

Explicit Roles of Diverse Directing Groups in Determining Transition State Energy and Reaction Exothermicity of C–H Activation Pathways

Lei Zhang, De-Cai Fang*

College of Chemistry, Beijing Normal University, Beijing 100875, China

E-mail: dcfang@bnu.edu.cn

Table S1. Cartesian coordinates of some stationary points in C–H activation pathways, optimized at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent.

Names	Cartesian Coordinates							
CAT	H	-4.35032	0.89789	-0.47243	O	1.79274	1.09248	0.01755
	C	-3.96283	0.00006	0.01346	C	2.46729	0.00007	0.01677
	C	-2.46731	-0.00004	-0.01621	O	1.79272	-1.09235	0.01762
	H	-4.29388	0.00105	1.05787	C	3.96284	-0.00004	-0.01280
	H	-4.35035	-0.89880	-0.47058	H	4.35022	-0.89659	0.47559
	O	-1.79278	-1.09245	-0.01761	H	4.29393	-0.00436	-1.05720
	O	-1.79270	1.09235	-0.01753	H	4.35036	0.90020	0.46857
	Pd	0.00001	0.00000	-0.00021				
TS-1	C	1.97163	1.60570	1.40407	H	3.70790	-2.26770	0.27565
	C	2.84049	1.89606	0.34997	O	0.86545	-2.23163	0.86827
	C	2.33323	2.32715	-0.88761	O	1.30435	-1.06794	-0.94554
	C	0.95698	2.47157	-1.07069	Pd	-0.42753	-0.51647	-0.02253
	C	0.07482	2.17932	-0.01534	O	-2.47268	0.03462	-1.26265
	C	0.58437	1.74222	1.22587	C	-2.96767	0.04454	-0.10877
	H	2.36345	1.27843	2.36430	O	-2.19317	-0.17120	0.91868
	H	0.56314	2.81483	-2.02442	C	-4.43214	0.27092	0.15402
	H	-0.98991	2.36412	-0.13294	H	-4.86873	0.86844	-0.64885
	H	-0.09229	1.57027	2.05979	H	-4.93978	-0.69961	0.17878
	H	3.21561	-2.72597	-1.36707	H	-4.58294	0.75826	1.11992
	C	2.92128	-2.74887	-0.31576	H	3.91460	1.79263	0.48776
	C	1.63558	-2.00218	-0.10812	H	3.01642	2.55377	-1.70309
	H	2.81556	-3.77943	0.03040				
INT-1	C	0.66212	-1.92060	-0.85363	H	1.51739	4.08785	1.23110
	C	2.00072	-1.78384	-1.29655	O	-0.32230	2.40039	-0.24896
	C	3.02741	-1.67792	-0.36875	O	1.56235	1.34174	0.13313
	C	2.74986	-1.71249	1.01819	Pd	-0.16710	0.21720	-0.20224
	C	1.44667	-1.85526	1.47149	O	-2.69951	0.06386	1.38560
	C	0.38232	-1.95785	0.53956	C	-2.92064	-0.36382	0.24600
	H	-0.12753	-2.13409	-1.56936	O	-2.00154	-0.50526	-0.68510

	H	3.56768	-1.63654	1.73091	C	-4.31122	-0.76239	-0.22403
	H	1.23177	-1.90388	2.53593	H	-4.72055	0.04188	-0.84466
	H	-0.61352	-2.21870	0.88724	H	-4.27536	-1.66748	-0.83521
	H	1.19346	4.52582	-0.45503	H	-4.96523	-0.91163	0.63689
	C	1.63574	3.76431	0.19112	H	2.21453	-1.77532	-2.36229
	C	0.92614	2.45607	0.00924	H	4.05596	-1.57573	-0.70688
