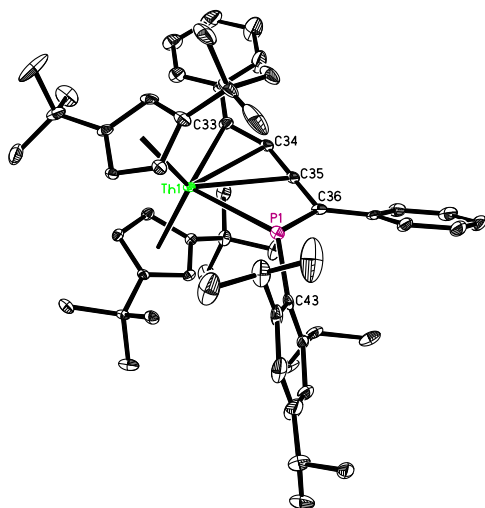


Figure S4 Molecular structure of **7** (thermal ellipsoids drawn at the 35% probability level).

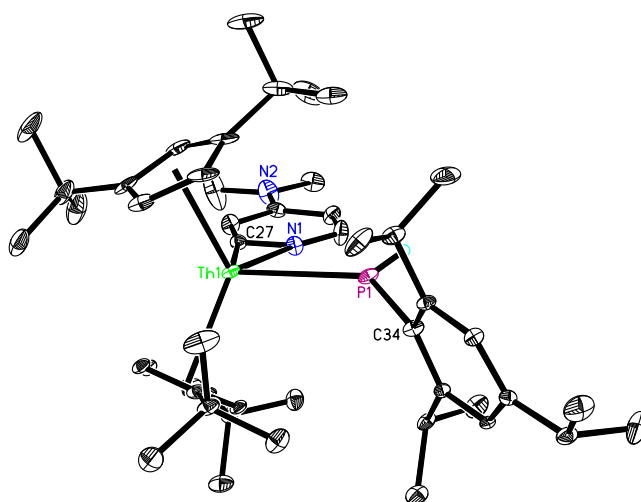


Figure S5 Molecular structure of **14** (thermal ellipsoids drawn at the 35% probability level).

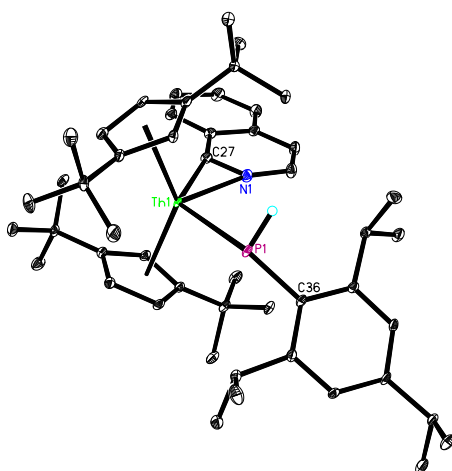


Figure S6 Molecular structure of **15** (thermal ellipsoids drawn at the 35% probability level).

2. Crystal parameters

Table S1. Crystal Data and Experimental Parameters for Compounds 2-5

Compound	2 $2C_6H_6$	3	4a	5a
Formula	$C_{94}H_{142}Cl_2K_2P_2Th_2$	$C_{56}H_{75}PTh$	$C_{50}H_{73}PTh$	$C_{55}H_{81}PTh$
Fw	1947.19	999.16	937.09	1005.20
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	$P2_1/c$	$P2_1/c$	$P2_1/n$	$P2_1/n$
<i>a</i> (Å)	11.599(1)	11.993(1)	11.872(1)	10.943(1)
<i>b</i> (Å)	19.420(1)	17.917(1)	18.664(1)	23.039(1)
<i>c</i> (Å)	20.564(1)	24.087(1)	23.870(1)	19.901(1)
α (deg)	90	90	90	90
β (deg)	92.15(1)	102.41(1)	98.70(1)	90.37(1)
γ (deg)	90	90	90	90
<i>V</i> (Å ³)	4628.6(3)	5054.8(3)	5227.94(8)	5017.02(17)
<i>Z</i>	2	4	4	4
<i>D</i> _{calc} (g/cm ³)	1.397	1.313	1.191	1.331
$\mu(Mo/K\alpha)_{calc}$ (cm ⁻¹)	3.433	3.014	9.673	10.116
size (mm)	0.20 × 0.15 × 0.10	0.25 × 0.20 × 0.20	0.30 × 0.20 × 0.20	0.25 × 0.20 × 0.20
<i>F</i> (000)	1976	2040	1912	2064
2θ range (deg)	6.60 to 59.73	6.91 to 59.72	7.49 to 146.40	7.67 to 146.78
no. of reflns, collected	25377	2825	22145	37967
no of obsd reflns	11042	12102	10256	9973
no of variables	466	562	488	532
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.85	1.00, 0.63	1.00, 0.46	1.00, 0.50
<i>R</i>	0.047	0.041	0.027	0.043
<i>R</i> _w	0.064	0.061	0.068	0.110
<i>R</i> _{all}	0.071	0.063	0.030	0.048
Gof	1.01	1.03	1.04	1.03
CCDC	1904635	1904623	1904628	1904626

Table S2. Crystal Data and Experimental Parameters for Compounds 6-8

Compound	6b	7	8
Formula	C ₅₂ H ₇₉ PSiTh	C ₅₇ H ₇₅ PTh	C ₅₁ H ₈₃ P ₂ Si ₂ Th
Fw	995.25	1023.18	1015.36
crystal system	monoclinic	monoclinic	orthorhombic
space group	<i>P2₁/n</i>	<i>P2₁/c</i>	<i>P2₁2₁2₁</i>
<i>a</i> (Å)	14.445(1)	14.779(1)	10.493(1)
<i>b</i> (Å)	16.993(1)	16.968(1)	20.177(1)
<i>c</i> (Å)	20.973(1)	20.157(1)	24.535(1)
α (deg)	90	90	90
β (deg)	106.37(1)	100.28(1)	90
γ (deg)	90	90	90
<i>V</i> (Å ³)	4939.32(9)	4973.4(3)	5194.8(2)
<i>Z</i>	4	4	4
<i>D</i> _{calc} (g/cm ³)	1.338	1.366	1.298
μ (Mo/K α) _{calc} (cm ⁻¹)	10.493	3.065	2.977
size (mm)	0.10 × 0.10 × 0.10	0.25 × 0.20 × 0.20	0.25 × 0.10 × 0.10
<i>F</i> (000)	2040	2088	2088
2 θ range (deg)	6.81 to 144.07	6.61 to 59.65	6.41 to 59.67
no. of reflns, collected	21029	49330	35914
no of obsd reflns	9510	12321	12714
no of variables	462	580	533
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.89	1.00, 0.74	1.00, 0.86
<i>R</i>	0.057	0.038	0.036
<i>R</i> _w	0.142	0.062	0.050
<i>R</i> _{all}	0.065	0.060	0.043
Gof	1.05	1.04	1.01
CCDC	1904624	1904633	1904625

Table S3. Crystal Data and Experimental Parameters for Compounds 10-12

Compound	10	11	12 0.5C ₆ H ₆
Formula	C ₄₂ H ₅₂ Th	C ₉₆ H ₁₄₀ Cl ₂ K ₂ N ₂ P ₂ Th ₂	C ₄₅ H ₆₈ ClKPS ₂ Th
Fw	788.87	1997.21	1010.67
crystal system	monoclinic	monoclinic	monoclinic
space group	<i>P2₁/c</i>	<i>C2/c</i>	<i>P2₁/n</i>
<i>a</i> (Å)	11.177(1)	24.882(1)	12.034(1)
<i>b</i> (Å)	9.597(1)	11.683(1)	14.361(1)
<i>c</i> (Å)	33.637(1)	32.216(1)	27.388(2)
α (deg)	90	90	90
β (deg)	91.08(1)	92.28(1)	100.61(1)
γ (deg)	90	90	90
<i>V</i> (Å ³)	3607.41(16)	9357.9(4)	4652.6(4)
<i>Z</i>	4	4	4
<i>D</i> _{calc} (g/cm ³)	1.453	1.418	1.443
μ (Mo/K α) _{calc} (cm ⁻¹)	4.160	12.144	13.029
size (mm)	0.25 × 0.20 × 0.15	0.10 × 0.08 × 0.02	0.10 × 0.05 × 0.05
<i>F</i> (000)	1576	4040	2044
2 θ range (deg)	6.64 to 59.75	8.36 to 146.59	6.98 to 146.46
no. of reflns, collected	22887	17598	19129
no of obsd reflns	8853	9078	9071
no of variables	400	496	478
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.84	1.00, 0.93	1.00, 0.81
<i>R</i>	0.035	0.044	0.064
<i>R</i> _w	0.055	0.093	0.125
<i>R</i> _{all}	0.049	0.062	0.097
Gof	1.04	1.03	1.04
CCDC	1904630	1904627	1904629

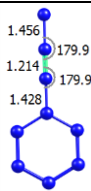
Table S4. Crystal Data and Experimental Parameters for Compounds 13-15

Compound	13	14	15
Formula	C ₄₅ H ₇₁ N ₂ PTh	C ₄₈ H ₇₅ N ₂ PTh	C ₅₀ H ₇₂ NPTh
Fw	903.04	943.11	950.09
crystal system	monoclinic	triclinic	triclinic
space group	<i>P2₁/c</i>	<i>P(-1)</i>	<i>P(-1)</i>
<i>a</i> (Å)	19.024(1)	10.605(1)	10.456(1)
<i>b</i> (Å)	10.958(1)	14.088(1)	13.392(1)
<i>c</i> (Å)	22.775(1)	17.095(1)	18.267(1)
α (deg)	90	79.43(1)	103.60(1)
β (deg)	110.36(1)	88.35(1)	101.98(1)
γ (deg)	90	70.87(1)	106.92(1)
<i>V</i> (Å ³)	4451.3(3)	2370.6(3)	2271.18(10)
<i>Z</i>	4	2	2
<i>D</i> _{calc} (g/cm ³)	1.348	1.321	1.389
μ (Mo/K α) _{calc} (cm ⁻¹)	3.416	3.210	11.148
size (mm)	0.25 × 0.20 × 0.20	0.30 × 0.25 × 0.20	0.20 × 0.15 × 0.15
<i>F</i> (000)	1840	964	968
2 θ range (deg)	6.66 to 59.85	6.63 to 59.56	7.27 to 146.31
no. of reflns, collected	30844	22442	15968
no of obsd reflns	10926	11321	8825
no of variables	465	493	500
abscorr (<i>T</i> _{max} , <i>T</i> _{min})	1.00, 0.93	1.00, 0.89	1.00, 0.57
<i>R</i>	0.040	0.056	0.032
<i>R</i> _w	0.057	0.112	0.079
<i>R</i> _{all}	0.062	0.070	0.032
Gof	1.04	1.09	1.02
CCDC	1904632	1904634	1904631

3. Computational details

Table S5. The optimized Cartesian Coordinates (in Å) of stationary points for 2'+PhCCMe, obtained with B3PW91-PCM method.

