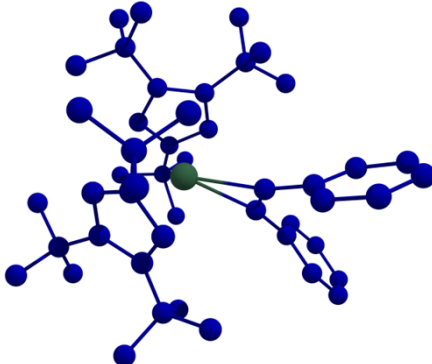
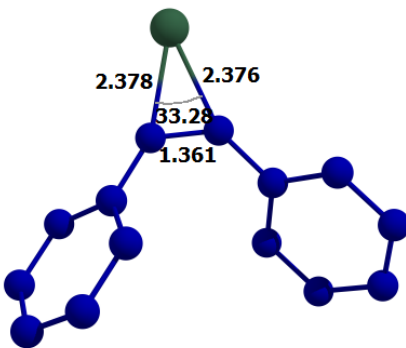


Supporting Information for

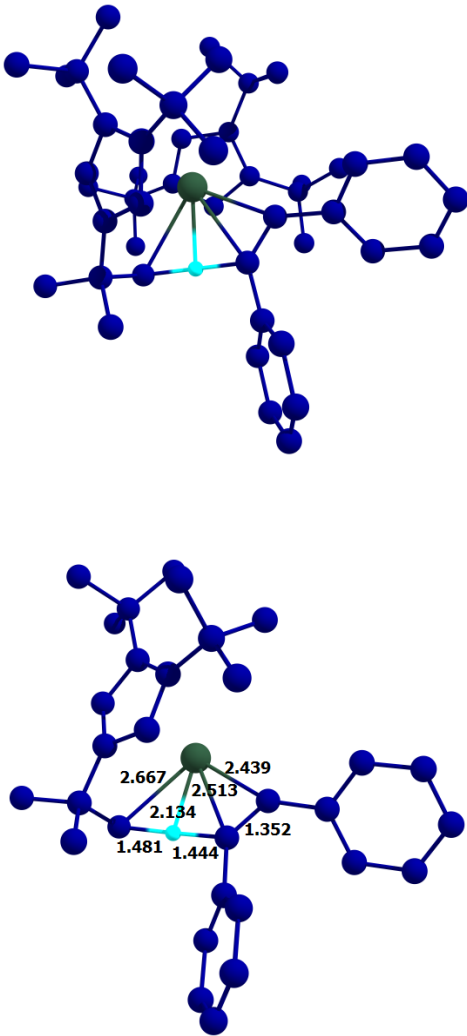
**C-H Bond Activation Induced by Thorium
Metallacyclopropene Complexes: A Combined
Experimental and Computational Study**

Bo Fang, Lei Zhang, Guohua Hou, Guofu Zi,* De-Cai Fang,* and Marc D. Walter*

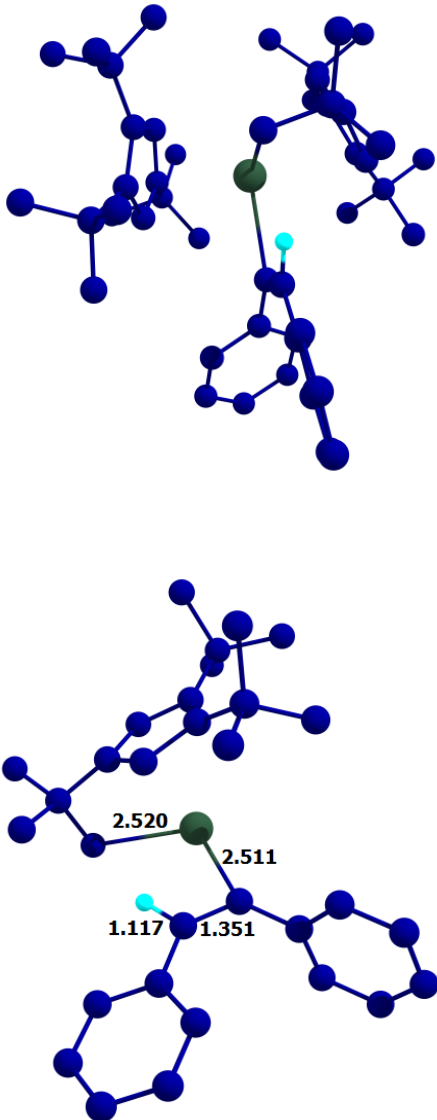
Table S1. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for conversion of **2**, obtained with B3PW91-PCM/6-31G(d)+sdd method.

Species	Cartesian coordinates				
2	C	-0.50362	2.89095	-0.23088	
	C	-1.89087	2.49331	-0.05584	
	C	-2.25016	1.78102	-1.24194	
	H	-3.24399	1.40789	-1.44960	
	C	-1.17650	1.74063	-2.15577	
	C	-0.10101	2.39133	-1.50580	
	H	0.87329	2.55223	-1.94313	
	C	0.42330	3.84235	0.55696	
	C	-0.17912	5.26117	0.60756	
	H	-1.09470	5.31485	1.19979	
	H	-0.40973	5.62106	-0.40194	
	H	0.54212	5.95545	1.05722	
	C	0.74562	3.35335	1.97984	
	H	1.38030	4.08635	2.49441	
	H	1.29971	2.40826	1.94788	
	H	-0.14464	3.20580	2.59188	
	C	1.77981	3.98520	-0.16053	
	H	2.43681	4.62708	0.43782	
	H	1.67570	4.44929	-1.14781	
	H	2.27806	3.01788	-0.27878	
	C	-3.03518	2.95026	0.87864	
	C	-3.67089	4.21789	0.26115	
	H	-4.52410	4.54933	0.86754	
	H	-4.03283	4.01247	-0.75230	
	H	-2.95870	5.04526	0.19897	
	C	-2.65795	3.25418	2.33529	
	H	-1.95623	4.08314	2.43336	
	H	-2.22916	2.38006	2.83721	
	H	-3.56229	3.53426	2.88929	
	C	-4.14545	1.88039	0.94380	
	H	-3.75505	0.91688	1.28829	
	H	-4.63696	1.72011	-0.02032	
	H	-4.92227	2.20093	1.64804	
	C	-1.21112	1.28459	-3.61325	
	C	-0.68951	2.43192	-4.50055	
	H	-1.29041	3.33787	-4.36222	
	H	-0.73822	2.14673	-5.55913	
	H	0.35198	2.67978	-4.26917	
	C	-2.64630	0.95758	-4.05021	
	H	-3.06987	0.12527	-3.47628	
H	-2.65807	0.66594	-5.10717		
H	-3.30764	1.82339	-3.93121		
C	-0.33133	0.04582	-3.84305		
H	0.70538	0.21351	-3.53420		
H	-0.32508	-0.23777	-4.90347		
H	-0.71490	-0.82047	-3.28783		
C	1.97516	0.04159	0.69082		
Th	-0.28992	-0.00782	-0.03197		
C	1.99833	-0.10829	-0.66204		
C	3.16982	-0.26881	-1.53633		
C	4.14773	-1.25437	-1.29680		
					

H	4.04761	-1.89479	-0.42511
C	5.23528	-1.41683	-2.15123
H	5.96972	-2.19175	-1.94191
C	5.39556	-0.58564	-3.26094
H	6.24861	-0.70963	-3.92340
C	4.44710	0.40694	-3.50751
H	4.55902	1.06713	-4.36503
C	3.34620	0.55183	-2.66620
H	2.61213	1.32588	-2.87399
C	-0.61534	-2.87238	0.24455
C	-1.98758	-2.43864	0.03143
C	-2.35627	-1.70298	1.19998
H	-3.34416	-1.30053	1.37891
C	-1.30263	-1.67712	2.13811
C	-0.22999	-2.36613	1.52251
H	0.72868	-2.54853	1.98565
C	0.30701	-3.84898	-0.51863
C	-0.33104	-5.25138	-0.58681
H	-1.23593	-5.28151	-1.19681
H	-0.59096	-5.60665	0.41720
H	0.38105	-5.96343	-1.02306
C	0.68175	-3.36683	-1.93280
H	1.30274	-4.12029	-2.43435
H	1.26973	-2.44279	-1.88507
H	-0.18794	-3.18750	-2.56573
C	1.63814	-4.03073	0.23696
H	2.29122	-4.69563	-0.34026
H	1.49064	-4.48722	1.22219
H	2.16429	-3.07985	0.36747
C	-3.11845	-2.86904	-0.93132
C	-3.80606	-4.11437	-0.32464
H	-4.65061	-4.42832	-0.95218
H	-4.19005	-3.89256	0.67722
H	-3.11788	-4.95965	-0.23655
C	-2.71097	-3.19138	-2.37589
H	-2.02482	-4.03546	-2.45162
H	-2.25119	-2.32949	-2.87203
H	-3.60694	-3.45469	-2.95125
C	-4.19467	-1.76745	-1.03511
H	-3.76737	-0.81911	-1.37938
H	-4.70553	-1.58238	-0.08583
H	-4.96219	-2.07231	-1.75630
C	-1.37255	-1.21746	3.59407
C	-0.95493	-2.39252	4.50019
H	-1.60475	-3.26075	4.34176
H	-1.02295	-2.10233	5.55640
H	0.07675	-2.70406	4.30467
C	-2.80493	-0.81108	3.97016
H	-3.15528	0.04586	3.38360
H	-2.84573	-0.52294	5.02736
H	-3.50892	-1.63733	3.81908
C	-0.43715	-0.02965	3.86929
H	0.61030	-0.27744	3.67228
H	-0.51552	0.29498	4.91476
H	-0.69823	0.83269	3.24261
C	3.12088	0.17215	1.60367
C	4.13426	1.12765	1.39114
C	3.23850	-0.64890	2.74078

	C 5.19845 1.26340 2.27897 H 4.08134 1.76579 0.51372 C 4.31616 -0.53134 3.61591 H 2.47712 -1.40161 2.92777 C 5.29951 0.43320 3.39627 H 5.96110 2.01596 2.08991 H 4.38263 -1.19090 4.47862 H 6.13429 0.53603 4.08513	
TS2a	C 0.98993 -2.35690 1.48005 C 2.25745 -1.96227 0.99913 C 2.36827 -2.21275 -0.40374 C 1.08558 -2.74071 -0.82402 C 0.27149 -2.79991 0.34937 H -0.74732 -3.15889 0.37232 C 0.42404 -2.06516 2.86350 C 1.47334 -2.31071 3.95751 H 2.37303 -1.70330 3.80878 H 1.78031 -3.36450 3.98214 H 1.06034 -2.05129 4.94016 C 0.00749 -0.57838 2.79552 H -0.71803 -0.32101 3.57925 H -1.04013 -0.41822 1.76172 H 0.88067 0.06458 2.98142 C -0.79061 -2.95422 3.15847 H -1.17500 -2.73876 4.16264 H -0.51528 -4.01516 3.11895 H -1.61141 -2.78735 2.45526 C -2.05695 -0.39293 0.73676 Th 0.37292 -0.01943 0.21343 C -1.92484 -0.16808 -0.58973 C -3.02559 -0.07566 -1.56753 C -4.27818 0.48112 -1.23469 H -4.44818 0.83684 -0.22348 C -5.29450 0.59438 -2.17851 H -6.24640 1.03524 -1.89079 C -5.10139 0.14080 -3.48467 H -5.89883 0.22286 -4.21910 C -3.86942 -0.40786 -3.83829 H -3.69856 -0.75718 -4.85412 C -2.84554 -0.49624 -2.89738 H -1.88454 -0.90564 -3.19150 C 0.03183 2.87176 -0.17714 C 1.21368 2.53923 -0.94590 C 2.22771 2.18901 0.00095 H 3.25305 1.95807 -0.25867 C 1.75246 2.32969 1.32455 C 0.38968 2.68231 1.19567 H 3.06261 -1.59409 1.62171 C 0.59764 -3.39046 -2.13571 C 3.78620 -2.20759 -1.02096 C 2.62757 2.47713 2.56863 C 1.54909 2.64134 -2.44774 C -1.26010 3.66158 -0.48848 H -0.26325 2.90066 2.03097 C 3.44962 3.77315 2.38060 H 2.79005 4.63690 2.23960 H 4.07536 3.96058 3.26298 H 4.10568 3.70419 1.50599	

C	3.61194	1.31124	2.74079
H	4.28406	1.50091	3.58693
H	3.08904	0.36948	2.93688
H	4.23222	1.17586	1.84775
C	1.79431	2.64140	3.84821
H	1.14878	3.52519	3.79127
H	1.16096	1.77223	4.05177
H	2.46070	2.77475	4.70892
C	3.01498	2.24158	-2.70994
H	3.21385	2.28584	-3.78725
H	3.72032	2.91845	-2.21523
H	3.23258	1.21932	-2.38033
C	0.68587	1.70257	-3.30967
H	0.93335	0.65211	-3.10268
H	-0.38368	1.83196	-3.14448
H	0.88743	1.86692	-4.37624
C	1.42841	4.09601	-2.94483
H	1.77945	4.16609	-3.98217
H	0.40568	4.47312	-2.92025
H	2.04750	4.76218	-2.33291
C	-1.91849	3.39994	-1.85094
H	-2.21137	2.35322	-1.96422
H	-2.82960	4.00591	-1.92840
H	-1.28460	3.67617	-2.69491
C	-0.91373	5.16597	-0.38397
H	-1.81414	5.77317	-0.54611
H	-0.51813	5.40415	0.61005
H	-0.16521	5.46940	-1.12125
C	-2.34408	3.38240	0.57394
H	-3.26585	3.90824	0.29856
H	-2.56978	2.31461	0.64372
H	-2.05909	3.74302	1.56769
C	4.45319	-3.55578	-0.66190
H	4.49358	-3.68906	0.42467
H	3.90562	-4.40486	-1.08056
H	5.48002	-3.58838	-1.04924
C	4.65446	-1.09651	-0.39484
H	4.22061	-0.10511	-0.56340
H	4.79903	-1.22622	0.68129
H	5.65007	-1.10695	-0.85412
C	3.88465	-2.00618	-2.53949
H	4.94212	-1.96414	-2.82787
H	3.43439	-2.82058	-3.10869
H	3.42370	-1.06462	-2.85808
C	1.40384	-4.67182	-2.43433
H	2.45143	-4.47090	-2.66903
H	1.37642	-5.35440	-1.57716
H	0.96927	-5.19423	-3.29623
C	0.64502	-2.44871	-3.35157
H	1.64224	-2.06767	-3.56532
H	0.29006	-2.97309	-4.24818
H	-0.01323	-1.58779	-3.19563
C	-0.87278	-3.83570	-1.99946
H	-1.21403	-4.24880	-2.95601
H	-0.99434	-4.61820	-1.24253
H	-1.53212	-2.99885	-1.74433
C	-3.24913	-0.73721	1.53461
C	-4.05679	-1.83673	1.18957