	H	2.70153	3.65380	-0.01888				
TS-2	C	-1.05157	0.96853	-0.00141	H	4.99703	-0.66641	-0.43443
	C	-1.15103	1.68452	1.21819	O	2.52565	-1.34805	-0.01182
	C	-1.35119	3.06588	1.22321	O	2.10951	0.81617	-0.01789
	C	-1.44532	3.75971	0.00775	Pd	0.48268	-0.52499	-0.00539
	C	-1.35113	3.07382	-1.21224	O	-2.68079	-1.10231	-0.00706
	C	-1.15075	1.69253	-1.21626	C	-1.99857	-2.17920	0.00030
	H	-1.83103	-0.10073	-0.00529	O	-0.72594	-2.21685	0.00367
	H	-1.59736	4.83724	0.01126	C	-2.74718	-3.49369	0.01318
	H	-1.43622	3.61682	-2.15102	H	-3.45666	-3.51385	-0.81831
	H	-1.09179	1.16240	-2.16521	H	-2.05801	-4.33475	-0.05765
	H	4.75075	0.24168	1.06935	H	-3.32306	-3.56331	0.94092
	C	4.43441	0.14916	0.02444	H	-1.09248	1.14814	2.16365
	C	2.96211	-0.14890	-0.01136	H	-1.43627	3.60274	2.16552
	H	4.64576	1.09391	-0.48105				
INT-2	C	-3.12879	-2.83451	0.03349	H	4.80331	-1.30127	-0.94474
	C	-1.95695	-3.09139	0.75564	H	5.19400	-0.18158	0.37450
	C	-0.87526	-2.20006	0.69195	H	4.57008	-1.82655	0.72869
	C	-0.97734	-1.04226	-0.08971	C	-1.22716	2.66572	0.26252
	C	-2.14522	-0.77853	-0.81675	O	-0.64644	1.91362	-0.53159
	C	-3.21852	-1.68117	-0.75432	O	-1.26782	2.47160	1.57519
	H	-1.87627	-3.98933	1.36568	H	-0.77552	1.64396	1.81857
	H	-2.22977	0.11146	-1.43533	C	-1.96406	3.89540	-0.18299
	H	-4.12280	-1.47735	-1.32503	H	-3.02139	3.79884	0.08223
	Pd	0.60170	0.17525	-0.18366	H	-1.57117	4.76937	0.34439
	C	3.09390	-0.43985	-0.00599	H	-1.85886	4.02448	-1.25906
	O	2.11899	-1.28118	0.09954	H	0.03902	-2.42031	1.23777
	O	2.85645	0.79165	-0.18319	H	-3.96375	-3.53028	0.08081
	C	4.50702	-0.96810	0.05621				
1A	H	-0.01416	-2.15304	0.21775	C	1.85716	1.23138	-0.13759
	H	2.47774	-2.09700	0.26905	C	0.45909	1.19752	-0.15139
	H	3.67458	0.07562	0.03321	C	-0.22189	-0.02457	-0.01472
	C	-1.72222	-0.12860	-0.03279	C	0.51799	-1.21039	0.12573
	O	-2.29571	-1.19245	-0.30930	C	1.91402	-1.17437	0.15040
	N	-2.42532	1.00918	0.24380	C	2.58721	0.04724	0.01909
	H	-3.43340	0.91627	0.33349	H	2.37535	2.18044	-0.25439
	H	-1.99657	1.79837	0.71461	H	-0.08883	2.12545	-0.29831
TS5-1A	H	-3.47145	-3.52259	1.25811	C	2.04787	-1.58097	0.06154

	O	-3.34992	-0.82309	0.18949	C	2.55314	-0.35197	0.51655
	O	-1.45504	-1.87422	-0.14165	C	3.80646	0.09176	0.05963
	Pd	-1.42683	0.19804	-0.08066	C	4.54494	-0.68756	-0.83534
	O	0.48165	0.33574	1.53337	C	4.04295	-1.91887	-1.27379
	H	1.07557	-1.91819	0.40721	C	2.79355	-2.36336	-0.82318