Species	Cartesian coordinates				
2'	C	8.070957	13.133265	14.745395	
	C	6.814200	13.113977	15.410977	
	H	5.879366	12.786719	14.974662	
	C	6.960762	13.620901	16.729691	
	C	8.342354	13.922118	16.894047	
	H	8.794292	14.364073	17.774753	
	C	9.015817	13.640394	15.677103	
	H	10.065997	13.820259	15.483502	
	C	8.304934	12.811050	13.272321	
	C	9.799531	12.829592	12.923422	
	H	10.250450	13.806942	13.128417	
	H	9.937821	12.617107	11.856915	
	H	10.363025	12.071378	13.483061	
	C	7.726235	11.433908	12.901523	
	H	8.236761	10.614095	13.429042	
	H	7.848233	11.244648	11.827780	
	H	6.659510	11.364200	13.136762	
	C	7.592837	13.887816	12.427796	
	H	6.514408	13.890970	12.619810	
	H	7.747331	13.702371	11.357212	
	H	7.979973	14.885974	12.661882	
	C	5.852213	13.987266	17.710105	
	C	5.731441	15.525886	17.726893	
	H	6.662443	15.996371	18.063858	
	H	4.927502	15.838047	18.405622	
	H	5.501637	15.911711	16.726995	
	C	6.184032	13.501470	19.131156	
	H	6.230588	12.405278	19.163476	
	H	5.407645	13.822382	19.836621	
	H	7.139733	13.904748	19.488012	
	C	4.506817	13.389389	17.280457	
	H	4.186422	13.783371	16.308588	
	H	3.731789	13.649270	18.011575	
	H	4.565735	12.297668	17.209349	
	C	11.023388	11.375170	18.006437	
	C	10.932364	10.047104	17.507984	
	H	11.595200	9.618005	16.762501	
	C	9.956984	9.310276	18.238930	
	C	9.380849	10.223317	19.159920	
	H	8.598719	9.996150	19.875492	
C	10.019380	11.487847	19.006140		
H	9.818138	12.363847	19.613620		
C	12.194876	12.319466	17.755753		
C	11.873605	13.770620	18.136305		
H	11.084298	14.193933	17.508676		
H	12.766791	14.394800	18.013094		
H	11.559486	13.852172	19.182976		
C	12.672759	12.267415	16.296410		
H	12.986183	11.257445	16.009479		
H	13.536466	12.928672	16.157123		
H	11.891102	12.589624	15.599818		
C	13.354166	11.835428	18.657559		
H	13.065219	11.863259	19.714180		
H	14.235955	12.475911	18.526265		

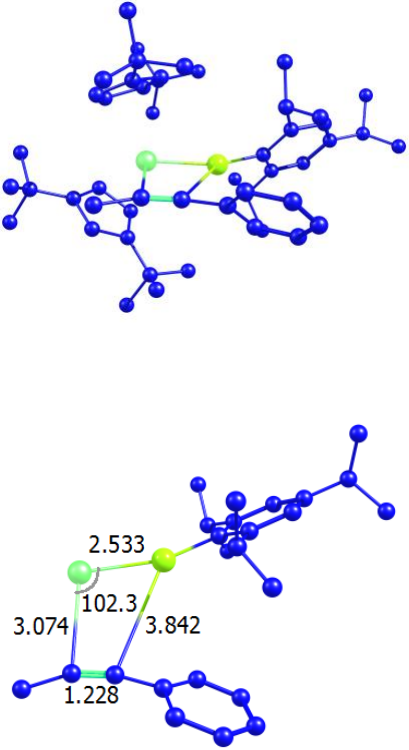
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PhCCMe	C 15.444614 -0.133992 9.031285 C 16.404072 0.164835 9.712369 C 17.532026 0.517826 10.513769 C 18.830187 0.129601 10.134692 C 17.364812 1.260871 11.696776 C 19.926346 0.476770 10.918358 C 18.466094 1.604091 12.474901 C 19.749675 1.214370 12.089852	

	H 18.966005 -0.444430 9.222563	
	H 16.365081 1.563423 11.994986	
	H 20.923495 0.169924 10.612953	
	H 18.321602 2.178621 13.386349	
	H 20.607992 1.483991 12.699714	
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	H 14.586007 -0.676482 7.175026	
	H 13.808818 -1.403174 8.590552	
	H 13.542490 0.306630 8.215745	
TS4a	C 3.385105 3.725627 17.373232	
	C 4.676733 4.236201 17.082749	
	H 5.236669 4.035967 16.179066	
	C 5.165072 4.974499 18.192619	
	C 4.127202 4.972791 19.162572	
	H 4.188796 5.403796 20.153331	
	C 3.038209 4.211987 18.664007	
	H 2.134560 3.973878 19.212300	
	C 2.683658 2.628966 16.577996	
	C 3.623831 1.404648 16.530342	
	H 4.552717 1.634386 15.997587	
	H 3.135174 0.568237 16.013881	
	H 3.887709 1.074672 17.541633	
	C 1.386257 2.193426 17.271418	
	H 1.592645 1.746138 18.250672	
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	H 0.702979 3.034012 17.429200	
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	H 1.679494 3.899172 15.097352	
	H 1.958741 2.232332 14.561024	
	H 3.302705 3.385467 14.623790	
	C 6.600954 5.428928 18.433162	
	C 7.441953 5.326278 17.155217	
	H 7.514841 4.288289 16.808921	
	H 8.461974 5.679924 17.349504	
	H 7.015236 5.931826 16.348891	
	C 6.656227 6.872003 18.955353	
	H 6.261432 7.568776 18.207075	
	H 7.692097 7.159550 19.176512	
	H 6.078271 6.988293 19.879740	
	C 7.212284 4.492879 19.497952	
	H 6.673049 4.562960 20.449646	
	H 8.261540 4.757673 19.682067	
	H 7.177606 3.448378 19.167026	
	C 2.222202 9.321628 17.907480	
	C 1.190088 8.500375 18.440387	
	H 0.150092 8.534466 18.136695	
	C 1.682337 7.748307 19.544103	
	C 3.066232 8.043407 19.633577	
	H 3.751845 7.668269 20.382486	
	C 3.398423 8.997766 18.633088	
	H 4.374750 9.448117 18.500281	
	C 2.014032 10.521179 16.985391	
	C 3.343674 11.217711 16.679053	
	H 3.829543 11.577567 17.593682	
	H 3.170012 12.085572 16.031257	
	H 4.027373 10.537733 16.162263	
	C 1.348140 10.138472 15.656626	
	H 2.000109 9.479039 15.074480	
	H 1.146194 11.038288 15.061304	
	H 0.394750 9.623896 15.815903	
	C 1.100461 11.519381 17.729075	
	H 0.113913 11.086547 17.930955	

H	0.956172	12.425547	17.126520
H	1.540476	11.814606	18.688711
C	0.809188	7.052264	20.585838
C	0.054387	8.159485	21.356206
H	0.757101	8.851251	21.834774
H	-0.579065	7.720439	22.138084
H	-0.586451	8.741915	20.685282
C	1.639850	6.257018	21.601407
H	2.177113	5.427036	21.132923
H	0.980584	5.832883	22.368430
H	2.370293	6.894581	22.112479
C	-0.228244	6.119173	19.943460
H	-0.864631	6.650153	19.228473
H	-0.880851	5.688781	20.713553
H	0.249379	5.287646	19.412762
C	6.071590	7.574015	14.195874
C	6.969273	8.670774	14.329987
C	8.062763	8.784828	13.466953
H	8.737427	9.631739	13.587749
C	8.328082	7.863089	12.456835
C	7.444416	6.790235	12.332200
H	7.624207	6.047622	11.556429
C	6.337542	6.623425	13.166479
C	6.796073	9.751016	15.385344
H	5.911559	9.477949	15.973323
C	7.989631	9.814640	16.347836
H	8.175854	8.840587	16.812651
H	7.801869	10.543699	17.146397
H	8.909195	10.120068	15.833243
C	6.533271	11.121615	14.746815
H	7.390995	11.456750	14.150299
H	6.348016	11.879967	15.517587
H	5.659817	11.088178	14.086074
C	9.529270	8.024337	11.543003
H	10.042484	8.948214	11.845691
C	10.528055	6.869568	11.705522
H	10.857368	6.775193	12.746245
H	11.414139	7.031075	11.079199
H	10.080099	5.913313	11.409243
C	9.114731	8.188821	10.074057
H	8.609364	7.289740	9.701097
H	9.992874	8.363708	9.440150
H	8.428582	9.033790	9.948424
C	5.464474	5.400522	12.928099
H	4.641615	5.456325	13.652197
C	4.863122	5.387305	11.515492
H	4.325861	6.317451	11.298881
H	4.163185	4.549736	11.399473
H	5.639166	5.272088	10.748962
C	6.231441	4.098440	13.197814
H	7.064462	3.970991	12.495452
H	5.571855	3.227943	13.088556
H	6.649970	4.088667	14.209936
C	1.864670	6.980251	13.256961
H	1.027939	6.982368	12.543115
H	2.573251	6.203087	12.964468
H	2.387130	7.938013	13.208441
C	1.332624	6.728086	14.598126
C	0.526480	6.459366	15.489873
C	-0.729132	6.205284	16.150847
C	-1.593539	7.269472	16.470507
H	-1.281789	8.288696	16.267551

	C -2.850849 7.019769 17.011418 H -3.507160 7.853864 17.245344 C -3.272864 5.709610 17.243108 H -4.254916 5.518442 17.666819 C -2.431492 4.647545 16.912261 H -2.758124 3.622792 17.067962 C -1.173719 4.889739 16.367787 H -0.539605 4.059988 16.076691 P 4.618874 7.395673 15.318010 Th 3.069330 6.634368 17.197473	
4a	C 3.701616 3.702099 17.992027 C 4.987573 4.213076 17.657629 H 5.511475 4.020469 16.730711 C 5.517669 4.946370 18.754504 C 4.524633 4.932220 19.764307 H 4.606155 5.388678 20.744351 C 3.411801 4.183227 19.299140 H 2.527826 3.950469 19.881851 C 2.956883 2.605500 17.239539 C 3.549387 1.253936 17.696121 H 4.622723 1.202189 17.481540 H 3.055404 0.422778 17.176228 H 3.413793 1.110522 18.774345 C 1.456549 2.606746 17.556800 H 1.264499 2.493805 18.629825 H 0.964309 1.769328 17.047217 H 0.976473 3.530102 17.216443 C 3.143361 2.734725 15.721570 H 2.778134 3.700605 15.354165 H 2.592007 1.939812 15.204188 H 4.196669 2.640871 15.436629 C 6.924614 5.517047 18.895980 C 7.704799 5.410954 17.579689 H 7.824755 4.366141 17.270512 H 8.707664 5.837706 17.701505 H 7.199739 5.952778 16.772251 C 6.886370 6.991832 19.332740 H 6.410509 7.623539 18.570775 H 7.904169 7.373659 19.483377 H 6.341693 7.118794 20.275288 C 7.665591 4.701541 19.975559 H 7.166833 4.780842 20.948213 H 8.695134 5.064170 20.091562 H 7.705852 3.640416 19.704063 C 2.595680 9.151021 18.792137 C 1.347340 8.478300 18.677407 H 0.548459 8.752925 17.998915 C 1.250965 7.471463 19.680608 C 2.488808 7.465971 20.365249 H 2.750739 6.827847 21.199566 C 3.315389 8.482152 19.819270 H 4.302485 8.746333 20.182641 C 2.948324 10.501907 18.180909 C 4.462503 10.749428 18.197773 H 4.860987 10.743485 19.218871 H 4.686999 11.731987 17.765201 H 4.995715 9.991706 17.613536 C 2.426999 10.635195 16.743503 H 2.874744 9.878470 16.090600 H 2.674624 11.626277 16.343622 H 1.337088 10.528171 16.699889 C 2.269881 11.583234 19.051431	