	C -3.58050 -0.01370 2.69368 C -5.15204 -2.19376 1.97107 H -3.81498 -2.40988 0.29835 C -4.68749 -0.36263 3.46613 H -2.97067 0.84022 2.98020 C -5.47584 -1.45702 3.11204 H -5.75856 -3.05042 1.68609 H -4.92994 0.21968 4.35219 H -6.33298 -1.73553 3.71984	
P2	C -1.34298 -1.12164 -2.48592 C -2.51822 -1.02042 -1.71150 C -2.54849 -2.02368 -0.68875 C -1.30410 -2.75285 -0.80533 C -0.58494 -2.15212 -1.88784 H 0.38853 -2.47460 -2.23197 C -0.84437 -0.07000 -3.46759 C -1.95879 0.35417 -4.43556 H -2.83211 0.74616 -3.90104 H -2.29553 -0.48784 -5.05581 H -1.59778 1.14880 -5.10071 C -0.39869 1.07902 -2.52964 H 0.44202 1.65028 -2.94224 H 1.64671 0.06045 -1.56929 H -1.23245 1.78993 -2.42132 C 0.33360 -0.59712 -4.29483 H 0.66988 0.17732 -4.99503 H 0.04845 -1.48187 -4.87776 H 1.19378 -0.86929 -3.67292 C 2.38352 -0.31793 -0.81980 Th -0.40719 0.05957 -0.22479 C 1.91319 -0.67360 0.39583 C -1.39453 2.77654 0.45973 C 0.02605 2.84181 0.72209 C 0.28272 1.92998 1.79452 H 1.25076 1.77004 2.24931 C -0.91784 1.34777 2.25806 C -1.92846 1.83173 1.39575 H -3.31935 -0.31793 -1.90504 C -0.79668 -4.06520 -0.17697 C -3.90491 -2.30613 -0.00342 C -1.09607 0.59984 3.57604 C 1.13000 3.82221 0.26791 C -2.40822 3.67249 -0.29422 H -2.98443 1.62097 1.51209 C -0.79853 1.59250 4.72029 H -1.46431 2.46170 4.66796 H -0.94348 1.10765 5.69444 H 0.23413 1.95438 4.67181 C -0.12686 -0.58475 3.69578 H -0.24851 -1.08360 4.66560 H -0.30491 -1.33592 2.91694 H 0.91635 -0.26662 3.61050 C -2.53529 0.09963 3.74428 H -3.25326 0.92781 3.75040 H -2.82169 -0.58885 2.94204 H -2.63918 -0.43744 4.69450 C 2.47954 3.47265 0.92593 H 3.24290 4.17575 0.57235	

H	2.44330	3.55039	2.01807
H	2.81088	2.46516	0.65323
C	1.40724	3.83295	-1.24526
H	1.87614	2.89208	-1.55215
H	0.51313	3.96915	-1.85018
H	2.10760	4.64324	-1.48619
C	0.77857	5.24023	0.76703
H	1.60038	5.93176	0.54118
H	-0.12643	5.64315	0.30869
H	0.62890	5.23664	1.85295
C	-1.90025	4.45943	-1.51191
H	-1.53302	3.80177	-2.30500
H	-2.73568	5.03610	-1.92817
H	-1.11433	5.17424	-1.26415
C	-2.95730	4.69211	0.73282
H	-3.70775	5.34010	0.26162
H	-3.43082	4.18120	1.57825
H	-2.16206	5.32963	1.13197
C	-3.60693	2.84458	-0.80387
H	-4.32928	3.51040	-1.29172
H	-3.29478	2.09981	-1.54443
H	-4.14016	2.32618	-0.00217
C	-4.75757	-3.13897	-0.98903
H	-4.88470	-2.60554	-1.93729
H	-4.29469	-4.10514	-1.21042
H	-5.75314	-3.32804	-0.56648
C	-4.66876	-0.99055	0.25625
H	-4.10130	-0.32061	0.91120
H	-4.90491	-0.44846	-0.66335
H	-5.62220	-1.21175	0.75082
C	-3.86839	-3.04015	1.34430
H	-4.88992	-3.11675	1.73640
H	-3.48036	-4.05698	1.27044
H	-3.27487	-2.50005	2.08893
C	-1.72647	-5.23632	-0.55712
H	-2.72545	-5.14561	-0.12695
H	-1.83541	-5.30279	-1.64588
H	-1.29953	-6.18311	-0.20199
C	-0.62749	-3.98960	1.35029
H	-1.54486	-3.71781	1.87041
H	-0.29713	-4.96017	1.74277
H	0.13773	-3.25212	1.61378
C	0.58861	-4.43390	-0.74648
H	0.95564	-5.33781	-0.24596
H	0.54610	-4.64694	-1.82033
H	1.32437	-3.63904	-0.58447
C	3.73200	-0.27971	-1.42267
C	4.83955	-0.95783	-0.88338
C	3.92064	0.45814	-2.60484
C	6.08573	-0.88168	-1.49867
H	4.72079	-1.55241	0.01512
C	5.16907	0.53913	-3.21532
H	3.07324	0.97837	-3.04638
C	6.26002	-0.13056	-2.66233
H	6.92789	-1.41648	-1.06616
H	5.28826	1.12225	-4.12516
H	7.23648	-0.07363	-3.13659
C	2.75858	-1.10489	1.52231

C	2.85321	-2.45359	1.91185
C	3.48058	-0.16338	2.28239
C	3.62955	-2.84090	3.00279
C	4.24941	-0.55083	3.37764
C	4.32915	-1.89306	3.74892
H	2.32749	-3.21076	1.33946
H	3.44739	0.88383	1.99734
H	3.68590	-3.89407	3.26914
H	4.79573	0.20367	3.93946
H	4.92945	-2.19551	4.60300

Table S2. Frequencies of the stationary points optimized for conversion of **2**, obtained with B3PW91-PCM/6-31G(d)+sdd method.

Species	Frequencies (cm ⁻¹)
2	6 19 24 31 34 43 44 49 61 65 67 74 77 80 87 91 94 102 105 110 124 130 133 135 137 155 169 175 175 184 191 200 202 203 204 210 214 218 241 242 245 250 252 255 257 264 266 271 271 282 285 286 289 305 310 316 316 329 330 346 346 350 353 367 368 372 373 373 378 380 387 390 402 402 414 415 419 424 427 434 452 453 470 473 478 480 486 487 553 554 555 559 562 566 567 588 596 597 608 630 635 648 649 679 682 685 689 696 710 711 769 785 796 800 805 828 828 832 834 840 842 850 852 854 855 900 914 932 933 937 942 944 946 946 947 949 950 950 951 953 957 962 964 965 966 967 972 973 974 976 988 988 1011 1012 1022 1022 1047 1049 1052 1052 1053 1055 1057 1058 1059 1061 1062 1063 1069 1074 1107 1108 1147 1148 1170 1185 1185 1199 1200 1205 1206 1207 1209 1223 1224 1229 1230 1234 1237 1242 1245 1247 1248 1261 1261 1263 1272 1273 1276 1279 1317 1319 1327 1329 1369 1370 1378 1382 1405 1406 1412 1412 1415 1416 1417 1419 1420 1421 1422 1423 1425 1426 1441 1441 1449 1450 1453 1454 1457 1457 1483 1485 1493 1496 1501 1501 1502 1503 1503 1504 1506 1507 1509 1511 1512 1513 1516 1517 1517 1518 1520 1520 1521 1523 1524 1527 1528 1531 1532 1532 1533 1534 1536 1536 1542 1543 1547 1551 1553 1557 1579 1591 1628 1631 1633 1660 1662 3049 3049 3051 3051 3052 3053 3053 3054 3055 3056 3057 3058 3059 3061 3061 3061 3066 3066 3119 3121 3121 3122 3123 3123 3123 3124 3124 3125 3126 3126 3128 3129 3129 3131 3131 3133 3133 3134 3137 3138 3145 3145 3146 3146 3149 3153 3156 3157 3168 3169 3183 3184 3184 3185 3191 3191 3192 3193 3205 3205 3213 3214 3221 3221 3268 3269 3286 3286
TS2a	-1318i 19 25 34 44 47 50 51 58 62 69 71 75 78 82 85 92 102 110 119 121 125 132 135 154 162 170 176 182 186 189 196 199 203 205 212 214 217 236 238 243 246 250 255 256 258 259 264 270 278 286 294 298 301 302 310 315 324 328 343 349 355 355 362 365 369 375 378 381 383 391 395 400 406 413 417 426 429 438 439 446 461 463 466 474 486 511 524 551 555 557 558 570 574 583 592 599 599 603 630 633 648 650 683 686 690 703 703 710 714 754 777 783 786 806 808 829 830 830 841 842 847 856 856 857 858 908 924 933 936 936 939 941 945 947 951 952 952 953 955 958 961 962 965 966 970 971 972 973 983 993 995 1012 1014 1018 1022 1027 1049 1051 1051 1052 1053 1055 1055 1060 1061 1061 1062 1067 1073 1090 1109 1112 1145 1151 1179 1186 1187 1196 1201 1203 1205 1206 1210 1223 1224 1229 1231 1232 1234 1241 1242 1243 1248 1261 1261 1261 1273 1275 1277 1285 1308 1315 1319 1333 1337 1370 1372 1386 1391 1403 1408 1411 1412 1412 1413 1415 1416 1420 1421 1422 1425 1428 1436 1443 1443 1446 1454 1455 1458 1461 1470 1485 1487 1497 1498 1500 1502 1502 1504 1505 1506 1509 1510 1511 1512 1513 1515 1516 1517 1518 1520 1521 1523 1523 1525 1526 1529 1530 1531 1532 1534 1535 1537 1539 1543 1546 1550 1552 1554 1555 1593 1623 1634 1636 1661 1663 1916 3037 3043 3046 3047 3049 3052 3054 3054 3055 3056 3057 3059 3060 3060 3063 3064 3066 3071 3087 3102 3116 3121 3121 3122 3123 3123 3124 3124 3126 3127 3127 3128 3128 3129 3131 3132 3136 3138 3144 3145 3145 3147 3152 3153 3155 3155 3162 3165 3177 3179 3187 3189 3189 3194 3195 3197 3204 3211 3211 3214 3220 3230 3232 3259 3263 3263 3285
P2	19 24 34 37 42 46 49 55 59 61 69 70 74 79 84 86 91 94 99 120 126 130 133 136 141 145 155 169

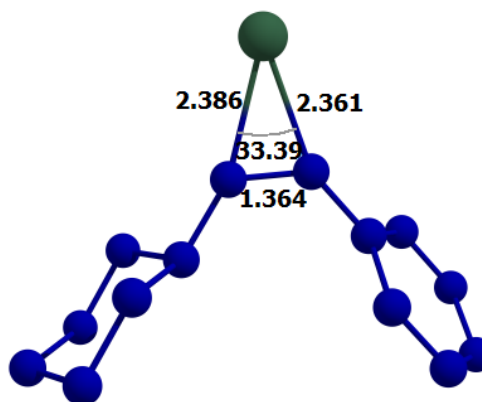
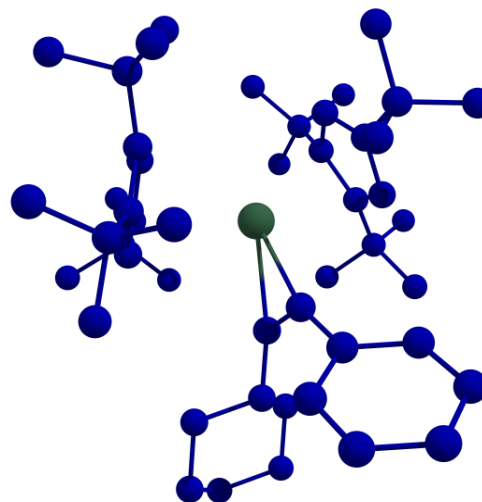
170	184	192	194	200	206	207	211	217	235	236	241	244	246
252	253	256	258	264	269	272	278	287	289	297	303	307	312
314	327	336	339	346	351	353	354	365	371	375	377	384	386
392	400	401	403	411	415	422	428	431	436	441	455	463	465
474	477	486	508	544	552	555	555	557	564	566	585	596	597
597	629	634	650	651	685	694	699	701	708	710	718	770	777
792	803	811	828	829	831	834	847	848	856	857	859	860	890
901	926	934	938	938	939	940	942	945	946	948	952	953	954
957	958	963	964	967	968	971	974	976	983	990	992	1001	1010
1014	1022	1024	1042	1048	1050	1050	1051	1052	1054	1054	1056	1058	1060
1061	1062	1063	1110	1118	1139	1142	1182	1186	1190	1193	1194	1195	1205
1211	1215	1221	1223	1224	1230	1231	1236	1238	1240	1241	1244	1253	1257
1259	1271	1273	1276	1281	1312	1313	1328	1342	1369	1379	1391	1392	1402
1403	1410	1410	1413	1413	1414	1415	1418	1422	1423	1425	1426	1429	1440
1443	1449	1450	1453	1455	1456	1459	1477	1483	1495	1497	1500	1501	1502
1503	1504	1506	1507	1507	1508	1508	1510	1512	1514	1515	1515	1516	1519
1520	1521	1522	1526	1528	1528	1530	1531	1534	1536	1537	1539	1540	1545
1546	1547	1551	1553	1554	1556	1631	1635	1662	1666	1678	2845	3023	3036
3046	3050	3050	3051	3053	3053	3054	3055	3056	3058	3061	3062	3062	3062
3068	3068	3093	3109	3119	3119	3121	3122	3122	3122	3124	3125	3125	3126
3127	3128	3129	3129	3130	3130	3135	3136	3137	3137	3142	3143	3146	3150
3150	3152	3157	3171	3171	3183	3184	3189	3191	3197	3198	3208	3211	3215
3218	3221	3225	3232	3248	3254	3259	3274	3276					

Table S3. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for conversion of **2**, obtained with B3PW91-PCM/6-31G(d)+sdd method