	C	-0.67262	2.58233	-0.78707	H	4.19907	1.05754	0.36975
	O	0.09578	1.71526	-1.26640	H	5.50763	-0.33132	-1.19457
	O	-1.69650	2.20353	-0.07230	H	4.62020	-2.52581	-1.96790
	C	-0.45995	4.06194	-0.96884	H	2.39925	-3.31805	-1.16373
	H	0.08732	4.24993	-1.89483	C	1.72276	0.44793	1.47275
	H	-1.41428	4.59347	-0.97424	H	-2.87181	-4.02544	-0.33589
	H	0.13597	4.43959	-0.13074	C	-3.42375	-3.24930	0.19824
	N	2.37483	1.31594	2.28754	C	-2.72597	-1.92893	0.07080
	H	1.82613	1.80980	2.98674	H	-4.44505	-3.17343	-0.18143
	H	3.37795	1.26725	2.43089				
INT5-1A	O	-2.19204	-1.70161	0.42856	C	3.45717	-0.12497	-0.04935
	Pd	-1.12575	0.13148	0.46208	C	4.01792	-0.55569	-1.25437
	O	0.40422	-0.18149	1.88428	C	3.40427	-1.57801	-1.98788
	H	0.73569	-2.19078	0.04171	C	2.22158	-2.16443	-1.52022
	C	-0.12943	2.49221	-0.85769	H	3.92852	0.68285	0.50613
	O	-0.07747	1.80343	-1.88390	H	4.92954	-0.09085	-1.62191
	O	-0.48652	2.05596	0.32889	H	3.84497	-1.91488	-2.92345
	C	0.20081	3.97999	-0.86573	H	1.74652	-2.96227	-2.08592
	H	0.71162	4.27823	0.05282	C	1.65283	-0.27089	1.70177
	H	0.81433	4.21902	-1.73646	H	-4.05956	-3.01881	-0.78345
	H	-0.73336	4.54868	-0.92831	C	-4.25735	-1.94606	-0.82705
	N	2.47299	0.02001	2.72195	C	-3.06138	-1.17593	-0.35530
	H	2.07097	0.32117	3.60797	H	-4.52353	-1.64483	-1.84272
	H	3.46157	-0.21242	2.69661	H	-5.10495	-1.71949	-0.17091
	C	1.64656	-1.72608	-0.32612	O	-2.88104	0.04577	-0.70435
C	2.26604	-0.70684	0.41707					
TSS-2A	O	-1.59756	1.60738	0.41506	C	2.29949	-0.66449	-0.17641
	O	-0.43689	2.72396	-1.14347	C	3.14249	-0.92770	0.91203
	Pd	-0.60752	0.04312	-0.39443	C	3.68328	0.13686	1.63978
	O	0.38976	-1.60554	-1.24834	C	3.38423	1.45991	1.28922
	H	1.45549	0.89007	-1.45566	C	2.54764	1.72586	0.20025
	C	-2.43747	-1.78276	0.83247	H	3.34601	-1.95196	1.21616
	O	-1.58686	-1.84188	1.72996	H	4.32825	-0.06756	2.49097
	O	-2.34342	-1.06281	-0.25784	H	3.80486	2.28101	1.86489
	C	-3.75223	-2.55289	0.92010	H	2.31768	2.74813	-0.08646
	H	-4.09387	-2.87462	-0.06590	C	1.60355	-1.75401	-0.91105
	H	-3.63139	-3.41306	1.58129	H	-1.44209	4.84160	-0.05063
	H	-4.51608	-1.89152	1.34301	C	-1.98849	3.94971	0.26155
	N	2.24969	-2.88492	-1.19815	C	-1.26555	2.70612	-0.21519

	H 1.75494 -3.63944 -1.67205	H -2.11162 3.93893 1.34724
	H 3.25028 -2.98216 -1.04692	H -2.98737 3.97316 -0.18744
	C 2.00358 0.66831 -0.53785	
INT5-2A	O -1.19679 1.60753 0.48481	C 2.26276 -0.70613 -0.11904