H	1.181400	11.456354	19.060085
H	2.494415	12.584694	18.661603
H	2.623962	11.532639	20.087581
C	-0.004766	6.688933	20.044386
C	-1.136451	7.690546	20.350712
H	-0.857772	8.358619	21.174016
H	-2.050901	7.156332	20.638663
H	-1.370838	8.309230	19.477761
C	0.224698	5.830594	21.296037
H	1.012828	5.084933	21.141603
H	-0.694721	5.291480	21.553238
H	0.505104	6.445682	22.159073
C	-0.440094	5.784186	18.883691
H	-0.663074	6.363111	17.982825
H	-1.337895	5.211623	19.150645
H	0.349576	5.064683	18.632707
C	5.669874	7.526072	14.088842
C	6.269484	8.772714	13.772779
C	7.093595	8.868470	12.645944
H	7.554977	9.827060	12.414522
C	7.341539	7.790131	11.801316
C	6.745559	6.571068	12.127026
H	6.927099	5.707859	11.489963
C	5.931482	6.407316	13.250045
C	6.075777	10.029830	14.607037
H	5.329936	9.792440	15.373917
C	7.372537	10.422890	15.328167
H	7.737377	9.605569	15.960570
H	7.208785	11.300273	15.965650
H	8.167702	10.672090	14.614595
C	5.525957	11.200367	13.781116
H	6.232695	11.528472	13.009220
H	5.327580	12.061224	14.431079
H	4.588903	10.928985	13.282132
C	8.219732	7.945534	10.573021
H	8.597134	8.977692	10.575790
C	9.435585	7.009679	10.609635
H	10.029096	7.164464	11.517423
H	10.083249	7.187741	9.742833
H	9.130142	5.956839	10.584207
C	7.414782	7.751495	9.279652
H	7.013426	6.733117	9.212108
H	8.049075	7.919520	8.400802
H	6.569995	8.447353	9.229448
C	5.389808	5.010868	13.521148
H	4.772792	5.068987	14.424411
C	4.503745	4.490131	12.380919
H	3.664139	5.163591	12.181081
H	4.091957	3.507368	12.639675
H	5.070231	4.375030	11.448779
C	6.535921	4.026993	13.802290
H	7.185890	3.907145	12.927123
H	6.140293	3.035319	14.054207
H	7.159957	4.369598	14.634610
C	2.575513	7.690828	13.686600
H	1.565549	7.437477	13.352180
H	3.297469	7.319841	12.953368
H	2.675448	8.784205	13.690693
C	2.846985	7.139397	15.073095
C	1.865925	6.613952	15.872826
C	0.456857	6.560804	15.442641
C	-0.326168	7.728230	15.344658

	H 0.139007 8.689225 15.550150 C -1.671584 7.674926 14.984443 H -2.245922 8.596804 14.919202 C -2.279747 6.451289 14.702882 H -3.329238 6.408197 14.422887 C -1.518675 5.284577 14.780972 H -1.973253 4.322481 14.554114 C -0.174937 5.338743 15.146534 H 0.404028 4.420598 15.194981 P 4.640855 7.369099 15.614714 Th 3.308418 6.556188 17.807837	
TS4b	C 3.859400 3.529724 17.845482 C 5.196413 3.987144 17.711337 H 5.827075 3.830639 16.846582 C 5.608688 4.640022 18.903550 C 4.484196 4.632677 19.771729 H 4.470190 5.020185 20.781728 C 3.411288 3.961076 19.127901 H 2.449099 3.740175 19.577279 C 3.185482 2.514498 16.928688 C 3.715390 1.119821 17.330574 H 4.803999 1.066365 17.219432 H 3.267848 0.341938 16.698167 H 3.472135 0.893218 18.375100 C 1.660293 2.512685 17.089136 H 1.358481 2.325267 18.125988 H 1.218055 1.721773 16.471075 H 1.227821 3.465147 16.767960 C 3.533424 2.760940 15.453191 H 3.195326 3.746249 15.114844 H 3.055584 2.001616 14.821463 H 4.612590 2.701011 15.279556 C 7.028523 5.033303 19.298111 C 7.981959 4.976391 18.099172 H 8.045202 3.961772 17.688224 H 8.992061 5.267725 18.411704 H 7.660223 5.655084 17.302754 C 7.073059 6.444733 19.902451 H 6.739327 7.188005 19.167660 H 8.096651 6.699827 20.205290 H 6.438556 6.523081 20.793131 C 7.514608 4.023202 20.359825 H 6.886133 4.052094 21.257456 H 8.545653 4.251059 20.659808 H 7.492862 3.000365 19.966110 C 2.625216 9.050451 18.538751 C 1.662602 8.194420 19.144858 H 0.608016 8.181730 18.892751 C 2.239886 7.504179 20.244455 C 3.612171 7.873750 20.260091 H 4.351543 7.553951 20.984203 C 3.845401 8.824670 19.228886 H 4.790427 9.317036 19.032437 C 2.295575 10.209992 17.602611 C 3.545686 10.755438 16.903755 H 4.273092 11.140073 17.627927 H 3.271489 11.585964 16.241362 H 4.038206 9.977041 16.310797 C 1.259709 9.817371 16.539411 H 1.644022 9.039991 15.871810 H 0.999585 10.689726 15.927007 H 0.331596 9.447580 16.991108	

C	1.692818	11.334632	18.474550
H	0.771105	11.004238	18.967569
H	1.454821	12.211375	17.858071
H	2.398302	11.646660	19.253115
C	1.442304	6.858625	21.377408
C	0.851062	8.017988	22.212811
H	1.647204	8.653072	22.617149
H	0.264049	7.626047	23.053886
H	0.195770	8.649270	21.602528
C	2.306647	5.999038	22.308885
H	2.661163	5.090895	21.812867
H	1.715758	5.687200	23.178668
H	3.174666	6.551523	22.685472
C	0.280513	5.998713	20.860089
H	-0.400771	6.572226	20.222045
H	-0.307192	5.610233	21.701025
H	0.648673	5.138739	20.289001
C	6.868014	7.512517	15.124783
C	7.676467	8.660947	15.352691
C	8.836122	8.853094	14.597013
H	9.447208	9.734585	14.789041
C	9.245171	7.964667	13.604689
C	8.441930	6.844647	13.383864
H	8.733625	6.130261	12.615364
C	7.277260	6.595263	14.113455
C	7.338927	9.709958	16.401787
H	6.396363	9.400387	16.869625
C	8.405043	9.775879	17.504149
H	8.547532	8.797372	17.975529
H	8.111703	10.491112	18.283428
H	9.375866	10.099079	17.107666
C	7.115562	11.091591	15.772505
H	8.027594	11.472347	15.295928
H	6.813227	11.819598	16.535739
H	6.330494	11.055051	15.009146
C	10.510443	8.214863	12.803758
H	10.949355	9.149835	13.180253
C	11.548566	7.102968	13.010621
H	11.792538	6.982340	14.071953
H	12.475645	7.330518	12.469839
H	11.176115	6.139397	12.642365
C	10.210935	8.415227	11.311391
H	9.777675	7.509736	10.869545
H	11.128618	8.650150	10.757804
H	9.499685	9.234424	11.157313
C	6.500521	5.327447	13.787513
H	5.617452	5.315289	14.439093
C	6.005912	5.311885	12.335693
H	5.397125	6.194314	12.116760
H	5.391448	4.422071	12.149850
H	6.840717	5.291481	11.623419
C	7.326629	4.069096	14.088709
H	8.215603	4.008253	13.448244
H	6.731959	3.163964	13.910555
H	7.669030	4.056408	15.129036
C	-0.007020	5.845154	17.091987
H	-0.699645	5.124200	16.640921
H	-0.555643	6.777420	17.265371
H	0.299065	5.452011	18.064193
C	1.110849	6.086153	16.168816
C	1.729555	6.341914	15.139188
C	2.145541	6.561557	13.783484

	C 1.701606 5.649390 12.807821 H 1.151529 4.764882 13.115587 C 1.951601 5.888642 11.459674 H 1.605565 5.177011 10.714799 C 2.636740 7.038406 11.068001 H 2.827508 7.226342 10.014700 C 3.087419 7.942255 12.032943 H 3.633478 8.832442 11.733063 C 2.853502 7.706451 13.382937 H 3.234893 8.384260 14.139088 P 5.339190 7.231776 16.109418 Th 3.668476 6.434201 17.838047	
4b	C 4.052011 3.512227 18.259555 C 5.401522 3.965261 18.191712 H 6.064027 3.826827 17.347190 C 5.773456 4.556107 19.431451 C 4.622411 4.515500 20.258133 H 4.560992 4.859984 21.283455 C 3.572096 3.885851 19.541713 H 2.590652 3.660448 19.940752 C 3.370221 2.548112 17.296896 C 3.877261 1.127897 17.631889 H 4.964342 1.059173 17.511522 H 3.412723 0.387869 16.967217 H 3.635092 0.857339 18.666243 C 1.845029 2.569998 17.463378 H 1.540614 2.274440 18.473928 H 1.380389 1.864666 16.763730 H 1.438071 3.565860 17.258612 C 3.716976 2.862226 15.836964 H 3.397274 3.875009 15.569800 H 3.220921 2.149201 15.166651 H 4.794549 2.787622 15.657658 C 7.160308 5.018901 19.863255 C 8.116598 5.116262 18.667581 H 8.263094 4.139084 18.193692 H 9.099322 5.473188 18.998493 H 7.739360 5.811271 17.908158 C 7.095152 6.390317 20.557300 H 6.749576 7.172604 19.869073 H 8.090295 6.688170 20.910355 H 6.425601 6.378821 21.424533 C 7.720071 3.986464 20.863367 H 7.084765 3.910505 21.753167 H 8.728715 4.273180 21.187987 H 7.777975 2.992254 20.405935 C 2.927459 8.995066 19.186859 C 1.754025 8.191450 19.139978 H 0.914339 8.359256 18.474630 C 1.782004 7.236311 20.195126 C 3.031790 7.397018 20.845889 H 3.375167 6.844294 21.711408 C 3.733282 8.466513 20.230731 H 4.698361 8.846556 20.547714 C 3.118879 10.330394 18.480835 C 4.577988 10.796617 18.565627 H 4.888498 10.963134 19.603995 H 4.702872 11.745564 18.030357 H 5.254819 10.061167 18.117488 C 2.688098 10.258797 17.010602 H 3.290855 9.525300 16.466558 H 2.809439 11.237434 16.529245	