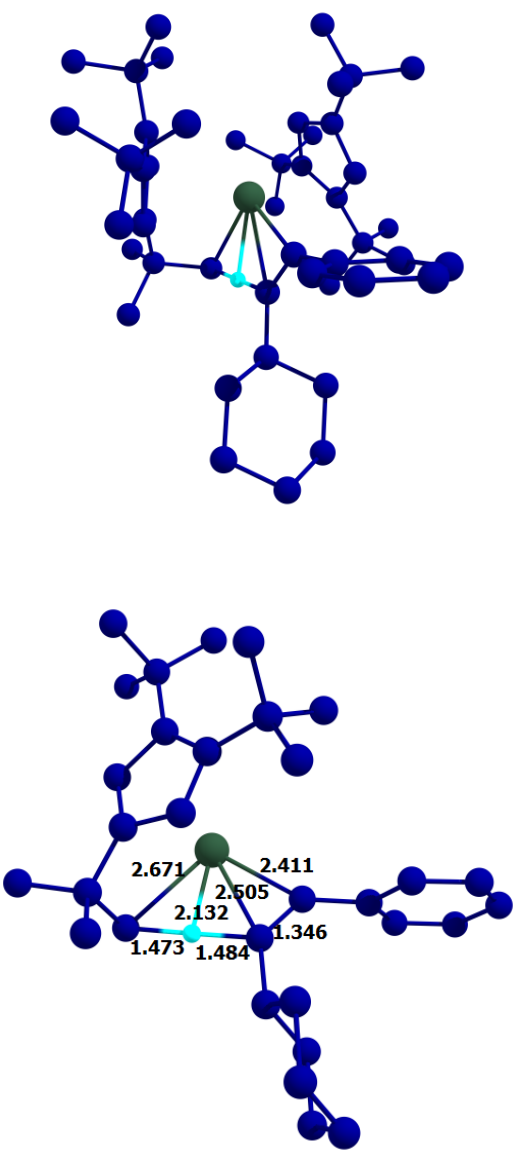
species	E	H	G (gas)	G (sol)
2	-2277.18902 (0.0)	-2276.09185 (0.0)	-2276.23475 (0.0)	-2276.22130 (0.0)
TS21	-2277.15058 (24.1)	-2276.05852 (20.9)	-2276.19664 (23.9)	-2276.18263 (24.3)
P2	-2277.18253 (4.1)	-2276.08739 (2.8)	-2276.22854 (3.9)	-2276.21513 (3.9)

Table S4. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for conversion of **5**, obtained with B3PW91-PCM/6-31G(d)+sdd method.

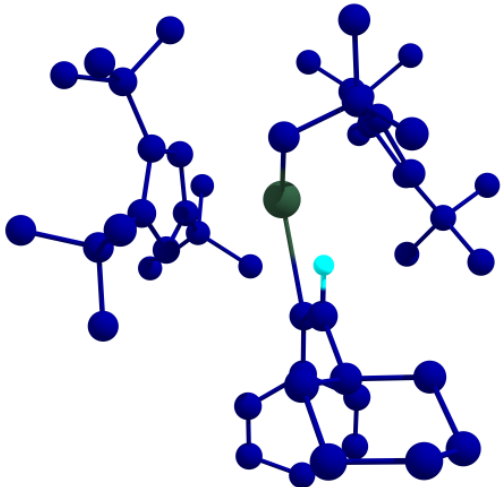
Species	Cartesian coordinates	
5	C	-0.71097 -1.99304 -2.08102
	C	-1.86684 -2.12843 -1.28379
	C	-1.55459 -2.70950 -0.01701
	C	-0.11790 -2.92695 -0.01577
	C	0.36122 -2.44584 -1.27290
	H	1.39310 -2.48657 -1.59011
	C	-0.65547 -1.65579 -3.57133
	C	-2.07025 -1.57053 -4.16235
	H	-2.66135 -0.77277 -3.69746
	H	-2.61448 -2.51324 -4.03477
	H	-2.01552 -1.35533 -5.23618
	C	0.06866 -0.32640 -3.83792
	H	0.14643 -0.13070 -4.91499
	H	1.07905 -0.32879 -3.41648
	H	-0.47870 0.51802 -3.39661
	C	0.10241 -2.78251 -4.30032
	H	0.11849 -2.59423 -5.38145
	H	-0.37896 -3.75191 -4.12854
	H	1.13988 -2.85586 -3.95712
	C	2.04561 0.33069 -0.39921
	Th	-0.28674 0.00085 -0.01819
	C	1.84297 0.32172 0.94956
	C	2.85601 0.46857 2.00294
	C	2.87390 1.60058 2.84196
	H	2.12826 2.37776 2.69426
	C	3.83375 1.75363 3.83966
	H	3.82265 2.64645 4.46151
	C	4.80184 0.77032 4.04769
	H	5.54613 0.88525 4.83167
	C	4.80081 -0.36109 3.23217
	H	5.55140 -1.13593 3.37500
	C	3.85020 -0.50598 2.22343
	H	3.87066 -1.39127 1.59379
	C	-2.42015 2.07595 -0.24626
	C	-1.17025 2.78133 -0.01094
	C	-0.76574 2.45046 1.31635
	H	0.11580 2.84140 1.80271
	C	-1.72037 1.61399 1.94212
	C	-2.70628 1.36995 0.96272
	H	-2.87190 -1.91851 -1.62318
	C	0.81845 -3.70261 0.93859
	C	-2.72165 -3.25875 0.83664
	C	-1.77287 1.25639 3.42668
	C	-0.40323 3.85309 -0.81299
	C	-3.55917 2.22881 -1.28150
	H	-3.61187 0.80483 1.13484
	C	-1.62107 2.55217 4.24845
	H	-2.40337 3.27506 3.99008
	H	-1.69693 2.33350 5.32127
	H	-0.65031 3.02835 4.07362
	C	-0.64496 0.29158 3.82598
	H	-0.68457 0.07134 4.90062



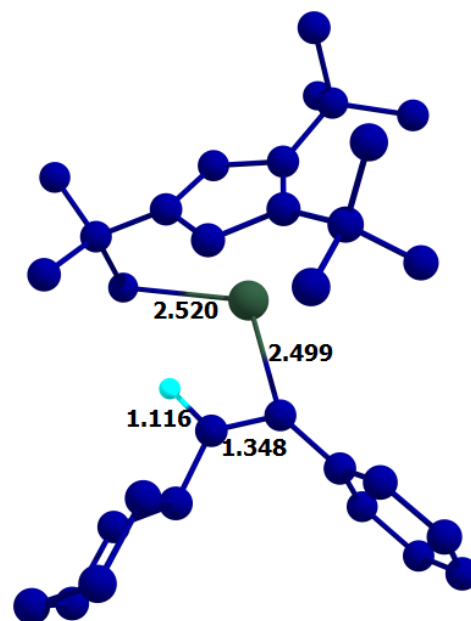
H	-0.73527	-0.66702	3.29763
H	0.34367	0.70295	3.60001
C	-3.12277	0.62019	3.78710
H	-3.95654	1.29499	3.56128
H	-3.29145	-0.31888	3.24747
H	-3.15455	0.39268	4.85928
C	0.84224	4.31879	-0.03235
H	1.39616	5.04587	-0.63797
H	0.57470	4.81138	0.90918
H	1.51798	3.48584	0.18919
C	0.11374	3.33888	-2.16718
H	0.83882	2.53151	-2.01358
H	-0.67878	2.97014	-2.81831
H	0.63521	4.14157	-2.70503
C	-1.27179	5.11027	-1.01697
H	-0.67131	5.90785	-1.47286
H	-2.12890	4.93496	-1.67034
H	-1.65059	5.47978	-0.05703
C	-3.13716	2.50442	-2.73157
H	-2.49427	1.70954	-3.12727
H	-4.03125	2.54364	-3.36587
H	-2.61982	3.45668	-2.85455
C	-4.47865	3.37867	-0.80842
H	-5.32839	3.49412	-1.49412
H	-4.87409	3.16784	0.19138
H	-3.94933	4.33415	-0.76156
C	-4.42782	0.95518	-1.33264
H	-5.20317	1.07122	-2.09930
H	-3.83220	0.07233	-1.58682
H	-4.94268	0.75560	-0.38858
C	-3.10723	-4.64892	0.27935
H	-3.39729	-4.57171	-0.77447
H	-2.28325	-5.36402	0.34435
H	-3.95868	-5.05993	0.83770
C	-3.97213	-2.36676	0.69963
H	-3.76807	-1.34146	1.02287
H	-4.35961	-2.33010	-0.32255
H	-4.77541	-2.76503	1.33089
C	-2.46430	-3.38122	2.34539
H	-3.37910	-3.72864	2.84111
H	-1.67823	-4.09526	2.59142
H	-2.20039	-2.41567	2.79139
C	0.37539	-5.17453	1.06607
H	-0.57654	-5.29300	1.58586
H	0.28066	-5.63809	0.07721
H	1.12702	-5.73927	1.63224
C	0.94624	-3.06374	2.33427
H	-0.00763	-2.98699	2.85753
H	1.61847	-3.66171	2.96320
H	1.37525	-2.05749	2.25771
C	2.24515	-3.75179	0.36038
H	2.90088	-4.28312	1.06019
H	2.28169	-4.28338	-0.59720
H	2.65322	-2.74759	0.21622
C	3.39839	0.50443	-1.06826
C	3.82875	-0.76153	-1.83500
C	3.45158	1.70955	-2.02367
H	4.16574	0.67739	-0.29261

	C 5.20598 -0.60629 -2.48750 H 3.08224 -0.98339 -2.61203 H 3.83839 -1.62288 -1.15688 C 4.83024 1.87692 -2.66962 H 2.69918 1.57331 -2.81485 H 3.17895 2.62472 -1.48419 C 5.25618 0.60998 -3.41379 H 5.46340 -1.51988 -3.04045 H 5.96704 -0.49250 -1.70122 H 4.82222 2.73691 -3.35289 H 5.57160 2.10489 -1.88928 H 6.26308 0.73052 -3.83503 H 4.57773 0.44515 -4.26477	
TS5a	C 0.79593 1.55415 -2.38450 C 2.05673 1.65050 -1.75481 C 1.99514 2.53744 -0.63236 C 0.62087 2.99127 -0.54808 C -0.07762 2.35277 -1.61594 H -1.12735 2.48861 -1.83000 C 0.37173 0.56204 -3.46089 C 1.50042 0.31541 -4.47094 H 2.40568 -0.06804 -3.98674 H 1.76876 1.23798 -5.00189 H 1.18541 -0.42869 -5.21279 C 0.00362 -0.72952 -2.69468 H -0.70272 -1.34814 -3.26460 H -1.01987 -0.47360 -1.66718 H 0.89487 -1.36566 -2.56878 C -0.85327 1.08169 -4.22537 H -1.12685 0.37313 -5.01677 H -0.64552 2.05247 -4.69082 H -1.72546 1.19761 -3.57390 C -2.04357 -0.18842 -0.63090 Th 0.40865 0.01053 -0.16036 C -1.85306 0.10764 0.66775 C -2.80601 0.30092 1.76904 C -3.06881 -0.73166 2.69235 H -2.59288 -1.69808 2.55355 C -3.93767 -0.54586 3.76505 H -4.12433 -1.37113 4.44906 C -4.56432 0.68415 3.96740 H -5.23816 0.83023 4.80762 C -4.30840 1.72308 3.07320 H -4.78622 2.69084 3.21084 C -3.44620 1.53560 1.99468 H -3.26380 2.35946 1.31188 C 2.10155 -2.44436 0.04763 C 0.78541 -2.86064 0.49365 C 0.52406 -2.14532 1.70076 H -0.36856 -2.25749 2.29988 C 1.63653 -1.35426 2.07123 C 2.57480 -1.51495 1.02726 H 2.96061 1.16766 -2.10406 C -0.07531 4.09261 0.28051 C 3.31930 3.02732 -0.00915 C 1.84184 -0.69029 3.43094 C -0.15274 -4.00780 0.05847 C 3.13462 -3.00050 -0.96209	

H	3.56742	-1.08314	1.02471
C	1.63847	-1.75821	4.52547
H	2.32106	-2.60307	4.37926
H	1.83101	-1.32904	5.51718
H	0.61436	-2.14616	4.52107
C	0.83596	0.44785	3.66907
H	0.94994	0.86283	4.67867
H	0.99276	1.27519	2.96383
H	-0.19902	0.10484	3.56051
C	3.26881	-0.14217	3.56338
H	4.01248	-0.94253	3.47440
H	3.49186	0.61119	2.79984
H	3.40086	0.33191	4.54330
C	-1.39566	-4.06728	0.96779
H	-2.05440	-4.87350	0.62365
H	-1.13474	-4.28005	2.01035
H	-1.96736	-3.13465	0.93028
C	-0.69310	-3.87443	-1.37549
H	-1.32416	-2.98334	-1.46101
H	0.09092	-3.79912	-2.12766
H	-1.31250	-4.74631	-1.62333
C	0.56300	-5.36264	0.24493
H	-0.13317	-6.18526	0.03661
H	1.42477	-5.48764	-0.41317
H	0.91412	-5.47081	1.27782
C	2.59459	-3.70637	-2.21465
H	1.99117	-3.03904	-2.83816
H	3.44318	-4.03810	-2.82554
H	2.00106	-4.59252	-1.98801
C	4.03098	-4.00406	-0.19876
H	4.80276	-4.41222	-0.86467
H	4.53214	-3.51857	0.64578
H	3.44859	-4.84171	0.19751
C	4.04489	-1.86905	-1.48409
H	4.77624	-2.27927	-2.19102
H	3.46424	-1.10408	-2.01244
H	4.61074	-1.37535	-0.68925
C	3.85160	4.20233	-0.86191
H	3.99201	3.88720	-1.90194
H	3.16840	5.05543	-0.86304
H	4.82091	4.54441	-0.47570
C	4.39302	1.92082	-0.06811
H	4.06427	1.01258	0.44807
H	4.66343	1.64987	-1.09297
H	5.30879	2.27239	0.42188
C	3.24818	3.46532	1.46110
H	4.25400	3.72867	1.81078
H	2.61678	4.33985	1.62044
H	2.87937	2.65931	2.10502
C	0.61187	5.45917	0.08152
H	1.61929	5.49977	0.49789
H	0.67710	5.70659	-0.98444
H	0.02409	6.24437	0.57395
C	-0.16945	3.75726	1.78039
H	0.80462	3.57038	2.23404
H	-0.63421	4.58887	2.32598
H	-0.79469	2.87127	1.93976
C	-1.52290	4.29323	-0.21091