	O -0.67239 2.64962 -1.44948	C 3.04927 -0.76138 1.03931
	Pd -0.43048 -0.08807 -0.30566	C 3.49590 0.42617 1.62595
	O 0.42892 -1.87647 -1.04976	C 3.15740 1.66874 1.07078
	H 1.46592 0.60314 -1.68091	C 2.38017 1.72952 -0.08708
	C -2.68077 -1.53550 0.71182	H 3.28116 -1.71830 1.50114
	O -1.95575 -1.72501 1.69838	H 4.09998 0.38252 2.52911
	O -2.34249 -0.86597 -0.36103	H 3.50667 2.58483 1.54074
	C -4.11140 -2.06363 0.65417	H 2.12814 2.68534 -0.53774
	H -4.79581 -1.25382 0.92899	C 1.64978 -1.92887 -0.71294
	H -4.37204 -2.39340 -0.35401	H -1.48572 4.77728 -0.23671
	H -4.23324 -2.88233 1.36572	C -1.82525 3.88227 0.28787
	N 2.36349 -3.04360 -0.85573	C -1.16675 2.64889 -0.31240
	H 1.91882 -3.88243 -1.22758	H -1.61217 3.96307 1.35641
	H 3.36556 -3.06228 -0.68236	H -2.91077 3.79546 0.16991
C 1.92379 0.54651 -0.69270		
TS5-3A	O -1.28188 1.86914 0.15649	C 2.24975 -0.80220 -0.18473
	O 0.42248 2.41882 -1.20810	C 3.51682 -1.03858 0.36281
	Pd -0.57129 -0.08078 -0.12450	C 4.08973 -0.10850 1.23685
	O 0.24716 -1.86807 -0.88399	C 3.38073 1.04278 1.58957
	H 0.86611 1.23348 -0.71646	C 2.11354 1.27974 1.04369
	C -3.04532 -1.24532 0.74991	H 4.04805 -1.96496 0.15440
	O -2.47240 -1.29680 1.85114	H 5.07305 -0.29896 1.65991
	O -2.51459 -0.76950 -0.34472	H 3.81154 1.75664 2.28809
	C -4.47565 -1.74039 0.56820	H 1.58809 2.19428 1.30876
	H -5.13035 -0.89196 0.34390	C 1.51742 -1.86161 -0.92088
	H -4.53526 -2.43120 -0.27770	H -0.41028 4.82778 -0.44148
	H -4.82279 -2.23384 1.47754	C -1.19609 4.10886 -0.68791
	N 2.16479 -2.83076 -1.57473	C -0.64893 2.70531 -0.57239
	H 1.62745 -3.55981 -2.04056	H -2.05634 4.24739 -0.03340
	H 3.17311 -2.82448 -1.69753	H -1.49206 4.28587 -1.72646
C 1.52787 0.38692 0.12895		
INT5-3A	O -0.94095 1.90396 0.09314	C 2.67839 -0.47351 -0.03379
	O -3.13987 1.56482 -0.33628	C 4.04720 -0.16111 0.02766
	Pd -0.17782 -0.10443 -0.05235	C 4.44523 1.16842 0.17045
	O 0.84724 -1.94472 -0.23252	C 3.47747 2.18029 0.25170
	H -2.87260 0.54116 -0.32685	C 2.10957 1.87567 0.19132
	C -2.86095 -1.84704 0.23262	H 4.80538 -0.94061 -0.03421
	O -2.26447 -2.78026 0.77663	H 5.50216 1.41812 0.21876
	O -2.27053 -0.76277 -0.22981	H 3.79068 3.21677 0.36325
	C -4.37098 -1.86913 0.02816	H 1.37105 2.66972 0.25598

	H -4.83209 -1.00329 0.51509	C 2.11470 -1.82398 -0.18419
	H -4.60304 -1.80367 -1.03979	H -2.89267 4.12222 -0.92510
	H -4.79832 -2.78517 0.43879	C -2.40619 3.79764 -0.00074