H	1.635525	9.970629	16.911001
C	2.233140	11.367025	19.206533
H	1.174345	11.090015	19.150286
H	2.350835	12.357557	18.748028
H	2.505669	11.446034	20.265381
C	0.583667	6.436652	20.699129
C	-0.470055	7.447838	21.201822
H	-0.055041	8.087514	21.989017
H	-1.341122	6.920425	21.611891
H	-0.817103	8.095420	20.389251
C	0.971307	5.533199	21.877981
H	1.749115	4.812887	21.604250
H	0.096923	4.968044	22.221953
H	1.339833	6.121419	22.726249
C	-0.058353	5.585175	19.593232
H	-0.367399	6.201103	18.741859
H	-0.953038	5.076994	19.974856
H	0.626875	4.815382	19.221332
C	6.515802	7.460434	14.798315
C	7.131632	8.728077	14.617136
C	8.122048	8.874025	13.639871
H	8.596818	9.845122	13.513671
C	8.526279	7.827122	12.816903
C	7.910175	6.590005	13.005432
H	8.216550	5.750369	12.385105
C	6.928224	6.377469	13.975626
C	6.801375	9.944519	15.468754
H	5.859080	9.725623	15.984841
C	7.874363	10.156568	16.546450
H	7.968499	9.273252	17.188499
H	7.625217	11.015926	17.181007
H	8.855047	10.345325	16.091957
C	6.593761	11.224500	14.648727
H	7.525354	11.586434	14.197636
H	6.216591	12.025534	15.295740
H	5.870074	11.070821	13.840610
C	9.602682	8.031153	11.766526
H	9.913295	9.083877	11.823938
C	10.841996	7.169136	12.046682
H	11.246346	7.368650	13.045256
H	11.629291	7.374382	11.311167
H	10.603968	6.100128	11.989625
C	9.069364	7.783757	10.348485
H	8.758074	6.740461	10.217422
H	9.844628	7.996241	9.602258
H	8.203626	8.419814	10.133762
C	6.401573	4.959876	14.132530
H	5.562864	4.994602	14.835146
C	5.887695	4.360517	12.816868
H	5.143621	5.009948	12.346658
H	5.422198	3.385246	13.004973
H	6.699681	4.198033	12.097918
C	7.486219	4.058547	14.741931
H	8.351771	3.978095	14.072956
H	7.102616	3.043994	14.908974
H	7.841915	4.455645	15.698246
C	1.147188	6.216817	15.852777
H	0.921447	5.161993	15.640335
H	0.923686	6.780658	14.937179
H	0.431117	6.528485	16.622573
C	2.563084	6.383380	16.340510
C	3.575406	6.874513	15.553235

	C	3.362019	7.244016	14.120805	
	C	2.839307	6.302282	13.220945	
	H	2.634927	5.293851	13.569707	
	C	2.588998	6.639296	11.891041	
	H	2.188107	5.889312	11.213147	
	C	2.847823	7.930497	11.433694	
	H	2.649582	8.196245	10.398376	
	C	3.365772	8.877522	12.317351	
	H	3.571172	9.888415	11.973230	
	C	3.629521	8.534904	13.641254	
	H	4.037744	9.278281	14.318986	
	P	5.332050	7.243842	16.198870	
	Th	3.895079	6.409431	18.322900	

Table S6. Frequencies of the stationary points optimized for **2'**+PhC₂Me.

Species	Frequencies (cm ⁻¹)													
2'	16	18	20	30	35	36	42	46	51	58	63	66	78	
	81	85	88	92	106	113	120	125	128	131	139	147		
	155	173	181	194	200	205	213	222	229	237	239	240		
	243	244	246	248	250	251	256	260	265	266	267	272		
	281	290	291	294	297	316	322	323	326	332	336	345		
	349	352	363	364	367	369	371	379	385	389	406	411		
	423	438	447	448	450	458	484	487	501	505	506	520		
	527	558	566	581	608	617	621	645	649	654	670	674		
	690	691	770	775	789	827	830	833	834	836	840	844		
	850	857	857	900	902	911	934	935	936	937	942	944		
	947	947	951	953	954	955	956	958	960	960	965	965		
	972	972	973	974	977	980	1048	1051	1053	1053	1055			
	1056	1062	1071	1075	1079	1083	1088	1100	1117	1122	1130			
	1139	1141	1143	1165	1190	1201	1201	1206	1214	1218	1224			
	1233	1241	1242	1244	1245	1248	1273	1274	1275	1287	1287			
	1289	1296	1333	1344	1349	1357	1366	1368	1376	1396	1398			
	1402	1403	1404	1413	1413	1414	1414	1415	1416	1417	1418			
	1421	1425	1429	1432	1433	1434	1442	1445	1450	1453	1471			
	1475	1476	1484	1501	1501	1503	1504	1506	1506	1507	1508			
	1508	1510	1511	1511	1512	1512	1512	1514	1514	1515	1521			
	1522	1523	1523	1524	1525	1525	1526	1528	1528	1530	1533			
	1536	1539	1543	1546	1549	1555	1588	1604	1608	1660	3035			
	3039	3041	3042	3043	3044	3045	3045	3046	3046	3046	3047			
	3050	3050	3051	3052	3053	3054	3056	3057	3063	3106	3111			
	3111	3112	3115	3116	3116	3117	3118	3119	3120	3120	3123			
	3123	3124	3124	3125	3126	3127	3129	3130	3131	3131	3132			
	3132	3133	3134	3134	3137	3138	3139	3139	3141	3145	3145			
	3159	3170	3172	3222	3237	3245	3255	3264	3270					
	PhCCMe	21	92	96	249	295	395	404	411	521	547	633	706	716
		772	857	929	974	998	1001	1015	1057	1060	1063	1111		
		1190	1208	1309	1337	1373	1433	1489	1494	1495	1543	1637		
		1670	2353	3047	3117	3122	3197	3205	3216	3223	3228			
	TS4a	-72	18	23	25	29	34	36	41	45	49	53	54	
60		62	67	70	77	79	84	86	92	96	98	99		
101		105	114	122	130	133	143	144	150	160	172	177		
182		193	197	202	212	224	229	233	234	236	239	247		
247		248	250	251	251	259	259	260	263	270	272	275		
297		300	301	303	307	312	319	321	322	325	327	334		
338		349	350	352	357	358	365	368	373	381	384	392		
406		408	415	422	424	426	436	449	449	458	478	487		
500		502	505	511	516	527	558	560	583	607	611	622		
632		643	648	655	662	668	683	686	706	725	766	771		
778		790	831	831	832	834	838	842	857	857	858	865		
873		901	904	915	932	935	937	937	938	939	943	945		
949		950	953	954	956	957	959	959	961	966	966	970		
972		972	972	974	975	980	985	1003	1016	1035	1048			
1051		1052	1053	1056	1058	1059	1061	1063	1063	1069	1080			
1083		1089	1094	1112	1117	1118	1132	1137	1139	1140	1163			
1191		1192	1199	1204	1207	1210	1217	1218	1222	1236	1236			
1243		1243	1246	1248	1271	1272	1273	1275	1279	1286	1288			
1294		1337	1337	1343	1343	1356	1362	1364	1370	1374	1390			
1399		1403	1404	1405	1413	1413	1415	1415	1415	1416	1417			
1418		1419	1422	1424	1425	1434	1435	1437	1442	1444	1448			
1449		1469	1471	1475	1482	1482	1488	1488	1500	1502	1503			
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1513		1514	1514	1515	1521	1523	1524	1524	1525	1525	1526			
1526		1528	1529	1530	1531	1532	1535	1536	1538	1539	1544			
1550		1554	1566	1602	1635	1660	1663	2219	3040	3041	3043			
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		3137	3138	3138	3138	3141	3143	3147	3148	3148	3151	3153	
		3155	3171	3178	3183	3204	3212	3225	3236	3246	3248	3249	
		3250	3267	3273	3274								
4a	17	20	24	30	33	34	37	43	46	49	51	53	63
		68	73	79	81	85	85	90	91	95	106	110	114
		126	128	131	137	142	146	154	170	172	182	187	192
		197	201	204	216	229	230	233	239	243	244	245	247
		248	251	253	256	261	263	267	273	275	284	293	294
		297	298	303	309	319	323	327	328	340	341	345	353
		358	361	363	367	373	376	381	386	393	414	417	418
		421	441	444	446	450	464	477	488	498	500	506	516
		526	528	551	561	566	575	585	612	614	621	632	650
		654	662	671	677	691	694	695	717	774	777	778	787
		831	832	833	837	838	841	843	852	855	857	859	860
		903	907	919	921	938	939	939	940	942	943	945	947
		949	951	952	956	959	960	960	961	965	967	969	969
		971	972	974	974	975	980	989	1011	1040	1050	1050	
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		1101	1105	1118	1119	1123	1132	1137	1139	1143	1168	1184	
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		1243	1245	1249	1271	1274	1278	1288	1288	1292	1298	1327	
		1343	1344	1351	1357	1364	1368	1370	1372	1395	1399	1400	
		1404	1406	1411	1412	1413	1415	1415	1416	1417	1418	1421	
		1421	1422	1425	1435	1436	1437	1443	1447	1448	1449	1471	
		1478	1482	1483	1485	1486	1499	1501	1501	1502	1502	1505	
		1506	1506	1507	1507	1508	1510	1510	1511	1512	1512	1513	
		1513	1514	1516	1521	1521	1522	1523	1523	1524	1525	1526	
		1527	1529	1529	1530	1532	1535	1541	1541	1543	1550	1551	
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		3048	3050	3050	3050	3051	3051	3052	3053	3054	3055	3055	
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		3265	3272										
TS4b	-13	12	18	20	24	30	35	37	42	46	48	53	
		55	56	58	61	68	69	74	76	85	87	89	90
		103	113	118	126	127	130	139	147	152	154	161	174
		184	188	197	201	207	214	221	223	229	233	235	238
		241	245	246	247	251	251	252	257	258	266	267	270
		286	289	290	291	297	299	301	303	314	319	328	334
		340	343	344	353	361	363	366	368	380	382	386	389
		406	407	413	418	426	436	438	446	451	457	476	487
		500	501	511	511	529	537	559	560	583	605	613	621
		630	647	648	654	661	665	684	687	695	725	752	769
		771	773	818	826	829	831	833	837	841	844	849	858
		862	903	904	914	932	933	936	937	938	939	940	946
		947	948	953	954	955	957	958	960	961	965	967	968
		969	973	973	973	975	981	987	1002	1015	1037	1047	
		1051	1052	1053	1053	1054	1056	1057	1062	1071	1083	1084	
		1085	1088	1104	1113	1116	1120	1133	1138	1140	1141	1166	
	1191	1192	1200	1202	1205	1210	1215	1218	1227	1233	1238		
		1239	1244	1245	1249	1274	1274	1276	1281	1287	1288	1289	
		1298	1336	1341	1342	1352	1357	1365	1370	1375	1377	1397	
		1401	1402	1402	1405	1410	1413	1413	1414	1414	1415	1416	
		1418	1421	1422	1424	1434	1435	1435	1436	1443	1445	1446	
		1452	1472	1475	1476	1481	1488	1496	1497	1500	1501	1502	
		1503	1506	1506	1507	1508	1508	1508	1509	1510	1510	1512	
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	1549	1552	1572	1603	1636	1660	1664	2247	3040	3042	3042	
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	3116	3117	3118	3119	3119	3119	3120	3120	3123	3123	3123	
	3123	3124	3129	3129	3129	3131	3131	3131	3132	3132	3133	
	3133	3133	3134	3134	3136	3138	3144	3146	3146	3150	3151	
	3157	3167	3172	3175	3202	3212	3221	3229	3239	3239	3241	
	3246	3261	3274	3279								
4b	1620	25	28	37	41	44	46	48	54	59	62	66
	71	74	78	81	83	87	89	92	94	100	108	113
	122	130	132	137	141	144	147	167	177	181	183	188
	197	204	211	223	232	234	236	237	240	247	249	252
	255	256	260	261	264	265	266	271	275	285	296	299
	301	305	310	311	312	313	319	321	330	332	335	342
	344	350	356	360	366	367	368	371	380	390	392	418
	422	428	428	439	447	449	461	481	487	489	501	506
	506	529	544	558	559	582	604	611	616	621	633	650
	654	662	664	677	686	697	699	714	772	777	780	799
	830	830	832	835	836	842	847	857	859	860	870	882
	901	904	913	931	936	937	937	937	938	940	942	946
	948	950	952	956	958	960	960	962	965	966	967	969
	971	972	974	974	975	994	996	1015	1037	1048	1050	
	1050	1052	1053	1054	1055	1060	1060	1064	1084	1086	1091	
	1101	1111	1116	1127	1129	1134	1136	1140	1141	1170	1188	
	1192	1202	1203	1205	1210	1214	1220	1229	1230	1238	1239	
	1241	1242	1245	1246	1273	1275	1283	1287	1289	1289	1303	
	1339	1342	1346	1350	1354	1357	1360	1373	1375	1394	1397	
	1400	1402	1408	1410	1412	1413	1413	1414	1416	1416	1416	
	1417	1418	1421	1424	1435	1435	1436	1442	1443	1443	1448	
	1470	1474	1479	1484	1488	1488	1500	1501	1501	1502	1503	
	1505	1506	1506	1506	1507	1508	1508	1510	1511	1511	1512	
	1513	1513	1514	1518	1522	1522	1523	1523	1524	1525	1525	
	1525	1526	1528	1529	1530	1530	1531	1535	1538	1539	1544	
	1545	1552	1554	1613	1641	1663	1664	3026	3044	3045	3045	
	3045	3046	3047	3048	3050	3050	3050	3052	3053	3053	3055	
	3055	3056	3056	3058	3061	3065	3084	3094	3104	3117	3119	
	3119	3120	3120	3121	3122	3122	3123	3124	3124	3125	3125	
	3126	3127	3127	3128	3129	3129	3132	3133	3133	3134	3134	
	3134	3135	3136	3137	3141	3142	3143	3143	3147	3147	3150	
	3153	3187	3189	3191	3199	3213	3220	3228	3239	3241	3248	
	3263	3269	3276									