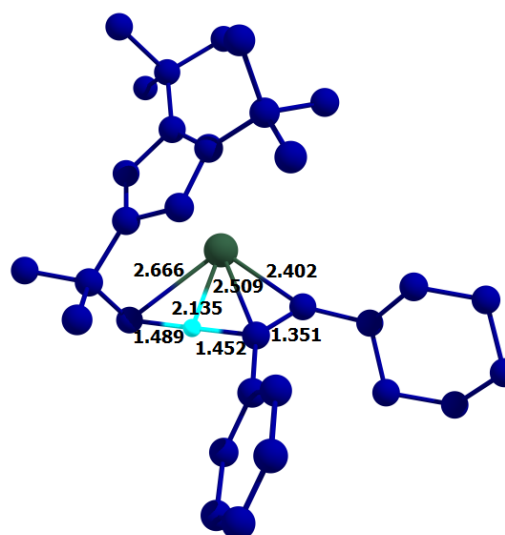
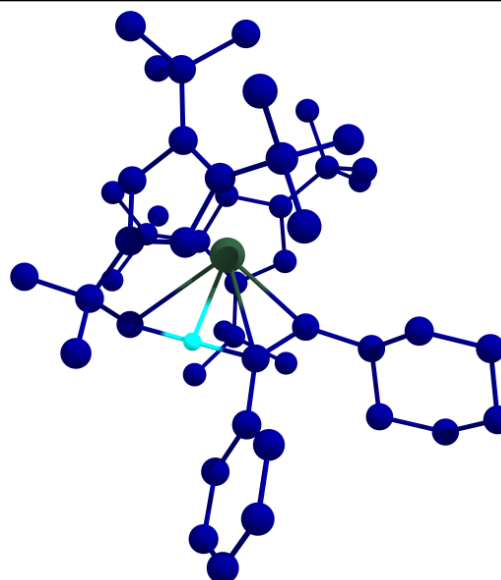
	H -2.01365 5.05262 0.40926 H -1.55510 4.63985 -1.24997 H -2.11077 3.37354 -0.13748 C -3.31736 -0.42404 -1.42215 C -4.22961 -1.50572 -0.81407 C -4.12044 0.87884 -1.61370 H -3.03996 -0.77345 -2.43268 C -5.47887 -1.73639 -1.67012 H -4.52589 -1.19566 0.19630 H -3.67221 -2.44415 -0.70382 C -5.36701 0.65373 -2.47477 H -4.42005 1.25408 -0.62631 H -3.48428 1.65171 -2.06474 C -6.26196 -0.43935 -1.88632 H -6.11945 -2.49429 -1.20008 H -5.17877 -2.14438 -2.64751 H -5.92698 1.59301 -2.57522 H -5.05931 0.36355 -3.49093 H -7.12539 -0.61858 -2.54051 H -6.66427 -0.09532 -0.92190	
8	C 0.49061 2.96058 -0.71566 C 1.88307 2.57202 -0.78667 C 1.98187 1.63804 -1.86860 H 2.90606 1.17594 -2.19339 C 0.73294 1.45971 -2.49984 C -0.17950 2.23731 -1.75292 H -1.23689 2.31232 -1.96647 C -0.25824 4.06009 0.06669 C -1.73665 4.11150 -0.36903 H -1.84413 4.38866 -1.42370 H -2.26190 4.86738 0.22672 H -2.24113 3.15230 -0.21224 C -0.27049 3.83750 1.58976 H -0.79476 2.90937 1.84366 H -0.80282 4.66074 2.08402 H 0.72856 3.78709 2.02275 C 0.31802 5.45276 -0.26100 H 1.33293 5.59378 0.11512 H -0.30884 6.23158 0.19188 H 0.33441 5.62062 -1.34411 C 3.19040 3.16922 -0.22121 C 3.12371 3.72098 1.20958 H 4.12386 4.04960 1.51771 H 2.79569 2.95743 1.92283 H 2.46272 4.58317 1.30619 C 3.64644 4.30007 -1.17233 H 4.59885 4.72479 -0.82858 H 2.91506 5.11078 -1.22745 H 3.79262 3.91316 -2.18686 C 4.31760 2.11535 -0.21643 H 4.57789 1.76931 -1.22101 H 4.04912 1.24073 0.38525 H 5.22535 2.55282 0.21576 C 0.39005 0.35236 -3.48804 C 1.46737 0.22689 -4.57484 H 1.22743 -0.60851 -5.24442 H 2.45604 0.02820 -4.14506 H 1.54185 1.14232 -5.17766	

C	0.31013	-0.90130	-2.58082
H	1.26356	-1.44679	-2.64066
H	-0.46784	-1.60208	-2.90916
C	-0.95264	0.62102	-4.17554
H	-1.78123	0.65798	-3.45955
H	-1.17261	-0.18413	-4.88706
H	-0.94022	1.57066	-4.72523
C	2.17454	-2.38516	0.07915
C	0.88772	-2.81017	0.58380
C	0.63208	-2.02567	1.75226
H	-0.23649	-2.13488	2.38488
C	1.72267	-1.17547	2.03843
C	2.63246	-1.36192	0.97265
H	3.60949	-0.89995	0.91459
C	3.21650	-2.98832	-0.89411
C	4.07789	-1.88084	-1.53753
H	4.83192	-2.33895	-2.18895
H	4.61623	-1.27587	-0.80223
H	3.47213	-1.20821	-2.15465
C	2.69669	-3.84329	-2.05995
H	2.05081	-3.27476	-2.73521
H	2.15574	-4.73129	-1.73094
H	3.55475	-4.19279	-2.64784
C	4.16155	-3.87273	-0.04532
H	3.61897	-4.69026	0.43986
H	4.64952	-3.28494	0.73982
H	4.94333	-4.31228	-0.67846
C	-0.02634	-4.01094	0.25356
C	-0.56490	-4.02783	-1.18724
H	-1.24598	-3.18595	-1.34931
H	-1.13266	-4.95173	-1.35885
H	0.21623	-3.96905	-1.94276
C	0.72160	-5.32392	0.56906
H	0.04999	-6.18101	0.43073
H	1.06501	-5.32841	1.61018
H	1.59310	-5.48161	-0.06874
C	-1.27463	-4.01358	1.15894
H	-1.86109	-3.09585	1.04153
H	-1.02021	-4.13663	2.21754
H	-1.91815	-4.85584	0.87841
C	1.94978	-0.41577	3.34468
C	1.76815	-1.40297	4.51554
H	0.74608	-1.79417	4.55581
H	1.97246	-0.90156	5.47015
H	2.45315	-2.25333	4.42159
C	0.94940	0.73680	3.51907
H	1.08129	1.50169	2.74373
H	1.09340	1.23284	4.48767
H	-0.08674	0.38475	3.47337
C	3.37730	0.14341	3.41322
H	4.12416	-0.65619	3.34720
H	3.52862	0.66683	4.36486
H	3.57653	0.86060	2.60940
C	-3.26439	1.50932	2.31297
H	-3.20327	2.31233	1.58461
C	-3.97099	1.71202	3.49687
H	-4.44968	2.67252	3.67511
C	-4.07374	0.69357	4.44379



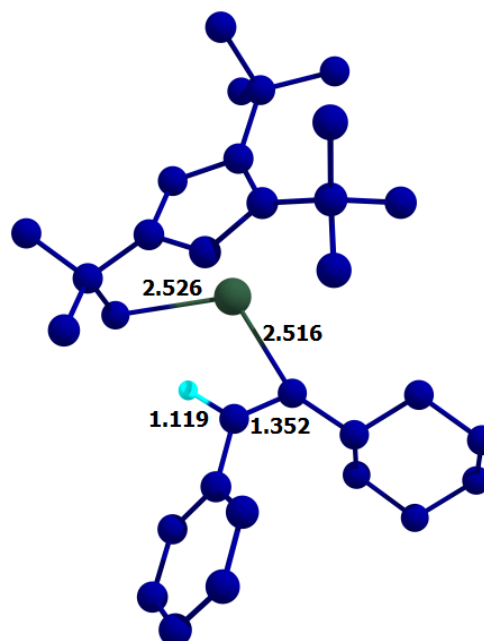
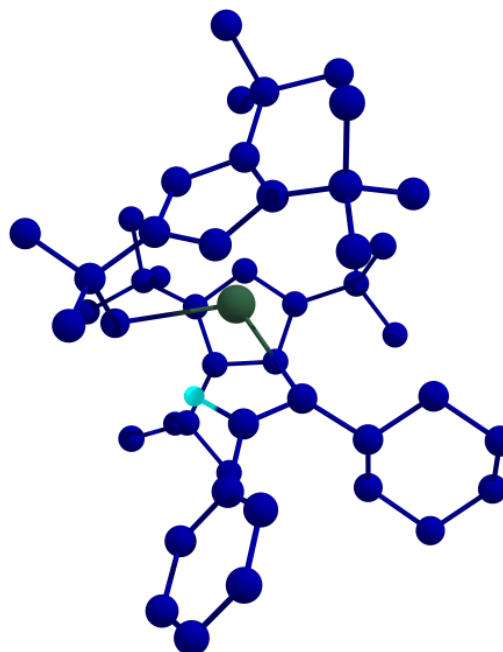
	H -4.62574 0.85114 5.36675 C -3.46167 -0.53236 4.18440 H -3.54036 -1.34403 4.90438 C -2.74768 -0.73195 3.00417 H -2.29236 -1.69962 2.81663 C -2.62883 0.28367 2.03662 C -1.85739 0.08622 0.79383 C -2.46192 -0.19635 -0.37723 C -3.92840 -0.39677 -0.69078 H -4.47007 -0.42887 0.26531 C -4.49279 0.77976 -1.51158 H -4.35680 1.71514 -0.95473 H -3.91377 0.88010 -2.44226 C -5.97119 0.57891 -1.85724 H -6.32970 1.41999 -2.46495 H -6.56215 0.58873 -0.92937 C -6.20247 -0.74538 -2.58819 H -7.27207 -0.88803 -2.78950 H -5.70072 -0.71159 -3.56701 C -5.65182 -1.92198 -1.77950 H -6.23109 -2.02457 -0.84983 H -5.78173 -2.86103 -2.33307 C -4.17381 -1.72292 -1.43195 H -3.57944 -1.72915 -2.35895 H -3.81219 -2.56037 -0.82218 Th 0.42175 -0.00640 -0.22768 H -1.83762 -0.31601 -1.29499	
TS5b	C 0.72571 1.72969 -2.20899 C 2.01484 1.77525 -1.63637 C 2.01603 2.56555 -0.44539 C 0.64502 2.99899 -0.24427 C -0.10941 2.45292 -1.32862 H -1.16674 2.61228 -1.48346 C 0.26344 0.85017 -3.36579 C 1.36026 0.70657 -4.42984 H 2.27495 0.26472 -4.01792 H 1.62247 1.67966 -4.86517 H 1.01485 0.05092 -5.23868 C -0.08042 -0.51221 -2.72187 H -0.80656 -1.07598 -3.32132 H -1.09920 -0.28937 -1.65882 H 0.81567 -1.15373 -2.67538 C -0.98241 1.44700 -4.03475 H -1.29194 0.81587 -4.87687 H -0.77479 2.45296 -4.41904 H -1.83231 1.51202 -3.34848 C -2.08333 -0.06796 -0.61490 Th 0.37981 -0.02674 -0.14123 C -1.86117 -0.16023 0.71430 C 2.09943 -2.44576 -0.10855 C 0.80685 -2.90073 0.36675 C 0.58653 -2.25849 1.62158 H -0.28432 -2.41117 2.24412 C 1.70760 -1.47926 1.99087 C 2.60342 -1.56635 0.90318 H 2.90025 1.33478 -2.07770 C -0.00216 4.04358 0.69183 C 3.37746 3.02245 0.12106	

C	1.95857	-0.88231	3.37284
C	-0.14572	-4.02147	-0.10108
C	3.09295	-2.93412	-1.19051
H	3.59072	-1.12277	0.88514
C	1.78270	-1.99713	4.42405
H	2.46283	-2.83313	4.22537
H	1.99828	-1.61130	5.42880
H	0.75962	-2.38810	4.42668
C	0.96489	0.24678	3.68653
H	1.10882	0.62588	4.70648
H	1.10119	1.09584	3.00426
H	-0.07196	-0.09748	3.59717
C	3.39056	-0.34380	3.48728
H	4.12748	-1.13986	3.33022
H	3.59008	0.44840	2.75751
H	3.55738	0.07666	4.48624
C	-1.34892	-4.14427	0.85513
H	-2.02622	-4.92198	0.48254
H	-1.04236	-4.43341	1.86646
H	-1.91662	-3.21044	0.91737
C	-0.74186	-3.78862	-1.49922
H	-1.35737	-2.88277	-1.49622
H	0.01172	-3.67472	-2.27707
H	-1.38831	-4.63108	-1.77776
C	0.57491	-5.38422	-0.03549
H	-0.12853	-6.19152	-0.27680
H	1.41447	-5.46251	-0.72855
H	0.96029	-5.56355	0.97501
C	2.50464	-3.56455	-2.46155
H	1.87199	-2.86350	-3.01527
H	3.32865	-3.84979	-3.12715
H	1.92631	-4.46858	-2.26833
C	4.02446	-3.97445	-0.52591
H	4.77606	-4.33062	-1.24275
H	4.54975	-3.53635	0.32979
H	3.46463	-4.84233	-0.16331
C	3.97300	-1.76580	-1.67967
H	4.67333	-2.12267	-2.44465
H	3.36164	-0.97618	-2.13039
H	4.57108	-1.31754	-0.88169
C	3.86469	4.22449	-0.72136
H	3.94905	3.94484	-1.77733
H	3.17984	5.07452	-0.65698
H	4.85244	4.55740	-0.37580
C	4.43617	1.91142	-0.03601
H	4.13317	0.99422	0.47930
H	4.63507	1.66278	-1.08238
H	5.38584	2.24422	0.39976
C	3.40057	3.41958	1.60360
H	4.42974	3.65885	1.89827
H	2.79557	4.30112	1.81872
H	3.05719	2.60279	2.24769
C	0.62408	5.43498	0.46406
H	1.66711	5.48980	0.78150
H	0.58029	5.70968	-0.59611
H	0.06887	6.19221	1.03245
C	0.06202	3.67523	2.18439
H	1.07573	3.49869	2.54266