	N 2.88031 -2.91854 -0.27320	C -2.10851 2.32390 -0.08109
	H 2.43352 -3.82820 -0.36542	H -1.49040 4.36498 0.16137
	H 3.89368 -2.88371 -0.23020	H -3.10708 3.97934 0.81983
	C 1.70174 0.54845 0.04788	
TS5-4A	O 0.76399 -1.89263 -0.72371	C 3.25892 2.06624 0.80525
	H -2.77511 0.43016 -1.42236	C 1.90236 1.74341 0.65480
	C -2.78982 -0.04933 1.04984	H 4.69090 -0.83866 -0.24864
	O -1.93140 0.58689 1.71049	H 5.30550 1.39865 0.59895
	O -2.49002 -0.61091 -0.08608	H 3.53762 3.05001 1.17790
	C -4.21101 -0.20264 1.54797	H 1.13563 2.47383 0.90614
	H -4.91641 0.09436 0.76588	C 2.02326 -1.75033 -0.64207
	H -4.40222 -1.25713 1.77291	H -2.31438 2.79659 -4.03984
	H -4.37671 0.39491 2.44574	C -2.17019 3.18963 -3.02938
	N 2.83423 -2.75887 -0.99691	C -1.96040 2.05368 -2.06064
	H 2.42441 -3.63010 -1.32510	H -1.31471 3.86406 -3.00591
	H 3.84562 -2.69515 -0.94482	H -3.07901 3.73586 -2.75765
	C 1.55098 0.48167 0.17835	O -0.99980 1.98649 -1.29171
	C 2.54914 -0.46247 -0.15338	O -2.92628 1.13385 -2.12131
	C 3.90544 -0.12623 -0.00005	Pd -0.31092 -0.09501 -0.05587
	C 4.25742 1.13637 0.47885	
INT5-4A	C -4.59139 0.82039 0.02659	C 2.15082 -0.11220 0.00347
	C -3.18328 0.27892 -0.00663	C 3.40973 0.51315 0.00659
	H -4.68831 1.66816 -0.65647	C 3.48703 1.90659 0.00414
	H -4.81136 1.18146 1.03711	C 2.31191 2.67303 -0.00136
	O -2.20066 1.11795 -0.01024	C 1.05182 2.05662 -0.00432
	O -2.94777 -0.96649 -0.01178	H 4.32878 -0.07147 0.01073
	Pd -0.71336 -0.38306 -0.00582	H 4.45729 2.39686 0.00639
	O 0.69762 -1.97062 0.00065	H 2.37766 3.75946 -0.00337
	N 2.90030 -2.46122 0.01024	H 0.14782 2.66162 -0.00856
	H 2.67396 -3.45323 0.01145	C 1.90566 -1.56496 0.00491
	H 3.87908 -2.19230 0.01453	H -5.30798 0.03961 -0.23360
	C 0.96809 0.66390 -0.00193	
II	N 0.46079 -0.52160 0.12195	C -2.72185 1.21668 -0.43825
	C 1.83933 -0.22298 0.06937	C -1.85381 0.16919 -0.07802
	C 2.71053 -1.22780 -0.39397	C -2.40052 -1.05656 0.35355
	C 2.38347 1.00153 0.50783	C -3.78294 -1.22424 0.41975
	C 4.08630 -0.99724 -0.46286	C -4.64151 -0.17356 0.05838
	H 2.28995 -2.18039 -0.70784	H -4.76978 1.86351 -0.65118
	C 3.76375 1.21961 0.45244	H -2.30766 2.16679 -0.77226
	H 1.73151 1.76746 0.92195	H -1.72932 -1.86441 0.63196
	C 4.62078 0.22787 -0.04068	H -4.19856 -2.17265 0.75325

	H	4.74444	-1.77829	-0.83764	H	-5.71960	-0.30867	0.11221
	H	4.17134	2.16474	0.80526	C	-0.40143	0.38797	-0.16372
	H	5.69368	0.40129	-0.08079	H	-0.09431	1.38654	-0.50871