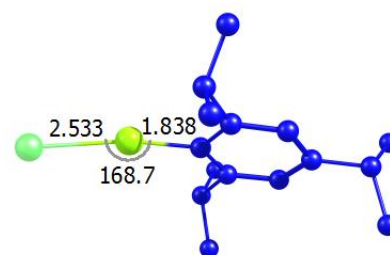
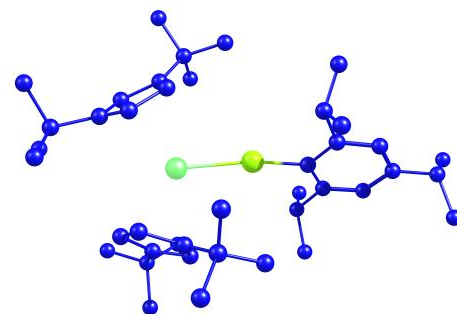
Table S7. The energies (with ZPE correction), enthalpies and free energies (in au at 298K) and corresponding relative values (in kcal/mol) for **2'**+PhC₂Me, obtained with B3PW91-PCM method

Species	E	H	G
2'	-2349.159052	-2349.106058	-2349.222640
PhCCMe	-347.441330	-347.432017	-347.461270
2'+PhCCMe	-2696.600382(0.0)	-2696.538075(0.0)	-2696.683910(0.0)
TS4a	-2696.581665(11.7)	-2696.519131(11.9)	-2696.654360(18.5)
4a	-2696.644418(-27.6)	-2696.582465(-27.9)	-2696.715570(-19.9)
TS4b	-2696.576494(15.0)	-2696.513684(15.3)	-2696.647910(22.6)
4b	-2696.637640(-23.4)	-2696.575530(-23.5)	-2696.708710(-15.6)

^a : The relative energies in parentheses are with respect to the corresponding energies of **2'**+ PhCCMe.

Table S8. The optimized Cartesian Coordinates (in Å) of stationary points for **2'**+Ph₂C₄, obtained with B3PW91-PCM method.

Species	Cartesian coordinates			
2'	C	8.070957	13.133265	14.745395
	C	6.814200	13.113977	15.410977
	H	5.879366	12.786719	14.974662
	C	6.960762	13.620901	16.729691
	C	8.342354	13.922118	16.894047
	H	8.794292	14.364073	17.774753
	C	9.015817	13.640394	15.677103
	H	10.065997	13.820259	15.483502
	C	8.304934	12.811050	13.272321
	C	9.799531	12.829592	12.923422
	H	10.250450	13.806942	13.128417
	H	9.937821	12.617107	11.856915
	H	10.363025	12.071378	13.483061
	C	7.726235	11.433908	12.901523
	H	8.236761	10.614095	13.429042
	H	7.848233	11.244648	11.827780
	H	6.659510	11.364200	13.136762
	C	7.592837	13.887816	12.427796
	H	6.514408	13.890970	12.619810
	H	7.747331	13.702371	11.357212
	H	7.979973	14.885974	12.661882
	C	5.852213	13.987266	17.710105
	C	5.731441	15.525886	17.726893
	H	6.662443	15.996371	18.063858
	H	4.927502	15.838047	18.405622
	H	5.501637	15.911711	16.726995
	C	6.184032	13.501470	19.131156
	H	6.230588	12.405278	19.163476
	H	5.407645	13.822382	19.836621
	H	7.139733	13.904748	19.488012
	C	4.506817	13.389389	17.280457
	H	4.186422	13.783371	16.308588
	H	3.731789	13.649270	18.011575
	H	4.565735	12.297668	17.209349
	C	11.023388	11.375170	18.006437
	C	10.932364	10.047104	17.507984
	H	11.595200	9.618005	16.762501
	C	9.956984	9.310276	18.238930
	C	9.380849	10.223317	19.159920
	H	8.598719	9.996150	19.875492
	C	10.019380	11.487847	19.006140
	H	9.818138	12.363847	19.613620
C	12.194876	12.319466	17.755753	
C	11.873605	13.770620	18.136305	
H	11.084298	14.193933	17.508676	
H	12.766791	14.394800	18.013094	
H	11.559486	13.852172	19.182976	
C	12.672759	12.267415	16.296410	
H	12.986183	11.257445	16.009479	
H	13.536466	12.928672	16.157123	
H	11.891102	12.589624	15.599818	
C	13.354166	11.835428	18.657559	
H	13.065219	11.863259	19.714180	
H	14.235955	12.475911	18.526265	
H	13.639414	10.806050	18.413644	
C	9.776605	7.797487	18.174425	
C	9.556113	7.322144	16.728525	
H	8.615679	7.727258	16.330961	

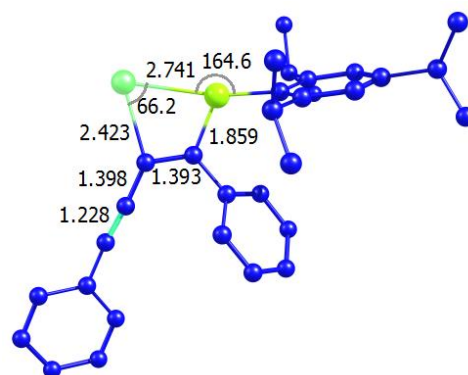
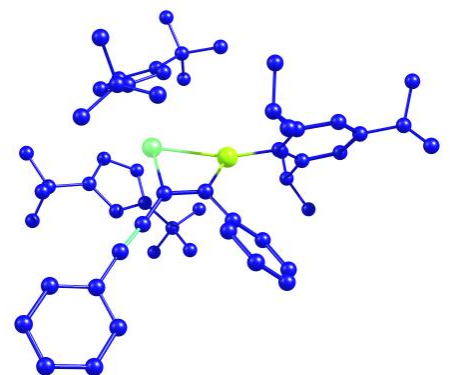