	H -0.36783 4.48400 2.78978 H -0.52808 2.77349 2.38088 C -1.50118 4.20279 0.36605 H -1.94704 4.92221 1.06320 H -1.66272 4.58212 -0.64879 H -2.04287 3.25720 0.47449 C -3.31905 0.03147 -1.41697 C -4.09933 1.20257 -1.37835 C -3.72169 -0.99042 -2.29553 C -5.23842 1.33766 -2.16930 H -3.80050 2.01367 -0.71967 C -4.86672 -0.85835 -3.07849 H -3.14121 -1.90745 -2.35007 C -5.63175 0.30663 -3.02283 H -5.82186 2.25417 -2.11623 H -5.16088 -1.67156 -3.73832 H -6.52160 0.41090 -3.63826 C -2.85799 -0.32581 1.84339 C -3.26313 1.02149 2.47491 C -4.12815 -1.12321 1.49337 H -2.34331 -0.88668 2.64375 C -4.16053 0.82531 3.70202 H -3.79667 1.62000 1.72279 H -2.36696 1.59011 2.75192 C -5.00818 -1.34433 2.72644 H -4.70222 -0.57878 0.73363 H -3.85665 -2.08602 1.04289 C -5.39829 -0.01314 3.37250 H -4.45749 1.80144 4.10845 H -3.58292 0.32150 4.49187 H -5.90761 -1.91140 2.45193 H -4.46383 -1.95877 3.46026 H -5.99350 -0.18423 4.27929 H -6.04028 0.54847 2.67738	
P5	C -1.19600 -1.43932 -2.35473 C -2.38243 -1.43284 -1.59035 C -2.30220 -2.36317 -0.50308 C -0.97210 -2.92929 -0.56250 C -0.32028 -2.31797 -1.68157 H 0.68966 -2.53913 -1.99877 C -0.83009 -0.42095 -3.42529 C -1.98351 -0.22940 -4.42130 H -2.90465 0.08870 -3.91935 H -2.20279 -1.15716 -4.96762 H -1.72244 0.54691 -5.15152 C -0.54111 0.85619 -2.59770 H 0.21529 1.49365 -3.07202 H 1.49977 0.22669 -1.62026 H -1.46343 1.45574 -2.54636 C 0.40948 -0.86348 -4.21191 H 0.64447 -0.11846 -4.98165 H 0.24244 -1.82680 -4.71017 H 1.29597 -0.96424 -3.57660 C 2.30774 -0.08561 -0.91171 Th -0.40680 0.03581 -0.21232 C 2.00786 -0.34989 0.38008 C -1.84188 2.60970 0.23834 C -0.45608 2.93814 0.48579	

C	-0.06566	2.19466	1.64416
H	0.90729	2.25760	2.10835
C	-1.14838	1.45130	2.15653
C	-2.21443	1.66473	1.24762
H	-3.27267	-0.87187	-1.84824
C	-0.31871	-4.14034	0.13257
C	-3.63405	-2.77031	0.17190
C	-1.23111	0.75304	3.51275
C	0.47575	4.04036	-0.06272
C	-2.98152	3.25793	-0.58453
H	-3.21982	1.28499	1.37949
C	-0.02808	1.13287	4.38816
H	0.02328	2.21625	4.54472
H	-0.11175	0.65127	5.36990
H	0.91761	0.80872	3.94031
C	-1.26902	-0.77354	3.36312
H	-1.36368	-1.26457	4.34055
H	-2.12228	-1.08978	2.75302
H	-0.35054	-1.15345	2.89943
C	-2.51375	1.21027	4.23334
H	-2.53412	2.30029	4.34373
H	-3.41497	0.90951	3.68745
H	-2.56719	0.76359	5.23429
C	1.85347	3.98422	0.62825
H	2.50496	4.74855	0.18802
H	1.78773	4.19078	1.70213
H	2.33994	3.01298	0.49051
C	0.76627	3.93752	-1.56922
H	1.35300	3.03705	-1.77892
H	-0.13173	3.89077	-2.18239
H	1.35581	4.80458	-1.89479
C	-0.10544	5.42774	0.28443
H	0.60075	6.21438	-0.01112
H	-1.05435	5.63440	-0.21422
H	-0.27214	5.51293	1.36462
C	-2.60310	3.99325	-1.87917
H	-2.13541	3.32921	-2.61149
H	-3.51841	4.38914	-2.33633
H	-1.93977	4.84298	-1.71243
C	-3.68718	4.27227	0.34712
H	-4.53560	4.73896	-0.17044
H	-4.06687	3.77739	1.24747
H	-3.00675	5.06792	0.66651
C	-4.03134	2.20259	-0.99114
H	-4.82941	2.68100	-1.57162
H	-3.58820	1.41991	-1.61614
H	-4.50607	1.72211	-0.13106
C	-4.39386	-3.66582	-0.83579
H	-4.57279	-3.13454	-1.77653
H	-3.82800	-4.57353	-1.06954
H	-5.36527	-3.96763	-0.42247
C	-4.50930	-1.52888	0.44502
H	-4.02406	-0.85003	1.15619
H	-4.74006	-0.96143	-0.46017
H	-5.46574	-1.84073	0.88229
C	-3.56513	-3.52621	1.50559
H	-4.58764	-3.71814	1.85347
H	-3.07152	-4.49587	1.42442



H	-3.06293	-2.94515	2.28464
C	-1.04846	-5.43278	-0.29164
H	-2.08599	-5.46526	0.04848
H	-1.05341	-5.52922	-1.38352
H	-0.53542	-6.31004	0.12354
C	-0.26262	-4.03807	1.66589
H	-1.23856	-3.90361	2.12715
H	0.18158	-4.95044	2.08496
H	0.36873	-3.19755	1.96913
C	1.14383	-4.30850	-0.32880
H	1.60092	-5.13932	0.22188
H	1.21654	-4.54487	-1.39588
H	1.73697	-3.40835	-0.13191
C	3.60886	-0.09652	-1.63543
C	4.38585	-1.26287	-1.71838
C	4.07220	1.05721	-2.28653
C	5.59622	-1.26738	-2.40970
H	4.02602	-2.17629	-1.25186
C	5.28412	1.05446	-2.97410
H	3.47906	1.96760	-2.24322
C	6.05276	-0.10801	-3.03635
H	6.18052	-2.18282	-2.46445
H	5.62710	1.96221	-3.46472
H	6.99672	-0.11236	-3.57535
C	3.12984	-0.64069	1.36284
C	3.68962	0.67998	1.93225
C	2.74584	-1.58091	2.51308
H	3.97059	-1.11649	0.83324
C	4.85372	0.44360	2.89793
H	2.88505	1.21558	2.45581
H	4.01274	1.32455	1.10595
C	3.90949	-1.81818	3.48048
H	1.89762	-1.14947	3.06338
H	2.40294	-2.54009	2.10780
C	4.46039	-0.50247	4.03382
H	5.20357	1.40287	3.30213
H	5.69971	0.01095	2.34346
H	3.58791	-2.47438	4.30000
H	4.71472	-2.35108	2.95241
H	5.32036	-0.69274	4.68931
H	3.69193	-0.02062	4.65711

Table S5. Frequencies of the stationary points optimized for conversion of **5**, obtained with B3PW91-PCM/6-31G(d)+sdd method.

Species	Frequencies (cm ⁻¹)
5	23 31 32 35 43 49 52 54 57 60 63 69 70 73 85 90 91 96 106 115 121 130 132 134 142 143 164 170 177 182 186 198 200 204 210 212 213 214 220 238 244 246 251 252 254 262 264 273 278 280 286 288 290 304 307 314 317 322 323 336 345 348 350 354 367 373 376 377 381 382 385 389 392 399 403 406 413 423 426 430 432 440 443 452 462 468 469 474 476 489 491 549 550 556 557 559 565 568 572 596 597 603 635 648 649 666 680 686 688 692 712 772 799 800 802 804 831 833 835 838 842 844 851 853 858 858 869 905 909 926 935 936 940 943 944 946 947 948 952 952 953 954 954 961 961 963 969 971 973 975 976 978 983 985 1010 1023 1024 1050 1051 1052 1052 1053 1056 1056 1058 1058 1061 1063 1068 1068 1069 1074 1093 1101 1107 1114 1147 1151 1168 1184 1200 1203 1204 1206 1206 1209 1224 1225 1226 1232 1234 1239 1239 1243 1248 1248 1250 1262 1262 1271 1273 1274 1276 1278 1296 1298 1319 1321 1326 1338 1342 1369 1375 1381 1381 1383 1392 1397 1400 1405 1406 1411 1414 1415 1416 1417 1418 1421 1421 1423 1425 1425 1427 1443 1444 1449 1451 1455 1456 1457 1459 1483 1493 1496 1497 1500 1501 1502 1503 1504 1504 1506 1507 1507 1508 1509 1512 1512 1513 1514 1517 1517 1518 1519 1520 1521 1524 1524 1524 1525 1529 1530 1532 1535 1536 1538 1538 1543 1545 1549 1551 1553 1553 1557 1568 1583 1597 1630 1661 2977 3029 3032 3034 3035 3039 3044 3047 3049 3049 3051 3052 3052 3054 3055 3055 3056 3056 3058 3058 3062 3064 3065 3067 3077 3078 3085 3096 3101 3108 3115 3119 3120 3121 3122 3122 3124 3124 3125 3125 3127 3127 3128 3129 3132 3132 3133 3135 3136 3138 3138 3141 3141 3146 3151 3155 3157 3158 3162 3165 3175 3180 3183 3183 3189 3191 3199 3204 3211 3218 3270 3272 3289 3293
TS5a	-1371i 19 26 33 42 46 48 49 52 58 62 63 66 69 70 81 85 92 99 110 123 127 127 130 140 146 152 162 174 176 181 187 191 196 197 203 209 216 223 235 237 238 242 250 254 256 260 264 266 272 276 283 289 297 298 303 305 315 317 322 329 335 347 348 352 366 370 372 378 381 385 386 390 392 398 405 410 419 423 427 429 431 439 450 456 458 468 472 495 498 523 541 554 555 557 562 575 586 592 597 597 602 635 648 649 679 681 691 699 711 723 743 766 769 798 798 799 819 829 829 833 839 842 845 852 855 856 871 900 905 918 933 933 939 940 942 945 945 946 949 951 953 954 958 960 962 966 967 969 971 975 983 986 986 1010 1011 1022 1023 1050 1050 1050 1050 1052 1053 1053 1055 1056 1059 1060 1063 1069 1072 1075 1078 1094 1107 1114 1141 1149 1167 1185 1196 1200 1201 1205 1206 1207 1223 1225 1227 1229 1231 1232 1238 1241 1242 1244 1246 1259 1262 1271 1272 1278 1278 1281 1296 1299 1301 1316 1318 1329 1337 1354 1368 1373 1382 1384 1388 1396 1398 1403 1404 1407 1410 1411 1412 1414 1414 1418 1419 1420 1421 1425 1426 1431 1441 1441 1449 1453 1454 1458 1460 1469 1483 1492 1496 1498 1501 1501 1502 1503 1504 1505 1506 1506 1507 1507 1509 1510 1511 1514 1516 1516 1517 1517 1519 1520 1521 1523 1525 1526 1527 1528 1530 1531 1533 1533 1537 1538 1544 1545 1550 1552 1553 1555 1628 1630 1642 1662 1908 2974 3014 3028 3030 3035 3043 3048 3050 3050 3050 3051 3053 3054 3055 3056 3056 3056 3059 3060 3061 3062 3062 3066 3068 3079 3079 3081 3086 3097 3107 3117 3118 3121 3121 3123 3124 3124 3124 3125 3125 3126 3127 3127 3129 3129 3130 3132 3133 3134 3135 3139 3141 3148 3149 3150 3150 3154 3163 3171 3176 3186 3186 3186 3192 3193 3206 3212 3220 3226 3259 3263 3282 3287

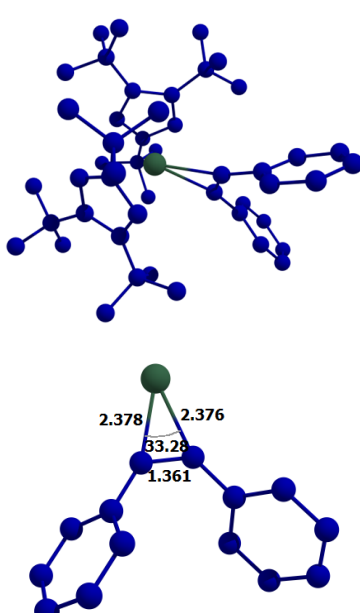
8	17 23 31 35 39 42 49 57 58 62 65 72 73 76 79 82 88 97 103 113 116 122 128 130 131 137 155 163 166 172 179 187 196 204 206 209 211 213 229 232 237 241 248 250 254 262 263 266 271 273 277 284 295 297 309 312 313 315 320 323 334 343 346 349 357 369 371 373 374 383 386 392 394 395 396 400 404 412 417 423 428 429 436 441 444 455 462 473 485 489 508 525 548 552 554 557 565 568 583 586 597 599 633 649 652 668 679 697 705 711 715 774 776 797 801 809 829 831 833 835 844 847 849 856 857 859 862 875 911 915 928 932 933 939 943 944 945 945 948 949 949 951 954 956 959 962 966 969 970 971 973 979 986 989 992 1011 1023 1026 1043 1047 1051 1051 1051 1053 1054 1055 1057 1060 1062 1063 1064 1064 1069 1096 1105 1110 1116 1144 1148 1168 1186 1194 1198 1199 1205 1208 1210 1217 1220 1223 1225 1230 1232 1239 1241 1242 1244 1247 1259 1260 1263 1269 1273 1276 1281 1298 1301 1314 1315 1326 1329 1341 1369 1374 1383 1390 1394 1396 1398 1402 1403 1403 1410 1411 1412 1413 1416 1417 1419 1419 1421 1424 1426 1429 1441 1443 1447 1450 1453 1453 1455 1459 1460 1483 1494 1496 1498 1500 1501 1502 1502 1504 1505 1505 1506 1507 1507 1508 1509 1510 1512 1514 1515 1516 1518 1519 1521 1521 1524 1524 1526 1528 1530 1530 1532 1534 1535 1537 1537 1542 1543 1545 1550 1552 1555 1558 1633 1654 1667 2861 3028 3030 3033 3035 3036 3037 3037 3048 3049 3049 3051 3051 3052 3052 3053 3054 3055 3056 3057 3061 3061 3062 3067 3068 3084 3084 3089 3091 3095 3097 3110 3119 3120 3121 3121 3122 3123 3123 3125 3125 3125 3126 3126 3127 3129 3129 3130 3133 3136 3137 3140 3141 3141 3142 3144 3146 3150 3159 3167 3171 3182 3186 3188 3195 3197 3214 3217 3223 3226 3254 3268 3275 3291
TS5b	-1324i 22 28 33 40 45 53 57 60 60 66 71 72 76 82 87 93 95 102 109 123 129 131 140 142 148 166 171 176 177 183 192 193 203 204 209 212 214 220 233 241 242 245 248 252 254 256 263 271 274 279 283 294 296 299 306 307 312 316 331 336 339 348 351 357 366 367 370 376 378 379 379 391 393 399 405 412 419 425 428 430 433 439 443 450 462 472 476 484 494 500 540 554 555 558 561 568 585 596 598 599 602 634 650 652 686 689 693 704 713 730 757 770 788 795 798 799 829 832 835 835 841 847 850 856 857 858 873 900 903 926 933 938 938 938 940 945 948 948 950 951 954 955 958 961 965 969 969 970 973 976 983 988 993 1012 1013 1024 1025 1047 1050 1051 1053 1053 1055 1056 1057 1059 1060 1062 1066 1068 1069 1074 1081 1093 1110 1113 1145 1150 1165 1187 1199 1200 1203 1206 1207 1210 1222 1224 1226 1230 1231 1234 1238 1242 1243 1245 1248 1259 1261 1270 1270 1275 1278 1280 1288 1297 1298 1316 1320 1331 1332 1342 1370 1372 1378 1386 1386 1394 1395 1401 1405 1406 1411 1412 1413 1414 1415 1418 1420 1420 1424 1425 1426 1436 1442 1444 1447 1452 1455 1460 1460 1469 1484 1495 1497 1497 1500 1502 1503 1503 1504 1505 1505 1507 1507 1508 1509 1509 1510 1513 1515 1516 1516 1517 1518 1519 1521 1523 1524 1527 1528 1529 1530 1530 1533 1534 1536 1538 1544 1545 1550 1551 1551 1553 1595 1598 1633 1663 1874 2972 3020 3025 3030 3033 3043 3044 3045 3049 3050 3051 3053 3053 3054 3055 3057 3057 3059 3062 3062 3064 3064 3066 3069 3078 3080 3085 3091 3098 3110 3115 3117 3121 3122 3123 3123 3123 3124 3124 3125 3125 3127 3127 3129 3129 3129 3133 3133 3134 3138 3139 3143 3144 3147 3149 3153 3157 3158 3170 3172 3183 3187 3189 3195 3199 3207 3209 3214 3221 3256 3257 3278 3287
P5	20 28 31 32 40 42 53 55 58 64 66 73 77 82 83 86 89 100 108 124 127 130 132 134 136 143 152 162 167 178 181 184 200 202 209 210 215 220 227 233 239 240 242 246 250 251 260 262 270 275 280 288 296 298 311 312 314 326 330 335 336 345 347 352 357 360 366 371 375 377