	C	-4.10829	1.04708	-0.37046				
TS5-II	C	1.16025	-1.08142	2.56137	C	-2.49946	0.88268	0.91394
	O	-0.09017	-0.93267	2.52363	C	-2.09775	1.81706	-0.06082
	O	1.78398	-1.40731	1.46844	C	-3.07374	2.61780	-0.68690
	C	1.96994	-0.87041	3.81021	C	-4.42647	2.46585	-0.37375
	H	2.27578	0.18045	3.85875	C	-4.81738	1.52492	0.58655
	H	1.36513	-1.09457	4.69135	C	-3.85020	0.74114	1.23259
	H	2.87049	-1.48828	3.79614	H	-2.76897	3.35597	-1.42706
	N	0.27685	1.20830	-0.21343	H	-5.17188	3.08236	-0.87074
	H	-0.49621	2.96935	-0.96719	H	-5.86919	1.40924	0.83912
	C	1.58993	1.64270	-0.54139	H	-4.15253	0.02330	1.99187
	C	2.06490	2.90433	-0.13422	C	-0.69372	2.02719	-0.43769
	C	2.44926	0.78559	-1.25132	H	-2.34568	-3.01567	-3.11543
	C	3.36583	3.30591	-0.45522	C	-1.25616	-2.99817	-3.18432
	H	1.42495	3.55532	0.45718	C	-0.65784	-2.46866	-1.91561
	C	3.74160	1.19860	-1.58138	H	-0.86850	-3.99792	-3.39303
	H	2.09531	-0.19555	-1.55710	H	-0.96838	-2.34102	-4.01229
	C	4.20768	2.45959	-1.18540	O	0.54585	-2.71537	-1.58162
	H	3.72218	4.27963	-0.12590	O	-1.35393	-1.71739	-1.12984
	H	4.38935	0.53037	-2.14458	Pd	0.19454	-1.44181	0.20531
	H	5.21942	2.77244	-1.43273	H	-1.75366	0.29338	1.43656
INT5-1I	O	-0.78695	-1.05276	2.79665	C	-1.52404	2.12585	-0.09292
	O	1.10297	-1.18035	1.55948	C	-2.18732	3.24146	-0.64879
	C	1.32364	-1.47090	3.89976	C	-3.55809	3.41705	-0.46091
	H	0.82431	-1.12858	4.80810	C	-4.27742	2.49682	0.31224
	H	1.49497	-2.54989	3.98057	C	-3.61955	1.40726	0.89937
	H	2.29664	-0.98585	3.79368	H	-1.62530	3.96197	-1.24039
	N	0.64683	0.95147	-0.34144	H	-4.06215	4.27122	-0.90638
	H	0.40387	2.95375	-0.63601	H	-5.34453	2.63678	0.47052
	C	2.06142	1.09992	-0.52792	H	-4.17345	0.71008	1.52370
	C	2.78508	2.02164	0.24401	C	-0.09098	2.01780	-0.35916
	C	2.72043	0.30686	-1.47965	H	-2.90767	-2.99797	-2.94740
	C	4.16211	2.16345	0.04477	C	-2.12287	-3.53384	-2.40905
	H	2.27895	2.60258	1.01144	C	-1.34357	-2.58537	-1.54667
	C	4.09422	0.45983	-1.67562	H	-2.55051	-4.33490	-1.80294
	H	2.15598	-0.40995	-2.07101	H	-1.44548	-3.97958	-3.14584
	C	4.81950	1.38753	-0.91602	O	-0.82205	-2.96865	-0.44070
	H	4.72039	2.87368	0.65023	O	-1.15910	-1.36641	-1.90628
	H	4.59909	-0.14728	-2.42332	Pd	-0.01283	-1.01900	-0.15056
	H	5.89089	1.49708	-1.06636	H	-1.75230	0.39089	1.20420
	C	-2.25193	1.21504	0.70177	C	0.43934	-1.20450	2.68809

TS5-2I	H	-1.74617	0.72877	-1.37600	H	6.04162	0.40347	-1.32976