	H 9.490775 6.227529 16.690797 H 10.382646 7.622487 16.071472 C 11.066252 7.149125 18.721392 H 11.938607 7.415689 18.113324 H 10.973022 6.055639 18.719018 H 11.261223 7.472022 19.750647 C 8.591787 7.341506 19.033191 H 8.739960 7.600097 20.088512 H 8.482606 6.252034 18.971995 H 7.661789 7.803009 18.683159 C 4.537080 9.082728 17.020549 C 3.765507 8.825418 15.852164 C 2.468778 8.323376 15.974849 H 1.898029 8.132904 15.066953 C 1.878724 8.059763 17.212751 C 2.648608 8.304394 18.348272 H 2.211981 8.100308 19.325523 C 3.955138 8.797655 18.285439 C 4.309030 9.063355 14.451308 H 5.307002 9.502559 14.571879 C 3.456911 10.064163 13.660147 H 2.443793 9.684411 13.478381 H 3.910564 10.267985 12.681609 H 3.363415 11.014249 14.198335 C 4.475933 7.746232 13.681504 H 5.123807 7.051555 14.228033 H 4.923581 7.926921 12.695708 H 3.511507 7.247649 13.522090 C 0.459794 7.532597 17.328847 H 0.255313 7.392064 18.399906 C 0.293768 6.167532 16.646373 H 0.466012 6.240275 15.565641 H -0.721581 5.779652 16.795587 H 1.002441 5.434985 17.048506 C -0.567308 8.540860 16.793526 H -0.478701 9.505460 17.305664 H -1.589576 8.169266 16.937479 H -0.424889 8.718518 15.720616 C 4.699150 9.004553 19.596288 H 5.706339 9.354593 19.336867 C 4.850734 7.694539 20.381275 H 3.878666 7.295904 20.697214 H 5.450901 7.855418 21.285882 H 5.345640 6.926479 19.777025 C 4.039481 10.087837 20.460244 H 3.968943 11.036637 19.917360 H 4.619384 10.260051 21.376167 H 3.024372 9.799091 20.760404 P 6.237509 9.769065 16.890442 Th 8.353830 11.155126 16.767561	
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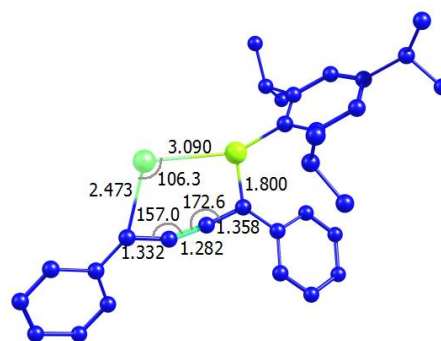
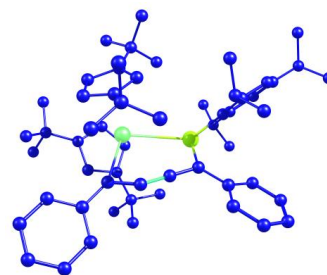
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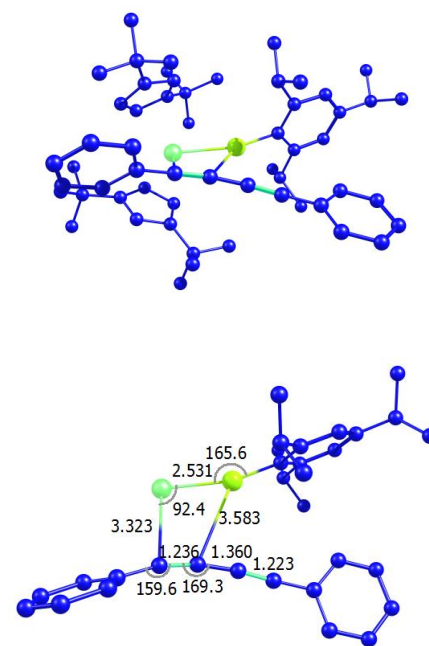
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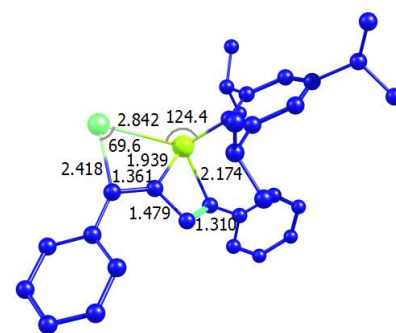
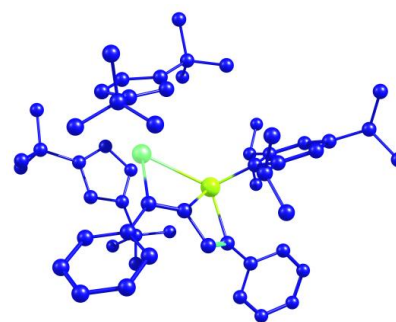


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H	3.872350	11.759798	14.735080
C	4.856732	9.143114	12.649457
H	5.483239	8.252192	12.755280
H	5.280338	9.770245	11.855697
H	3.862406	8.820138	12.317361
C	1.113706	7.104366	15.926797
H	0.909026	6.574526	16.867661
C	1.057632	6.071129	14.792856
H	1.241258	6.539053	13.818360
H	0.070494	5.594909	14.753190
H	1.809321	5.286504	14.932781
C	0.024121	8.171660	15.751761
H	0.040636	8.894280	16.575033
H	-0.969009	7.707310	15.723568
H	0.158663	8.726757	14.815702

	C	5.221035	7.892135	18.707496	
	H	6.214284	8.347398	18.627916	
	C	5.422142	6.397557	18.990487	
	H	4.466723	5.873799	19.115799	
	H	5.997737	6.259560	19.913618	
	H	5.968125	5.912414	18.174245	
	C	4.491055	8.584462	19.866829	
	H	4.391047	9.660962	19.686671	
	H	5.043148	8.445578	20.804614	
	H	3.483341	8.175598	20.010817	
	P	6.704542	9.698363	16.562890	
	Th	8.889298	11.216289	16.655007	
TS7b2	C	7.452992	11.331765	19.014816	
	C	6.094774	11.048215	18.692952	
	H	5.631570	11.234008	17.731379	
	C	5.409292	10.584565	19.851792	
	C	6.375175	10.508539	20.886094	
	H	6.187743	10.213294	21.911852	
	C	7.618910	10.959963	20.373833	
	H	8.524966	11.084928	20.954460	
	C	8.425588	12.180944	18.205676	
	C	9.885538	11.878430	18.568080	
	H	10.087248	12.053746	19.631349	
	H	10.554846	12.534736	17.998847	
	H	10.152502	10.844885	18.326505	
	C	8.231503	11.997754	16.696399	
	H	8.411123	10.961780	16.393035	
	H	8.932148	12.638972	16.147864	
	H	7.219571	12.278054	16.387229	
	C	8.129397	13.655913	18.560532	
	H	7.096426	13.922391	18.308977	
	H	8.799433	14.323316	18.003504	
	H	8.274801	13.841611	19.630978	
	C	3.909076	10.407629	20.043888	
	C	3.404280	11.588156	20.901075	
	H	3.883565	11.599441	21.886503	
	H	2.319495	11.514536	21.050796	
	H	3.616974	12.545768	20.412400	
	C	3.599648	9.096539	20.784884	
	H	3.924628	8.224298	20.202591	
	H	2.521160	8.996992	20.957201	
	H	4.094406	9.059089	21.762380	
	C	3.167826	10.426878	18.702811	
	H	3.313269	11.379937	18.181038	
	H	2.090345	10.305708	18.866776	
	H	3.501223	9.621118	18.040251	
	C	8.555960	7.451903	21.530635	
	C	8.978527	6.580475	20.485549	
	H	10.004544	6.459332	20.157279	
	C	7.896709	5.756229	20.073005	
	C	6.759616	6.196547	20.804429	
	H	5.758499	5.785993	20.735278	
	C	7.163543	7.225306	21.698094	
	H	6.518894	7.712905	22.420171	
	C	9.506178	8.165422	22.489942	
	C	8.775633	9.151239	23.410850	
	H	8.312714	9.971036	22.855290	
	H	9.484748	9.591023	24.122226	
	H	7.995642	8.650151	23.995463	
	C	10.640439	8.890557	21.748859	
	H	11.233656	8.195623	21.144237	
	H	11.322139	9.361213	22.467658	



H	10.262971	9.675726	21.084729
C	10.137932	7.070189	23.380379
H	9.366314	6.519970	23.930703
H	10.823034	7.520593	24.109974
H	10.703441	6.349093	22.780259
C	8.052745	4.443921	19.311423
C	9.026084	4.571362	18.131307
H	8.648046	5.254943	17.366257
H	9.174271	3.589148	17.665522
H	10.010002	4.931538	18.452117
C	8.638089	3.427134	20.319411
H	9.621757	3.747592	20.680868
H	8.753575	2.445799	19.841694
H	7.979966	3.308715	21.188059
C	6.708161	3.900251	18.815022
H	6.013783	3.724370	19.645208
H	6.859565	2.942052	18.304290
H	6.235742	4.587235	18.106776
C	11.064204	8.454813	17.522968
H	10.898776	8.332910	18.591011
C	12.362381	8.573825	17.033787
H	13.204543	8.541015	17.721264
C	12.580478	8.749608	15.666828
H	13.591903	8.855445	15.282183
C	11.488430	8.795721	14.799062
H	11.648064	8.935130	13.732252
C	10.191439	8.657784	15.286679
H	9.349411	8.673857	14.602983
C	9.949634	8.479580	16.663747
C	8.594220	8.344415	17.217521
C	7.606054	7.695532	16.543670
C	7.662508	6.817819	15.354730
C	6.659137	5.979075	15.434611
C	6.098615	4.799394	14.807027
C	6.925978	3.680118	14.596383
H	7.953324	3.715822	14.945687
C	6.439838	2.555269	13.937041
H	7.093431	1.701488	13.775938
C	5.119509	2.521599	13.485556
H	4.739894	1.641083	12.973328
C	4.290724	3.625934	13.688931
H	3.265048	3.610330	13.328758
C	4.773176	4.758062	14.339807
H	4.132993	5.623737	14.477247
C	4.389897	7.859909	16.152382
C	4.419301	8.731757	15.031586
C	3.240454	8.950225	14.311077
H	3.285278	9.609298	13.447165
C	2.021894	8.363288	14.644318
C	2.000216	7.553911	15.777891
H	1.055080	7.105333	16.075222
C	3.137692	7.291285	16.545276
C	5.655481	9.478558	14.546190
H	6.464592	9.313359	15.263784
C	5.406886	10.993835	14.482717
H	4.669924	11.253236	13.713668
H	6.336204	11.517793	14.232622
H	5.036984	11.385359	15.436874
C	6.129614	8.968736	13.176786
H	6.378249	7.904985	13.213537
H	7.026535	9.514112	12.858495
H	5.358263	9.122682	12.411960

C	0.764236	8.605499	13.829989
H	-0.037938	8.014677	14.294370
C	0.917248	8.118886	12.382304
H	1.696269	8.681264	11.853833
H	-0.020870	8.250855	11.829644
H	1.189014	7.058165	12.346296
C	0.333818	10.078959	13.871397
H	0.191241	10.421963	14.902175
H	-0.609138	10.221856	13.329819
H	1.086705	10.725540	13.404677
C	2.963594	6.380166	17.761652
H	3.808228	6.565435	18.437916
C	2.996462	4.891171	17.387010
H	2.181075	4.648399	16.694475
H	2.872957	4.270526	18.283238
H	3.937226	4.608301	16.906824
C	1.685915	6.680920	18.559577
H	1.577519	7.749569	18.768040
H	1.714007	6.146221	19.516452
H	0.784146	6.345523	18.034218
P	5.827976	7.134972	17.077711
Th	7.202639	8.446055	19.192138

Table S9. Frequencies of the stationary points optimized for for $2'+\text{Ph}_2\text{C}_4$.