381	389	392	396	402	411	413	418	428	430	432	435	439	445
450	458	464	476	482	491	515	531	548	552	556	558	567	568
583	588	598	598	631	650	652	671	682	695	698	707	714	766
794	799	802	807	819	829	830	834	836	847	851	852	856	861
861	868	910	918	935	935	936	938	942	943	946	947	948	949
949	950	954	956	964	965	970	971	974	974	975	984	986	999
1010	1015	1023	1024	1049	1050	1051	1051	1053	1055	1056	1057	1059	1061
1061	1062	1066	1068	1072	1094	1100	1110	1123	1146	1149	1167	1188	1194
1201	1202	1205	1208	1211	1220	1223	1224	1232	1232	1235	1239	1241	1242
1243	1251	1260	1261	1268	1272	1274	1277	1282	1295	1300	1313	1315	1331
1337	1344	1371	1372	1380	1390	1391	1395	1396	1403	1403	1405	1411	1412
1413	1414	1416	1416	1418	1422	1422	1424	1425	1431	1442	1444	1447	1453
1454	1455	1458	1459	1477	1494	1497	1497	1498	1499	1500	1500	1503	1503
1504	1505	1506	1506	1508	1508	1509	1510	1514	1515	1517	1517	1517	1518
1520	1521	1523	1524	1527	1528	1529	1530	1531	1534	1535	1539	1541	1545
1546	1548	1550	1552	1554	1572	1633	1655	1667	2805	3010	3029	3030	3032
3034	3035	3046	3048	3049	3050	3050	3051	3051	3051	3052	3054	3055	3057
3058	3061	3062	3064	3067	3069	3081	3081	3087	3094	3101	3104	3108	3118
3120	3120	3121	3122	3122	3123	3125	3126	3126	3127	3129	3129	3130	3130
3135	3136	3138	3138	3139	3140	3146	3146	3147	3147	3152	3159	3160	3169
3180	3186	3192	3197	3207	3213	3214	3222	3224	3250	3266	3279	3296	

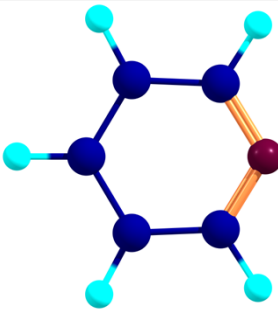
Table S6. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in kcal/mol) for conversion of **5**, obtained with B3PW91-PCM/6-31G(d)+sdd method

species	E	H	G (gas)	G (sol)
5	-2280.81471 (0.0)	-2279.64513 (0.0)	-2279.78732 (0.0)	-2279.77360 (0.0)
TS5a	-2280.78042 (21.5)	-2279.61723 (17.5)	-2279.75938 (17.5)	-2279.74565 (17.5)
8	-2280.81650 (-1.1)	-2279.64985 (-3.0)	-2279.79407 (-4.2)	-2279.78087 (-4.6)
TS5b	-2280.77716 (23.6)	-2279.61391 (19.6)	-2279.75432 (20.7)	-2279.74008 (21.0)
P5	-2280.80383 (6.8)	-2279.63667 (5.3)	-2279.77969 (4.8)	-2279.76605 (4.7)

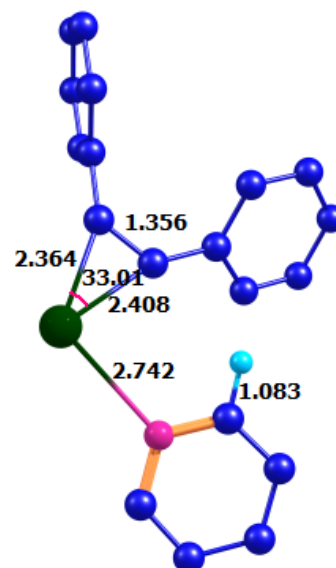
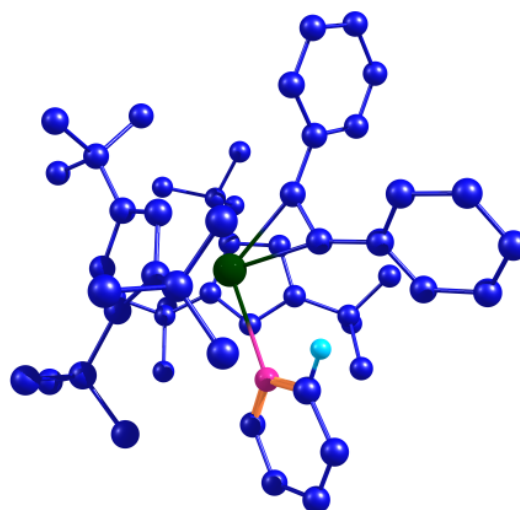
Table S7. The optimized Cartesian Coordinates (in Å) and structures (the hydrogen atoms omitted for clarity) of stationary points for **2**+Py, obtained with B3PW91-PCM/6-31G(d)+sdd method.

Species	Cartesian coordinates				
2	C	-0.50362	2.89095	-0.23088	
C	-1.89087	2.49331	-0.05584		
C	-2.25016	1.78102	-1.24194		
H	-3.24399	1.40789	-1.44960		
C	-1.17650	1.74063	-2.15577		
C	-0.10101	2.39133	-1.50580		
H	0.87329	2.55223	-1.94313		
C	0.42330	3.84235	0.55696		
C	-0.17912	5.26117	0.60756		
H	-1.09470	5.31485	1.19979		
H	-0.40973	5.62106	-0.40194		
H	0.54212	5.95545	1.05722		
C	0.74562	3.35335	1.97984		
H	1.38030	4.08635	2.49441		
H	1.29971	2.40826	1.94788		
H	-0.14464	3.20580	2.59188		
C	1.77981	3.98520	-0.16053		
H	2.43681	4.62708	0.43782		
H	1.67570	4.44929	-1.14781		
H	2.27806	3.01788	-0.27878		
C	-3.03518	2.95026	0.87864		
C	-3.67089	4.21789	0.26115		
H	-4.52410	4.54933	0.86754		
H	-4.03283	4.01247	-0.75230		
H	-2.95870	5.04526	0.19897		
C	-2.65795	3.25418	2.33529		
H	-1.95623	4.08314	2.43336		
H	-2.22916	2.38006	2.83721		
H	-3.56229	3.53426	2.88929		
C	-4.14545	1.88039	0.94380		
H	-3.75505	0.91688	1.28829		
H	-4.63696	1.72011	-0.02032		
H	-4.92227	2.20093	1.64804		
C	-1.21112	1.28459	-3.61325		
C	-0.68951	2.43192	-4.50055		
H	-1.29041	3.33787	-4.36222		
H	-0.73822	2.14673	-5.55913		
H	0.35198	2.67978	-4.26917		
C	-2.64630	0.95758	-4.05021		
H	-3.06987	0.12527	-3.47628		
H	-2.65807	0.66594	-5.10717		
H	-3.30764	1.82339	-3.93121		
C	-0.33133	0.04582	-3.84305		
H	0.70538	0.21351	-3.53420		
H	-0.32508	-0.23777	-4.90347		
H	-0.71490	-0.82047	-3.28783		
C	1.97516	0.04159	0.69082		
Th	-0.28992	-0.00782	-0.03197		
C	1.99833	-0.10829	-0.66204		
C	3.16982	-0.26881	-1.53633		
C	4.14773	-1.25437	-1.29680		
H	4.04761	-1.89479	-0.42511		

C	5.23528	-1.41683	-2.15123
H	5.96972	-2.19175	-1.94191
C	5.39556	-0.58564	-3.26094
H	6.24861	-0.70963	-3.92340
C	4.44710	0.40694	-3.50751
H	4.55902	1.06713	-4.36503
C	3.34620	0.55183	-2.66620
H	2.61213	1.32588	-2.87399
C	-0.61534	-2.87238	0.24455
C	-1.98758	-2.43864	0.03143
C	-2.35627	-1.70298	1.19998
H	-3.34416	-1.30053	1.37891
C	-1.30263	-1.67712	2.13811
C	-0.22999	-2.36613	1.52251
H	0.72868	-2.54853	1.98565
C	0.30701	-3.84898	-0.51863
C	-0.33104	-5.25138	-0.58681
H	-1.23593	-5.28151	-1.19681
H	-0.59096	-5.60665	0.41720
H	0.38105	-5.96343	-1.02306
C	0.68175	-3.36683	-1.93280
H	1.30274	-4.12029	-2.43435
H	1.26973	-2.44279	-1.88507
H	-0.18794	-3.18750	-2.56573
C	1.63814	-4.03073	0.23696
H	2.29122	-4.69563	-0.34026
H	1.49064	-4.48722	1.22219
H	2.16429	-3.07985	0.36747
C	-3.11845	-2.86904	-0.93132
C	-3.80606	-4.11437	-0.32464
H	-4.65061	-4.42832	-0.95218
H	-4.19005	-3.89256	0.67722
H	-3.11788	-4.95965	-0.23655
C	-2.71097	-3.19138	-2.37589
H	-2.02482	-4.03546	-2.45162
H	-2.25119	-2.32949	-2.87203
H	-3.60694	-3.45469	-2.95125
C	-4.19467	-1.76745	-1.03511
H	-3.76737	-0.81911	-1.37938
H	-4.70553	-1.58238	-0.08583
H	-4.96219	-2.07231	-1.75630
C	-1.37255	-1.21746	3.59407
C	-0.95493	-2.39252	4.50019
H	-1.60475	-3.26075	4.34176
H	-1.02295	-2.10233	5.55640
H	0.07675	-2.70406	4.30467
C	-2.80493	-0.81108	3.97016
H	-3.15528	0.04586	3.38360
H	-2.84573	-0.52294	5.02736
H	-3.50892	-1.63733	3.81908
C	-0.43715	-0.02965	3.86929
H	0.61030	-0.27744	3.67228
H	-0.51552	0.29498	4.91476
H	-0.69823	0.83269	3.24261
C	3.12088	0.17215	1.60367
C	4.13426	1.12765	1.39114
C	3.23850	-0.64890	2.74078
C	5.19845	1.26340	2.27897

	H 4.08134 1.76579 0.51372 C 4.31616 -0.53134 3.61591 H 2.47712 -1.40161 2.92777 C 5.29951 0.43320 3.39627 H 5.96110 2.01596 2.08991 H 4.38263 -1.19090 4.47862 H 6.13429 0.53603 4.08513	
Py	C -2.93685 0.00000 -3.14893 C -2.93685 1.19692 -2.43714 C -2.93685 1.14013 -1.04422 N -2.93685 0.00000 -0.34522 C -2.93685 -1.14013 -1.04422 C -2.93685 -1.19692 -2.43714 H -2.93685 0.00000 -4.23593 H -2.93685 2.15641 -2.94638 H -2.93685 2.05838 -0.45818 H -2.93685 -2.05838 -0.45818 H -2.93685 -2.15641 -2.94638	
COM10	C 2.00330 -2.40389 -0.52544 C 2.60986 -1.40456 -1.38815 C 1.63475 -1.10030 -2.38471 H 1.81887 -0.46529 -3.24045 C 0.47352 -1.89700 -2.22586 C 0.69223 -2.63276 -1.04288 H 0.00581 -3.36887 -0.64861 C -1.51961 -1.17366 0.91685 Th 0.25202 0.05187 -0.05604 C -2.11044 -0.41651 -0.04104 C -3.55417 -0.36721 -0.34422 C -4.52129 -0.31523 0.68218 H -4.19068 -0.33780 1.71591 C -5.88178 -0.23696 0.39858 H -6.59785 -0.19640 1.21674 C -6.33105 -0.22137 -0.92318 H -7.39441 -0.16779 -1.14373 C -5.39584 -0.27516 -1.95558 H -5.72640 -0.26800 -2.99231 C -4.03282 -0.33082 -1.66839 H -3.31980 -0.36652 -2.48642 C -0.21351 2.61717 1.51454 C 1.12274 2.86137 0.99576 C 1.96826 1.88598 1.60043 H 3.04087 1.84854 1.47841 C 1.24967 1.08764 2.52197 C -0.09638 1.50594 2.40424 H -0.90443 1.13664 3.02243 C -1.49170 3.48480 1.62992 C 1.76782 4.07407 0.28237 C 1.84472 0.35267 3.72536 C 2.56420 -3.46792 0.44750 C 4.04874 -0.86114 -1.52292 C -0.50457 -2.28988 -3.33249 C -2.11560 -2.19152 1.78883 C -2.31116 -1.96903 3.16536 C -2.50504 -3.44500 1.27745 C -2.86628 -2.94692 3.98803 H -2.04090 -1.00442 3.58816 C -3.04851 -4.42665 2.10286	