	C	1.23282	-1.42186	2.07130	C	-2.04082	1.45215	-0.60721
	O	0.57629	-0.57902	2.69761	C	-1.10843	2.37522	-0.07927
	O	1.10159	-1.69170	0.79658	C	-1.56424	3.45301	0.69929
	C	2.28840	-2.28658	2.75414	C	-2.92414	3.57131	0.99613
	H	1.84104	-3.25522	3.00163	C	-3.83890	2.62954	0.50591
	H	3.13928	-2.46909	2.09431	C	-3.39834	1.57538	-0.30433
	H	2.61832	-1.80677	3.67735	H	-0.85293	4.17519	1.09486
	N	0.83626	1.01147	-0.46017	H	-3.27172	4.39690	1.61243
	H	0.97121	3.06985	-0.31966	H	-4.89655	2.72957	0.73833
	C	2.24171	0.85464	-0.66924	H	-4.10747	0.86508	-0.72115
	C	3.17361	1.52951	0.13415	C	0.32307	2.18915	-0.29837
	C	2.67499	-0.00254	-1.69129	H	-3.75619	-3.69001	0.23189
	C	4.54011	1.36471	-0.10965	C	-3.39148	-3.53004	-0.78561
	H	2.83537	2.15396	0.95775	C	-2.44150	-2.35072	-0.84114
	C	4.04159	-0.15289	-1.93261	H	-2.85371	-4.43333	-1.09367
	H	1.94255	-0.53407	-2.29394	H	-4.22773	-3.37083	-1.46902
	C	4.97753	0.53010	-1.14482	O	-1.64490	-2.22987	0.18559
	H	5.26214	1.88198	0.51780	O	-2.41056	-1.56348	-1.80947
	H	4.37604	-0.80733	-2.73404	Pd	-0.41009	-0.63666	-0.14162
INT5-2I	C	1.33526	-1.90212	1.59767	C	-1.92670	1.42101	-0.53736
	O	0.88667	-1.15350	2.47780	C	-1.05567	2.40429	0.00117
	O	0.99799	-1.86727	0.33366	C	-1.58371	3.44785	0.77678
	C	2.35057	-2.99593	1.91203	C	-2.95339	3.48273	1.05367
	H	1.83648	-3.96276	1.92931	C	-3.80630	2.48730	0.55618
	H	3.12369	-3.04441	1.14161	C	-3.29557	1.46206	-0.24662
	H	2.80061	-2.81613	2.88987	H	-0.92238	4.20825	1.18677
	N	0.90976	1.10366	-0.36162	H	-3.35762	4.28642	1.66455
	H	1.01588	3.16897	-0.16211	H	-4.87029	2.52561	0.77681
	C	2.31807	0.94010	-0.51510	H	-3.95352	0.71183	-0.67603
	C	3.22507	1.64076	0.29685	C	0.38687	2.27506	-0.18503
	C	2.78392	0.05193	-1.49594	H	-3.07716	-4.26308	-0.63167
	C	4.59798	1.47369	0.09863	C	-3.61855	-3.31471	-0.54805
	H	2.86267	2.28602	1.09363	C	-2.65042	-2.16718	-0.79781
	C	4.15733	-0.09885	-1.69335	H	-4.42033	-3.29731	-1.28832
	H	2.07060	-0.50245	-2.09939	H	-4.03333	-3.26049	0.46174
	C	5.06750	0.61117	-0.89947	O	-1.84078	-1.94114	0.20437
	H	5.29999	2.01004	0.73263	O	-2.64443	-1.53178	-1.86588
	H	4.51732	-0.77661	-2.46371	Pd	-0.45613	-0.47002	-0.10975
	H	6.13697	0.48286	-1.04907	H	-1.60523	0.77292	-1.37181
TS5-3I	O	1.16095	-1.35656	2.48437	C	-1.23837	2.25435	-0.09172
	O	1.10812	-1.92672	0.29961	C	-1.84704	3.46249	0.28390
	C	2.68866	-3.04580	1.66541	C	-3.14598	3.45825	0.79994