Species	Frequencies (cm^{-1})											
2'	16	18	20	30	35	36	42	46	51	58	63	66
	78	81	85	88	92	106	113	120	125	128	131	
	139	147	155	173	181	194	200	205	213	222	229	
	237	239	240	243	244	246	248	250	251	256	260	
	265	266	267	272	281	290	291	294	297	316	322	
	323	326	332	336	345	349	352	363	364	367	369	
	371	379	385	389	406	411	423	438	447	448	450	
	458	484	487	501	505	506	520	527	558	566	581	
	608	617	621	645	649	654	670	674	690	691	770	
	775	789	827	830	833	834	836	840	844	850	857	
	857	900	902	911	934	935	936	937	942	944	947	
	947	951	953	954	955	956	958	960	960	965	965	
	972	972	973	974	977	980	1048	1051	1053	1053	1055	
	1056	1062	1071	1075	1079	1083	1088	1100	1117	1122	1130	
	1139	1141	1143	1165	1190	1201	1201	1206	1214	1218	1224	
	1233	1241	1242	1244	1245	1248	1273	1274	1275	1287	1287	
	1289	1296	1333	1344	1349	1357	1366	1368	1376	1396	1398	
	1402	1403	1404	1413	1413	1414	1414	1415	1416	1417	1418	
	1421	1425	1429	1432	1433	1434	1442	1445	1450	1453	1471	
	1475	1476	1484	1501	1501	1503	1504	1506	1506	1507	1508	
	1508	1510	1511	1511	1512	1512	1512	1514	1514	1515	1521	
	1522	1523	1523	1524	1525	1525	1526	1528	1528	1530	1533	
	1536	1539	1543	1546	1549	1555	1588	1604	1608	1660	3035	
	3039	3041	3042	3043	3044	3045	3045	3046	3046	3046	3047	
	3050	3050	3051	3052	3053	3054	3056	3057	3063	3106	3111	
	3111	3112	3115	3116	3116	3117	3118	3119	3120	3120	3123	
	3123	3124	3124	3125	3126	3127	3129	3130	3131	3131	3132	
	3132	3133	3134	3134	3137	3138	3139	3139	3141	3145	3145	
	3159	3170	3172	3222	3237	3245	3255	3264	3270			
	PhCCCCPh	13	27	34	82	95	190	213	232	312	406	406
463		473	512	518	557	620	631	649	675	702	702	
754		772	783	796	855	855	933	933	976	976	1004	
1004		1008	1014	1014	1059	1065	1113	1113	1193	1193	1209	
1211		1243	1338	1338	1375	1375	1400	1488	1489	1536	1550	
1634		1634	1666	1666	2249	2330	3201	3201	3210	3210	3220	
3220		3228	3228	3232	3232							
TS7a1	-56	12	13	20	21	27	29	31	32	36	42	
	47	54	55	58	59	60	63	64	69	72	75	
	77	86	88	89	94	96	105	113	123	126	129	
	131	140	149	159	166	178	182	188	195	199	207	
	223	227	228	230	234	234	240	242	244	248	248	
	250	251	257	260	263	264	265	267	271	291	293	
	296	299	300	305	318	318	319	324	326	336	338	
	347	352	354	358	365	367	369	373	379	383	393	
	403	407	407	409	429	430	436	448	449	455	458	
	473	479	484	485	499	502	507	513	528	533	552	
	559	561	581	598	606	613	621	630	633	645	647	
	655	664	667	681	683	685	699	701	770	770	771	
	775	786	794	830	830	831	834	836	841	851	854	
	856	857	865	869	902	903	915	934	936	936	937	
	937	939	941	942	946	948	948	954	955	957	958	
	959	960	961	965	966	968	971	972	973	974	977	
	978	980	1004	1006	1008	1014	1015	1050	1051	1052	1053	
	1054	1055	1056	1058	1059	1065	1068	1084	1084	1087	1099	
	1113	1114	1117	1122	1133	1138	1139	1142	1164	1191	1191	
	1192	1199	1203	1206	1208	1212	1215	1218	1225	1233	1234	
	1238	1242	1244	1245	1246	1273	1274	1275	1284	1287	1289	
	1297	1336	1338	1340	1344	1347	1357	1368	1369	1374	1375	
	1375	1389	1396	1397	1402	1403	1403	1412	1412	1413	1413	

		1414	1416	1416	1421	1421	1424	1424	1433	1434	1435	1446
		1447	1448	1448	1470	1474	1479	1483	1487	1487	1499	1500
		1502	1502	1504	1505	1505	1507	1507	1508	1510	1510	1511
		1511	1512	1512	1512	1515	1521	1522	1522	1522	1523	1523
		1525	1526	1526	1528	1529	1530	1530	1533	1535	1538	1543
		1544	1545	1549	1553	1560	1603	1633	1633	1660	1661	1664
		2189	2292	3040	3044	3044	3044	3044	3045	3046	3046	3047
		3047	3047	3050	3051	3052	3053	3055	3057	3057	3061	3063
		3065	3110	3113	3116	3117	3119	3119	3119	3120	3120	3120
		3122	3123	3124	3124	3124	3125	3127	3129	3129	3131	3132
		3132	3133	3133	3134	3136	3137	3138	3141	3142	3144	3146
		3146	3147	3149	3159	3171	3177	3203	3204	3212	3213	3221
		3221	3228	3229	3232	3233	3238	3247	3249	3264	3275	3278
9a	7	11	13	18	22	27	30	33	36	38	44	49
		50	53	56	58	60	62	70	72	74	79	84
		87	91	94	101	104	110	121	128	130	137	143
		147	150	173	177	182	188	192	199	203	209	227
		229	232	234	235	240	246	249	250	253	254	258
		259	260	262	264	273	274	291	295	295	299	310
		315	317	319	320	326	327	329	333	340	344	351
		352	355	365	366	368	369	381	388	391	409	413
		417	421	429	431	444	448	448	466	474	481	489
		491	498	500	513	522	526	543	552	560	580	584
		591	612	617	619	620	631	632	648	653	660	663
		677	685	694	705	707	721	760	770	772	780	784
		790	830	831	834	837	841	845	853	853	855	858
		860	862	901	903	904	914	921	935	936	936	937
		939	940	943	947	950	950	954	956	958	958	961
		961	962	965	966	966	971	971	971	974	975	975
		980	994	995	1012	1013	1037	1048	1050	1051	1052	1054
		1056	1057	1060	1061	1069	1083	1084	1085	1093	1095	1109
	1114	1119	1122	1133	1137	1138	1140	1168	1187	1188	1188	1192
		1201	1202	1205	1207	1209	1214	1215	1217	1226	1236	1239
		1239	1243	1247	1251	1272	1274	1277	1283	1288	1290	1303
		1308	1333	1340	1342	1344	1345	1356	1357	1358	1372	1374
		1375	1390	1398	1399	1402	1404	1411	1415	1415	1416	1416
		1417	1417	1417	1422	1423	1428	1436	1437	1437	1443	1447
		1449	1454	1456	1472	1477	1485	1487	1487	1488	1500	1502
		1503	1503	1505	1506	1506	1507	1508	1509	1510	1510	1510
		1512	1512	1512	1513	1515	1522	1523	1523	1523	1524	1525
		1526	1526	1527	1529	1530	1530	1531	1534	1536	1537	1543
		1545	1547	1550	1555	1613	1629	1640	1662	1662	1665	1732
		2239	3045	3045	3045	3046	3046	3048	3048	3050	3051	3051
		3051	3051	3051	3054	3054	3054	3057	3057	3058	3058	3091
		3114	3119	3120	3120	3121	3122	3123	3123	3123	3124	3125
		3125	3125	3126	3128	3128	3128	3129	3129	3130	3133	3133
		3134	3134	3135	3135	3136	3136	3138	3138	3138	3139	3145
		3146	3149	3153	3188	3189	3192	3193	3200	3202	3214	3215
		3222	3226	3227	3232	3234	3241	3252	3257	3263	3278	
TS7a2	-59	17	17	20	22	24	30	35	37	39	42	
	44	45	49	52	57	59	64	66	70	75	77	
	86	86	91	96	106	108	115	125	129	131	138	
	142	147	157	172	173	182	189	192	195	205	209	
	222	224	230	231	234	239	241	243	247	248	252	
	253	255	256	262	264	265	275	284	293	294	295	
	299	302	305	311	312	318	324	335	336	348	351	
	354	356	360	364	369	374	374	384	389	389	399	
	413	415	421	426	434	439	446	447	453	459	480	
	481	490	499	500	501	504	527	536	538	558	576	
	580	598	608	615	620	625	630	631	639	652	660	
	673	675	685	698	703	706	742	747	766	774	777	
	786	789	828	831	832	835	840	847	849	854	857	

	858	858	864	902	907	915	919	934	935	936	937
	939	941	941	947	949	950	952	955	957	959	959
	960	961	963	964	968	969	971	973	974	974	976
	977	977	993	994	1000	1010	1015	1048	1050	1053	1054
	1055	1058	1060	1060	1063	1063	1077	1081	1082	1087	1095
	1110	1115	1117	1117	1131	1133	1139	1142	1166	1187	1188
	1193	1199	1202	1204	1206	1208	1215	1215	1226	1229	1236
	1237	1240	1242	1246	1249	1272	1274	1275	1283	1286	1287
	1297	1306	1332	1334	1340	1343	1346	1357	1357	1359	1370
	1372	1379	1390	1397	1398	1399	1399	1413	1413	1414	1416
	1417	1417	1418	1420	1423	1426	1427	1434	1435	1436	1446
	1446	1448	1455	1469	1476	1478	1484	1487	1489	1500	1502
	1502	1502	1505	1506	1507	1507	1507	1508	1509	1510	1510
	1511	1511	1512	1512	1513	1520	1522	1522	1523	1523	1523
	1525	1525	1525	1526	1528	1529	1529	1531	1534	1534	1538
	1541	1543	1549	1551	1598	1609	1625	1640	1660	1661	1663
	1666	2132	3041	3042	3046	3046	3046	3048	3049	3049	3049
	3050	3053	3053	3053	3054	3055	3059	3061	3061	3063	3070
	3092	3117	3117	3118	3121	3122	3122	3122	3124	3124	3125
	3126	3126	3127	3127	3128	3129	3130	3130	3132	3132	3132
	3132	3133	3133	3133	3135	3135	3136	3139	3142	3145	3148
	3150	3151	3162	3163	3180	3183	3193	3194	3201	3203	3215
	3215	3221	3223	3226	3229	3239	3240	3246	3258	3273	3274
7	1618	20	27	28	32	34	35	36	39	44	49
	50	55	59	62	67	69	71	76	85	87	93
	101	105	106	116	127	128	130	133	141	143	146
	155	172	176	185	188	195	196	200	203	214	222
	228	232	235	238	240	242	244	246	247	249	252
	254	262	265	269	272	275	281	296	297	302	303
	305	310	311	317	325	333	337	340	345	352	353
	356	357	360	366	372	373	388	391	396	410	413
	420	420	423	440	445	446	448	460	470	473	480
	488	495	496	500	504	513	527	548	560	564	580
	593	605	613	619	628	629	638	639	651	660	667
	671	683	687	691	705	707	772	773	777	781	789
	829	831	831	832	834	837	844	849	853	856	857
	859	859	903	907	919	924	931	934	935	936	938
	940	941	942	948	948	950	952	953	956	957	959
	960	962	963	967	969	969	972	973	974	975	976
	976	995	1000	1013	1014	1024	1047	1049	1051	1053	1054
	1058	1059	1059	1060	1064	1072	1083	1084	1086	1097	1109
	1113	1114	1119	1130	1133	1139	1141	1166	1186	1189	1193
	1199	1202	1203	1205	1207	1214	1214	1227	1231	1235	1238
	1238	1241	1247	1249	1272	1273	1277	1284	1284	1287	1300
	1312	1333	1335	1337	1346	1346	1351	1358	1358	1372	1375
	1380	1392	1396	1399	1400	1404	1412	1413	1414	1415	1416
	1417	1417	1422	1423	1425	1427	1435	1436	1437	1446	1447
	1448	1455	1470	1477	1479	1483	1488	1491	1501	1502	1502
	1503	1505	1506	1506	1507	1508	1508	1509	1510	1511	1511
	1512	1512	1512	1513	1522	1523	1523	1523	1524	1525	1525
	1526	1527	1527	1528	1530	1530	1532	1532	1534	1538	1541
	1544	1550	1552	1606	1607	1611	1631	1641	1658	1662	1664
	2029	3043	3043	3046	3047	3047	3049	3049	3050	3051	3051
	3053	3054	3056	3056	3057	3057	3062	3064	3064	3065	3085
	3117	3118	3119	3121	3122	3122	3124	3124	3124	3125	3126
	3126	3127	3128	3129	3129	3131	3132	3132	3133	3133	3133
	3134	3134	3135	3135	3140	3140	3142	3147	3151	3153	3155
	3162	3164	3165	3180	3186	3190	3194	3197	3202	3208	3211
	3217	3221	3225	3232	3244	3249	3253	3265	3269	3280	
TS7b1	-42	14	20	21	24	29	30	31	35	37	43
	44	47	50	51	56	59	61	67	71	73	75
	78	83	86	90	92	94	101	110	112	124	129