H	-2.38490	-3.63965	0.21499
C	-3.23281	-4.18730	3.46520
H	-3.01257	-2.73686	5.04566
H	-3.33873	-5.38419	1.67495
H	-3.65955	-4.95322	4.10792
C	0.30805	1.96192	-3.17651
C	-1.78195	2.06226	-2.23330
C	-2.27380	2.81232	-3.29774
C	-1.41786	3.13608	-4.34602
C	-0.09618	2.70191	-4.28077
H	1.33195	1.61175	-3.09734
H	-2.42408	1.76614	-1.41339
H	-3.31364	3.12257	-3.29626
H	-1.77175	3.71306	-5.19587
H	0.61558	2.92876	-5.06807
N	-0.51024	1.63274	-2.16289
C	3.37475	0.27588	3.62810
H	3.82629	1.27457	3.64431
H	3.77823	-0.28578	4.47919
H	3.70450	-0.22289	2.71183
C	1.27254	-1.05459	3.92344
H	1.64569	-1.49305	4.85803
H	0.18011	-1.04603	3.97142
H	1.56234	-1.72397	3.10941
C	1.50503	1.18807	4.98081
H	1.97629	0.74926	5.87021
H	1.86479	2.21786	4.87507
H	0.42422	1.22434	5.15507
C	3.27757	3.84791	0.05836
H	3.68785	4.69968	-0.49740
H	3.83351	3.77415	0.99886
H	3.47596	2.94615	-0.53232
C	1.20033	4.41280	-1.10611
H	0.11261	4.42448	-1.14313
H	1.56126	5.39914	-1.42624
H	1.55011	3.68810	-1.84684
C	1.67287	5.31133	1.20288
H	2.07859	5.08415	2.19529
H	2.25569	6.13951	0.77871
H	0.64880	5.66536	1.33315
C	-1.38528	4.28903	2.94858
H	-2.27764	4.91449	3.08517
H	-1.30869	3.61539	3.80885
H	-0.50882	4.94345	2.96106
C	-2.75266	2.60814	1.74136
H	-2.72024	1.92524	2.59492
H	-3.63339	3.24877	1.87451
H	-2.90638	2.00274	0.84524
C	-1.76885	4.47585	0.49176
H	-1.00698	5.25171	0.40212
H	-1.86135	3.97197	-0.47459
H	-2.72127	4.98469	0.68646
C	1.44845	-4.03146	1.35544
H	0.72237	-4.62809	0.79600
H	1.89069	-4.69400	2.10894
H	0.89155	-3.24964	1.87886
C	3.06346	-4.65783	-0.40807
H	3.88399	-4.37494	-1.07292

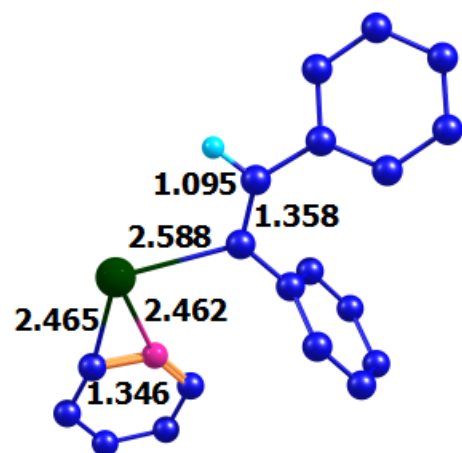
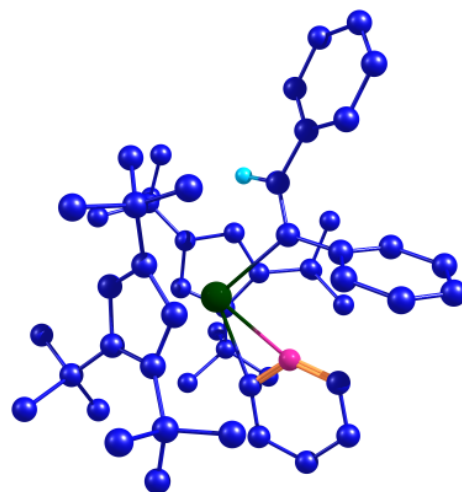


	H 3.41856 -5.46840 0.24225 H 2.25131 -5.05149 -1.02898 C 3.71089 -3.02906 1.36624 H 3.98260 -3.85907 2.02988 H 4.61328 -2.75467 0.81652 H 3.42421 -2.18603 2.00066 C 4.57398 -0.14555 -0.26785 H 4.52135 -0.76323 0.62757 H 5.62213 0.14840 -0.41067 H 3.99974 0.76622 -0.07795 C 4.13838 0.17600 -2.66092 H 5.15804 0.57619 -2.70578 H 3.91343 -0.25976 -3.64031 H 3.46409 1.02536 -2.49450 C 5.01862 -1.99577 -1.91308 H 4.65623 -2.52938 -2.79905 H 6.00722 -1.58009 -2.14689 H 5.15341 -2.72507 -1.11183 C 0.25055 -3.27981 -4.25084 H -0.40799 -3.63965 -5.05283 H 1.12294 -2.80377 -4.71353 H 0.60256 -4.14813 -3.68263 C -0.95060 -1.10538 -4.19773 H -0.09394 -0.58376 -4.63994 H -1.58017 -1.45913 -5.02384 H -1.52666 -0.37748 -3.62152 C -1.73597 -3.01411 -2.77357 H -2.43043 -3.26127 -3.58614 H -1.45464 -3.95623 -2.28917 H -2.26906 -2.40144 -2.04186	
TS10	C 1.42300 -2.79283 -0.32033 C 2.27007 -2.00357 -1.20402 C 1.42961 -1.56807 -2.26783 H 1.77112 -1.00009 -3.12192 C 0.11134 -2.06347 -2.11870 C 0.11752 -2.76132 -0.89138 H -0.72885 -3.30162 -0.49162 C -1.78461 -0.74645 0.84873 Th 0.28339 0.03053 -0.11804 C -2.23664 0.08704 -0.11757 C -3.64012 0.42223 -0.45013 C -4.59626 0.66404 0.55503 H -4.29995 0.58120 1.59561 C -5.90737 1.00730 0.23721 H -6.62194 1.19023 1.03661 C -6.30853 1.11369 -1.09548 H -7.33407 1.37729 -1.34193 C -5.37776 0.87910 -2.10645 H -5.67453 0.95437 -3.15028 C -4.06170 0.54942 -1.78631 H -3.35057 0.36857 -2.58735 C 0.35214 2.71200 1.31872 C 1.73520 2.60082 0.88949 C 2.27789 1.48212 1.58541 H 3.31594 1.18660 1.54486 C 1.33318 0.93044 2.48536 C 0.13881 1.65305 2.25399 H -0.77336 1.52179 2.82234	

C	-0.68702	3.86133	1.30402
C	2.69507	3.58102	0.17659
C	1.66434	0.13740	3.75146
C	1.69695	-3.91350	0.71147
C	3.79702	-1.79720	-1.29373
C	-0.90588	-2.26430	-3.24277
C	-2.60478	-1.58294	1.73682
C	-2.80662	-1.24864	3.08921
C	-3.20620	-2.76595	1.26702
C	-3.56917	-2.05627	3.93029
H	-2.37482	-0.32890	3.47651
C	-3.95937	-3.57849	2.11153
H	-3.08559	-3.03967	0.22251
C	-4.14580	-3.23226	3.45001
H	-3.71326	-1.76275	4.96799
H	-4.41149	-4.48594	1.71658
H	-4.73551	-3.86612	4.10733
C	0.99493	1.77581	-3.51814
C	-0.70082	1.77383	-1.90956
C	-1.46113	2.65896	-2.68887
C	-0.95234	3.11090	-3.90227
C	0.29772	2.65763	-4.33169
H	1.97308	1.39479	-3.80276
H	-1.45053	1.03221	-1.00033
H	-2.44137	2.97752	-2.34710
H	-1.52327	3.80368	-4.51579
H	0.72284	2.98229	-5.27639
N	0.50669	1.35963	-2.34111
C	3.14662	-0.26138	3.78151
H	3.79814	0.61969	3.80616
H	3.35636	-0.85636	4.67852
H	3.42799	-0.86101	2.91018
C	0.79943	-1.11380	3.92304
H	1.00458	-1.59836	4.88658
H	-0.26701	-0.87689	3.88742
H	1.00253	-1.84457	3.13665
C	1.41070	1.06907	4.95772
H	1.70848	0.57328	5.89100
H	1.98500	1.99795	4.86486
H	0.35137	1.33504	5.04102
C	4.11250	2.98352	0.05478
H	4.74763	3.68401	-0.50084
H	4.58477	2.81971	1.02927
H	4.11308	2.03550	-0.49466
C	2.30061	3.97632	-1.25686
H	1.24949	4.23667	-1.36430
H	2.89971	4.83629	-1.58398
H	2.50890	3.15338	-1.94572
C	2.85911	4.84333	1.05236
H	3.15828	4.56818	2.07030
H	3.63919	5.49205	0.63268
H	1.94441	5.43437	1.12379
C	-0.49985	4.65805	2.61814
H	-1.22027	5.48554	2.66737
H	-0.66052	4.01569	3.49073
H	0.50620	5.08124	2.69868
C	-2.12617	3.31335	1.30671
H	-2.32746	2.64556	2.14871

	H -2.83500 4.14769 1.37851 H -2.34735 2.76317 0.38930 C -0.62391 4.85497 0.13636 H 0.30699 5.42294 0.10108 H -0.76126 4.35578 -0.82614 H -1.43724 5.58342 0.24736 C 0.45015 -4.17218 1.58701 H -0.36397 -4.63069 1.01808 H 0.70552 -4.86976 2.39343 H 0.05351 -3.25995 2.03992 C 1.94316 -5.22082 -0.08146 H 2.83052 -5.15819 -0.71716 H 2.08147 -6.06186 0.61125 H 1.08636 -5.44814 -0.72515 C 2.88450 -3.71114 1.66150 H 2.93361 -4.55237 2.36360 H 3.84202 -3.67993 1.13752 H 2.78584 -2.79758 2.25425 C 4.42354 -1.17405 -0.03706 H 4.21057 -1.73924 0.86924 H 5.51420 -1.11574 -0.14691 H 4.05117 -0.15644 0.10957 C 4.14879 -0.84570 -2.45524 H 5.22981 -0.66280 -2.45897 H 3.88447 -1.26886 -3.43042 H 3.64969 0.12536 -2.35106 C 4.50131 -3.13319 -1.61019 H 4.05852 -3.60724 -2.49359 H 5.56515 -2.95678 -1.81589 H 4.44340 -3.84264 -0.78177 C -0.38536 -3.44192 -4.09978 H -1.09187 -3.67026 -4.90900 H 0.58515 -3.20394 -4.54998 H -0.26136 -4.34358 -3.48945 C -1.04078 -1.04319 -4.16018 H -0.07512 -0.74902 -4.58566 H -1.71240 -1.27324 -4.99692 H -1.45054 -0.17917 -3.62930 C -2.28893 -2.65176 -2.70259 H -2.99572 -2.77275 -3.53283 H -2.25298 -3.60628 -2.16498 H -2.68811 -1.89359 -2.02304	
10	C 2.48505 -1.89735 -1.12194 C 1.94737 -2.56283 0.04529 C 0.57533 -2.83578 -0.25317 H -0.08005 -3.40620 0.38996 C 0.25003 -2.45268 -1.57289 C 1.41156 -1.80879 -2.06558 H 1.52438 -1.44292 -3.07719 C 3.92661 -1.55756 -1.55425 C 3.94561 -0.90055 -2.94797 H 3.35088 0.01765 -2.97347 H 3.57975 -1.57261 -3.73204 C 4.75148 -2.85421 -1.69989 H 5.73525 -2.62226 -2.12810 H 4.92069 -3.36371 -0.75003 H 4.24788 -3.55814 -2.37254 C 4.64097 -0.56671 -0.62164	

H	4.18355	0.42321	-0.70649
H	4.60572	-0.85963	0.42636
H	5.69524	-0.46749	-0.91238
C	2.57854	-3.33953	1.22829
C	3.90204	-2.81048	1.79686
H	4.71760	-2.82139	1.07270
H	3.79379	-1.79552	2.18750
H	4.20997	-3.45217	2.63213
C	1.61035	-3.42437	2.42606
H	1.36785	-2.43575	2.82181
H	0.67329	-3.93218	2.18022
H	2.08196	-4.00209	3.23047
C	2.80906	-4.79037	0.73849
H	3.49502	-4.83334	-0.11253
H	3.23366	-5.40016	1.54711
H	1.86443	-5.24997	0.42727
C	-0.87239	-3.04578	-2.42441
C	-1.42710	-2.05910	-3.45796
H	-1.98159	-1.25082	-2.97318
H	-0.63085	-1.62160	-4.07103
C	-0.24930	-4.23764	-3.18842
H	-1.01354	-4.74605	-3.79097
H	0.54899	-3.90435	-3.86150
H	0.17950	-4.96819	-2.49308
C	-2.02826	-3.58099	-1.56993
H	-1.69349	-4.37810	-0.89560
H	-2.48429	-2.78760	-0.97154
C	1.30286	2.93419	-0.01209
C	-0.13753	3.00199	0.13586
C	-0.68746	2.52917	-1.09121
H	-1.74468	2.51705	-1.31195
C	0.32729	2.21944	-2.02538
C	1.54444	2.40508	-1.32020
H	2.52799	2.31499	-1.76682
C	2.47391	3.63685	0.71443
C	2.33857	3.83440	2.23110
H	2.22672	2.88139	2.75418
H	3.24995	4.31521	2.60897
H	1.50374	4.47899	2.50675
C	3.79466	2.87464	0.50324
H	4.08796	2.82358	-0.55001
H	4.60515	3.38964	1.03337
H	3.72557	1.85612	0.89250
C	2.64845	5.02655	0.05549
H	2.85251	4.92532	-1.01638
H	1.75522	5.64746	0.16670
H	3.49166	5.56023	0.51390
C	-1.06227	3.67799	1.17383
C	-0.80098	5.19966	1.20816
H	-1.55714	5.68958	1.83520
H	0.17679	5.46335	1.61427
H	-0.87256	5.62625	0.20071
C	-0.96003	3.08332	2.58855
H	-1.54692	3.68842	3.29242
H	-1.36899	2.06896	2.60251
H	0.06265	3.03253	2.96086
C	-2.54147	3.53369	0.75994
H	-3.17456	3.96253	1.54612