	132	144	152	163	171	178	183	186	194	196	204	
	212	214	225	226	231	234	238	239	242	246	247	
	248	251	256	260	262	264	264	267	271	286	289	
	297	297	298	305	307	316	316	317	324	327	337	
	342	348	351	356	363	364	365	366	368	380	391	
	393	404	407	409	424	427	437	443	449	451	457	
	474	478	487	489	501	503	509	516	528	532	543	
	557	561	582	604	615	617	621	631	633	646	648	
	654	667	668	680	682	687	701	702	763	769	769	
	774	786	788	823	828	829	830	834	834	840	848	
	855	857	859	863	901	903	916	932	934	935	936	
	936	937	938	940	946	948	950	954	956	957	958	
	959	961	963	964	965	966	971	972	973	974	976	
	979	981	1006	1006	1009	1013	1016	1047	1051	1051	1052	
	1053	1054	1056	1058	1059	1063	1064	1083	1089	1091	1102	
	1109	1113	1116	1123	1131	1139	1140	1142	1163	1190	1191	
	1192	1200	1202	1206	1206	1209	1215	1220	1224	1233	1233	
	1236	1238	1243	1245	1246	1272	1274	1274	1286	1287	1289	
	1295	1336	1337	1338	1343	1351	1358	1361	1370	1372	1373	
	1376	1388	1398	1398	1403	1405	1406	1411	1413	1413	1414	
	1414	1415	1416	1419	1420	1424	1424	1433	1434	1435	1444	
	1446	1447	1449	1470	1472	1477	1484	1488	1488	1498	1498	
	1502	1503	1504	1504	1506	1506	1507	1507	1507	1509	1511	
	1511	1511	1511	1512	1512	1520	1521	1521	1522	1522	1523	
	1523	1524	1527	1527	1528	1529	1530	1531	1533	1535	1536	
	1542	1544	1546	1551	1554	1600	1633	1634	1658	1662	1665	
	2181	2297	3041	3043	3043	3043	3044	3045	3045	3046	3046	
	3046	3048	3051	3052	3053	3053	3056	3056	3059	3060	3061	
	3062	3111	3112	3115	3117	3117	3118	3119	3119	3121	3121	
	3121	3123	3123	3124	3125	3127	3127	3128	3131	3131	3131	
	3132	3132	3133	3134	3134	3135	3136	3138	3139	3142	3147	
	3152	3154	3160	3162	3168	3177	3201	3205	3211	3213	3220	
	3225	3227	3231	3233	3234	3240	3248	3252	3267	3272	3276	
9b	11	15	18	19	27	29	30	33	36	37	41	44
	49	51	57	60	63	68	71	75	82	84	88	
	89	91	95	97	104	110	122	130	130	136	140	
	146	146	162	176	179	185	191	201	203	214	223	
	228	230	231	233	234	239	240	246	247	248	252	
	254	257	259	263	265	271	278	285	289	291	296	
	297	298	300	302	319	327	337	339	342	345	351	
	356	362	366	367	368	377	380	384	390	409	412	
	415	416	421	433	436	437	449	449	453	481	482	
	487	503	503	505	509	521	528	547	558	559	581	
	590	607	615	622	624	630	632	652	656	663	666	
	671	684	686	700	705	709	761	763	773	774	777	
	783	817	826	828	832	832	833	836	843	844	857	
	860	861	880	903	905	919	926	934	935	936	938	
	939	940	941	943	946	948	953	954	957	957	959	
	960	961	965	965	968	970	970	973	973	974	976	
	979	991	1002	1013	1014	1034	1048	1051	1052	1052	1052	
	1053	1054	1060	1062	1064	1067	1079	1083	1088	1098	1110	
	1111	1115	1122	1132	1137	1138	1142	1168	1185	1190	1192	
	1201	1202	1205	1206	1209	1212	1217	1219	1226	1233	1239	
	1239	1241	1244	1245	1273	1273	1279	1287	1289	1290	1302	
	1324	1335	1336	1339	1345	1349	1353	1358	1367	1372	1372	
	1375	1394	1398	1400	1403	1406	1412	1413	1414	1414	1415	
	1415	1418	1419	1420	1423	1425	1434	1435	1438	1443	1445	
	1447	1447	1462	1473	1477	1478	1486	1486	1489	1501	1501	
	1502	1502	1505	1506	1506	1507	1508	1508	1510	1510	1510	
	1511	1511	1512	1513	1514	1521	1521	1522	1522	1523	1523	
	1523	1524	1527	1528	1529	1530	1531	1535	1536	1537	1540	
	1542	1546	1550	1552	1571	1611	1631	1634	1659	1661	1667	

	2282	3044	3044	3045	3046	3046	3047	3049	3049	3051	3051
	3052	3054	3054	3054	3054	3056	3058	3061	3063	3078	3091
	3118	3119	3119	3120	3120	3122	3122	3122	3123	3124	3125
	3125	3126	3126	3127	3128	3128	3129	3129	3129	3132	3132
	3133	3135	3135	3135	3137	3137	3138	3139	3141	3147	3147
	3153	3160	3162	3180	3188	3189	3195	3197	3206	3213	3217
	3223	3226	3229	3230	3232	3245	3250	3252	3260	3266	
TS7b2	-347	16	21	23	27	29	31	33	36	40	47
	49	55	58	63	67	73	75	77	78	83	87
	90	92	97	99	103	108	121	128	133	136	141
	144	147	153	168	175	181	187	189	194	201	203
	208	227	229	232	236	236	242	244	248	254	254
	255	256	261	263	268	270	272	281	283	289	292
	296	300	302	303	310	319	325	329	338	339	343
	348	350	355	362	364	367	368	372	382	389	392
	393	412	416	420	425	427	433	447	447	451	474
	481	483	493	503	508	522	528	551	557	559	560
	579	588	604	605	614	616	628	631	643	645	652
	670	674	686	688	703	706	728	763	773	775	783
	787	793	828	829	831	834	836	838	843	849	853
	858	858	864	877	900	905	915	921	934	935	936
	937	938	942	942	945	947	949	952	954	956	958
	959	960	962	963	964	964	970	970	972	974	976
	978	980	991	1000	1008	1013	1014	1043	1049	1050	1051
	1052	1056	1057	1058	1060	1062	1063	1080	1083	1090	1100
	1111	1111	1118	1121	1132	1134	1139	1144	1165	1186	1189
	1191	1200	1201	1203	1205	1209	1214	1215	1217	1227	1233
	1234	1240	1242	1245	1245	1250	1273	1275	1275	1283	1286
	1289	1304	1333	1337	1338	1344	1345	1347	1355	1368	1372
	1373	1373	1398	1399	1404	1406	1408	1413	1413	1414	1414
	1416	1417	1418	1420	1422	1424	1425	1435	1435	1438	1447
	1447	1448	1449	1465	1476	1477	1485	1486	1488	1499	1501
	1502	1503	1503	1504	1504	1506	1507	1508	1508	1509	1510
	1510	1511	1512	1515	1515	1516	1521	1522	1523	1524	1525
	1525	1527	1527	1528	1529	1529	1530	1531	1532	1534	1536
	1540	1542	1543	1546	1549	1553	1606	1634	1635	1660	1660
	1661	1730	3042	3045	3045	3046	3048	3048	3049	3050	3051
	3053	3054	3055	3055	3056	3057	3058	3059	3060	3063	3065
	3100	3119	3119	3120	3121	3122	3122	3123	3123	3123	3124
	3124	3125	3127	3127	3127	3128	3131	3131	3133	3133	3133
	3135	3135	3135	3136	3138	3141	3146	3148	3149	3151	3156
	3158	3160	3162	3169	3187	3194	3195	3195	3196	3205	3205
	3217	3218	3231	3233	3237	3244	3246	3247	3259	3259	3262

Table S10. The energies (with ZPE correction), enthalpies and free energies (in au at 298K) and corresponding relative values (in kcal/mol) for **2'**+Ph₂C₄, obtained with B3PW91-PCM method

Species	E	H	G
2'	-2349.159052	-2349.106058	-2349.222640
PhCCCCPh	-615.165353	-615.151483	-615.191730
2+PhCCCCPh	-2964.324405(0.0)	-2964.257541(0.0)	-2964.414370(0.0)
TS7a1	-2964.306480(11.2)	-2964.238809(11.7)	-2964.383680(19.2)
9a	-2964.375125(-31.8)	-2964.307630(-31.4)	-2964.452850(-24.1)
TS7a2	-2964.364772(-25.3)	-2964.298020(-25.4)	-2964.440780(-16.6)
7	-2964.386801(-39.2)	-2964.319768(-39.0)	-2964.462670(-30.3)
TS7b1	-2964.300259(15.2)	-2964.232342(15.8)	-2964.377410(23.2)
9b	-2964.367938(-27.3)	-2964.300096(-26.7)	-2964.445560(-19.6)
TS7b2	-2964.291409(20.7)	-2964.224718(20.6)	-2964.366730(29.9)

^a : The relative energies in parentheses are with respect to the corresponding energies of **2'**+ PhCCCCPh.