H	-2.76395	4.07384	-0.16754
H	-2.83055	2.48646	0.62897
C	0.15300	2.24180	-3.54477
C	-1.24430	1.77854	-3.97489
H	-2.02948	2.40422	-3.53625
H	-1.34347	1.84663	-5.06517
H	-1.43375	0.74019	-3.68846
C	1.20679	1.41187	-4.28471
H	1.10853	0.34639	-4.05857
H	1.09357	1.53639	-5.36877
H	2.22381	1.72498	-4.02463
C	0.31784	3.71673	-3.98161
H	-0.42022	4.35682	-3.48552
H	1.31514	4.09323	-3.72818
H	0.18116	3.81327	-5.06690
C	-2.89676	-0.08436	-0.61958
H	-2.43229	0.38175	-1.49474
C	-2.07771	-0.38856	0.41941
C	-2.62472	-0.88924	1.69923
C	-3.37962	-0.04534	2.53962
H	-3.59822	0.96618	2.20914
C	-3.85533	-0.48261	3.77432
H	-4.43423	0.19739	4.39583
C	-3.60365	-1.78482	4.21013
H	-3.97780	-2.12806	5.17132
C	-2.86689	-2.63977	3.38931
H	-2.66523	-3.66029	3.70795
C	-2.37845	-2.19548	2.16158
H	-1.80575	-2.87406	1.53768
C	1.70871	0.22107	2.01648
C	2.67656	0.35337	3.02876
H	3.71044	0.57439	2.77580
C	2.30889	0.20531	4.36094
H	3.05080	0.30264	5.15086
C	0.97407	-0.06849	4.68709
H	0.65906	-0.18724	5.71928
C	0.05346	-0.18966	3.65920
H	-0.99567	-0.40248	3.83983
N	0.44052	-0.04700	2.37953
Th	0.42418	0.04699	-0.08029
C	-4.35229	-0.24976	-0.82469
C	-4.97039	0.51681	-1.83023
C	-5.15794	-1.15582	-0.11016
C	-6.33335	0.41246	-2.09322
C	-6.51958	-1.26722	-0.37813
C	-7.11788	-0.48110	-1.36411
H	-4.36456	1.20959	-2.41173
H	-4.71211	-1.78561	0.65122
H	-6.78211	1.02515	-2.87169
H	-7.11792	-1.97890	0.18611
H	-8.18209	-0.57077	-1.56760
H	-2.12066	-2.57114	-4.13642
H	-2.80423	-4.00646	-2.21789
H	4.97788	-0.63225	-3.20301

Table S8. Frequencies of the stationary points optimized for **2**+Py, obtained with B3PW91-PCM/6-31G(d)+sdd method.

Species	Frequencies (cm ⁻¹)
2	6 19 24 31 34 43 44 49 61 65 67 74 77 80 87 91 94 102 105 110 124 130 133 135 137 155 169 175 175 184 191 200 202 203 204 210 214 218 241 242 245 250 252 255 257 264 266 271 271 282 285 286 289 305 310 316 316 329 330 346 346 350 353 367 368 372 373 373 378 380 387 390 402 402 414 415 419 424 427 434 452 453 470 473 478 480 486 487 553 554 555 559 562 566 567 588 596 597 608 630 635 648 649 679 682 685 689 696 710 711 769 785 796 800 805 828 828 832 834 840 842 850 852 854 855 900 914 932 933 937 942 944 946 946 947 949 950 950 951 953 957 962 964 965 966 967 972 973 974 976 988 988 1011 1012 1022 1022 1047 1049 1052 1052 1053 1055 1057 1058 1059 1061 1062 1063 1069 1074 1107 1108 1147 1148 1170 1185 1185 1199 1200 1205 1206 1207 1209 1223 1224 1229 1230 1234 1237 1242 1245 1247 1248 1261 1261 1263 1272 1273 1276 1279 1317 1319 1327 1329 1369 1370 1378 1382 1405 1406 1412 1412 1415 1416 1417 1419 1420 1421 1422 1423 1425 1426 1441 1441 1449 1450 1453 1454 1457 1457 1483 1485 1493 1496 1501 1501 1502 1503 1503 1504 1506 1507 1509 1511 1512 1513 1516 1517 1517 1518 1520 1520 1521 1523 1524 1527 1528 1531 1532 1532 1533 1534 1536 1536 1542 1543 1547 1551 1553 1557 1579 1591 1628 1631 1633 1660 1662 3049 3049 3051 3051 3052 3053 3053 3054 3055 3056 3057 3058 3059 3061 3061 3061 3066 3066 3119 3121 3121 3122 3123 3123 3123 3124 3124 3125 3126 3126 3128 3129 3129 3131 3131 3133 3133 3134 3137 3138 3145 3145 3146 3146 3149 3153 3156 3157 3168 3169 3183 3184 3184 3185 3191 3191 3192 3193 3205 3205 3213 3214 3221 3221 3268 3269 3286 3286
Py	382 417 610 666 718 764 899 960 998 1014 1016 1053 1091 1104 1181 1255 1333 1394 1488 1533 1649 1656 3181 3184 3207 3222 3230
COM10	14 20 31 36 41 42 46 49 56 57 60 64 69 69 75 76 83 85 89 94 103 104 109 111 116 123 126 129 140 143 149 154 158 172 175 176 190 193 196 198 200 201 208 215 231 239 243 246 248 252 258 260 266 268 276 278 283 289 293 300 305 312 314 316 324 332 338 345 350 352 357 364 367 372 376 378 383 385 393 393 403 408 413 418 424 426 427 431 434 438 462 464 470 477 477 498 532 533 553 554 555 562 563 585 594 597 606 623 631 635 647 648 663 673 674 679 685 688 714 716 729 767 769 782 785 802 815 827 828 830 831 842 848 853 855 857 859 894 904 918 931 931 934 935 936 939 939 947 948 952 953 955 957 961 961 963 965 966 967 968 970 971 974 985 990 992 1010 1012 1019 1021 1023 1027 1028 1048 1048 1050 1050 1051 1052 1053 1055 1055 1056 1057 1060 1060 1060 1062 1097 1103 1105 1109 1139 1141 1173 1184 1184 1185 1197 1197 1205 1205 1208 1210 1221 1222 1225 1229 1232 1233 1234 1242 1243 1245 1246 1254 1260 1260 1270 1272 1277 1278 1317 1319 1326 1332 1334 1369 1370 1374 1378 1383 1403 1403 1408 1409 1411 1413 1415 1415 1416 1416 1421 1422 1424 1425 1441 1442 1443 1446 1452 1453 1457 1458 1482 1484 1488 1496 1498 1499 1500 1501 1501 1504 1505 1506 1507 1508 1509 1510 1514 1514 1515 1518 1519 1520 1521 1521 1522 1522 1523 1524 1527 1529 1530 1530 1531 1532 1535 1536 1538 1541 1543 1544 1548 1551 1553 1554 1588 1629 1632 1643 1659 1662 1669 3042 3045 3048 3050 3051 3051 3054 3055 3055 3057 3060 3062 3063 3063 3064 3066 3068 3072 3115 3119 3119 3120 3121 3123 3124 3124 3125 3125 3126 3133 3134 3134 3134 3136 3138 3138 3138 3139 3141 3142 3150 3153 3159 3161 3161

	3165 3169 3171 3171 3172 3179 3182 3182 3184 3188 3192 3201 3207 3210 3211 3216 3217 3219 3225 3228 3234 3241 3250 3260 3273 3275 3282 3286
TS10	-1353i 21 24 32 40 41 46 49 50 55 57 63 65 70 73 77 79 83 87 91 97 98 100 112 120 124 130 139 145 146 149 155 169 174 180 184 186 191 192 198 201 207 209 222 226 232 240 246 247 249 252 254 256 266 268 273 278 279 288 292 301 304 310 315 321 325 339 340 344 351 354 358 366 369 370 374 379 382 385 392 393 396 400 410 415 418 427 430 433 435 436 461 463 466 474 477 496 532 533 554 555 557 562 563 585 594 596 604 630 635 639 647 648 665 676 682 685 689 691 712 717 744 768 774 787 805 813 815 828 829 830 832 847 852 855 856 857 857 896 916 920 933 933 934 935 938 939 941 948 951 953 954 954 956 959 962 963 963 964 968 970 970 971 976 981 987 994 1010 1013 1020 1021 1025 1025 1047 1048 1049 1050 1051 1053 1054 1055 1056 1058 1060 1060 1060 1062 1068 1104 1106 1112 1141 1145 1149 1176 1185 1187 1188 1197 1201 1203 1205 1207 1209 1212 1222 1222 1228 1230 1233 1234 1235 1240 1243 1247 1253 1261 1261 1271 1275 1277 1279 1290 1316 1319 1321 1327 1335 1370 1372 1375 1376 1400 1404 1408 1410 1411 1412 1414 1415 1415 1418 1421 1422 1423 1425 1441 1442 1443 1444 1452 1453 1456 1459 1464 1483 1485 1494 1497 1499 1499 1499 1500 1502 1504 1505 1505 1507 1508 1508 1509 1513 1515 1516 1517 1519 1520 1521 1522 1523 1524 1524 1525 1526 1529 1529 1531 1534 1534 1535 1536 1542 1545 1545 1547 1551 1554 1555 1590 1614 1630 1636 1643 1661 1663 1892 3042 3046 3047 3048 3050 3051 3053 3054 3055 3056 3059 3062 3062 3064 3064 3065 3068 3071 3117 3119 3120 3120 3120 3123 3124 3124 3125 3126 3126 3132 3135 3135 3136 3137 3137 3139 3140 3141 3141 3142 3145 3149 3153 3155 3158 3165 3166 3170 3171 3174 3177 3184 3184 3188 3190 3196 3202 3203 3208 3209 3212 3213 3219 3220 3220 3228 3233 3235 3258 3271 3282 3293
10	20 23 30 32 43 45 46 49 54 60 62 68 71 75 75 78 82 87 89 95 98 100 111 117 123 124 127 137 146 153 158 166 168 176 185 190 194 198 204 205 209 216 219 232 237 241 243 248 249 255 257 258 263 270 271 272 276 282 290 292 296 303 308 312 315 319 329 334 346 349 352 357 364 370 372 379 382 388 393 397 403 404 405 411 417 425 427 431 434 436 464 465 466 472 474 476 530 537 538 553 554 554 561 562 596 596 598 629 633 637 647 647 675 678 679 693 695 698 711 715 737 773 775 782 796 803 809 828 831 831 831 846 854 856 856 858 862 876 910 921 923 931 932 934 938 940 945 949 949 950 951 953 956 958 960 963 964 968 969 970 971 972 974 976 982 986 1000 1011 1013 1020 1022 1022 1026 1049 1049 1050 1051 1053 1054 1054 1055 1057 1057 1058 1060 1061 1063 1063 1090 1106 1118 1138 1141 1143 1181 1185 1188 1188 1195 1199 1203 1206 1208 1215 1223 1224 1228 1231 1233 1237 1238 1241 1242 1244 1244 1261 1261 1274 1274 1276 1278 1289 1314 1316 1323 1326 1334 1367 1378 1381 1387 1400 1400 1408 1410 1411 1412 1413 1414 1414 1417 1418 1420 1421 1423 1424 1441 1442 1444 1445 1450 1451 1455 1458 1460 1482 1484 1492 1497 1499 1499 1500 1502 1504 1504 1505 1505 1506 1507 1508 1510 1511 1515 1518 1519 1520 1522 1522 1522 1523 1524 1525 1528 1528 1530 1531 1531 1534 1535 1539 1540 1542 1542 1545 1548 1551 1554 1555 1608 1617 1629 1640 1647 1659 1667 3044 3044 3048 3049 3052 3053 3054 3055 3057 3058 3060 3060 3061 3062 3063 3064 3067 3070 3105 3118 3118 3120 3120 3121 3122 3123 3124 3124 3124 3128 3128 3129 3132 3134 3137 3138 3139 3141 3142 3151 3152 3152 3154 3155 3155 3158 3165 3171 3175 3175 3179 3182 3186 3188 3190 3193 3194 3194 3201 3203 3210 3212 3213 3217 3220 3227 3228 3243 3244 3248 3278 3281 3289

Table S9. The energies, enthalpies and free energies (in au at 298 K) and corresponding relative values (in a.u.) for **2**+Py, obtained with B3PW91-PCM/6-31G(d)+sdd method.

species	E	H	G (gas)	G (sol)
2	-2277.18902	-2276.09185	-2276.23475	-2276.22130
Py	-248.19074	-248.09620	-248.12815	-248.11445
2 +Py	-2525.37976 (0.0)	-2524.18805 (0.0)	-2524.3629 (0.0)	-2524.33575 (0.0)
COM10	-2525.36609	-2524.17254	-2524.32772	-2524.31418
TS10	-2525.32528 (34.2)	-2524.13739 (31.8)	-2524.29058 (45.4)	-2524.27687 (36.9)
10	-2525.38220 (-1.5)	-2524.18892 (-0.5)	-2524.34294 (12.5)	-2524.32930 (4.0)

Table S10. The energies, zero-point (vibrational) energy (ZPE) and entropies (at 298 K) for **2**+Py, obtained with B3PW91-PCM(+D3)/6-31G(d)+sdd method.

species	E ^a	ZPE ^b	S (gas) ^c	S (sol) ^c
2	-1905.55025	1.04123	300.896	272.579
Py	-248.19591	0.08932	67.281	38.413
2 +Py	-2153.74616	1.13055	368.177	310.992
COM10	-2153.75561	1.13134	326.772	298.268
TS10	-2153.72198	1.12613	322.571	293.714
10	-2153.77532	1.13126	324.326	295.615

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

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

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