	H	2.36475	-4.01941	1.28591	C	-3.82363	2.24516	0.96197

	H	3.55081	-2.73261	1.06806	C	-3.22612	1.04142	0.56243
	H	2.98405	-3.13595	2.71213	H	-1.28965	4.39464	0.21367
	N	0.81817	1.09602	-0.33094	H	-3.61735	4.39253	1.09533
	H	0.71926	3.15277	-0.60142	H	-4.82626	2.23441	1.38373
	C	2.23124	1.05088	-0.51466	H	-3.79322	0.11815	0.65604
	C	3.07171	1.94471	0.16974	C	0.18201	2.22630	-0.38195
	C	2.77523	0.09835	-1.38978	H	-3.30143	-3.44536	-2.40885
	C	4.45158	1.90113	-0.04774	C	-3.49630	-3.16995	-1.36835
	H	2.65144	2.64884	0.88412	C	-2.61212	-2.00353	-0.99216
	C	4.15380	0.07074	-1.60823	H	-4.54447	-2.86454	-1.30023
	H	2.11786	-0.60280	-1.89442	H	-3.31262	-4.02449	-0.71740
	C	4.99557	0.97011	-0.94051	O	-1.81302	-2.13882	-0.00773
	H	5.10073	2.58959	0.48820	O	-2.71232	-0.92644	-1.67703
	H	4.57228	-0.65815	-2.29836	Pd	-0.42910	-0.54115	0.07317
	H	6.06979	0.93780	-1.10686	H	-2.08461	0.04643	-0.96872
	C	-1.94483	1.01498	-0.01411	C	1.56789	-2.02333	1.51679
	C	-1.50858	2.26548	0.91829	C	1.82547	-1.36947	0.03203
	O	-1.61251	1.56482	1.93119	C	1.15260	-2.61900	0.02094
	O	-0.71488	1.98175	-0.09621	C	1.86725	-3.82838	0.08990
	C	-2.32222	3.53950	0.73740	C	3.26123	-3.79496	0.17266
	H	-1.67092	4.37841	0.47212	C	3.92689	-2.56139	0.18524
	H	-3.02749	3.40315	-0.08909	C	3.21533	-1.34893	0.11727
	H	-2.87459	3.77615	1.64827	H	1.33647	-4.77896	0.08073
	N	-0.82438	-1.35691	-0.14760	H	3.82834	-4.72097	0.22699
	H	-0.90522	-3.43843	-0.14572	H	5.01341	-2.53822	0.24819
	C	-2.23729	-1.21165	-0.25544	H	3.75242	-0.40436	0.13057
	C	-3.10808	-1.96651	0.54894	C	-0.28512	-2.53999	-0.08632
	C	-2.75737	-0.30007	-1.18680	H	3.67402	4.06045	-1.38992
	C	-4.49057	-1.82574	0.39898	C	3.60546	3.54114	-0.43020
	H	-2.70629	-2.63690	1.30522	C	2.30626	2.78606	-0.35205
	C	-4.14015	-0.17104	-1.33409	H	4.44841	2.86269	-0.30388
	H	-2.07714	0.29435	-1.78923	H	3.62371	4.30181	0.35696
	C	-5.01165	-0.93256	-0.54466	O	2.28223	1.58227	-0.02069
	H	-5.15959	-2.40681	1.02961	O	1.24248	3.49443	-0.64850
	H	-4.53797	0.52828	-2.06603	Pd	0.59539	0.21161	-0.02309
	H	-6.08778	-0.82230	-0.65615	H	0.37774	2.94465	-0.48235
	C	-2.35433	-1.54281	0.76395	C	1.64476	0.42064	0.47552
	O	-1.64548	-1.04791	1.67474	C	2.83853	-0.02023	-0.14840
	O	-2.00269	-1.46399	-0.48771	C	4.07752	0.53847	0.21488
	C	-3.64773	-2.26498	1.07799	C	4.11983	1.53063	1.19723
	H	-4.46020	-1.86359	0.46459	C	2.93399	1.96043	1.81076
	H	-3.54067	-3.32392	0.82042	C	1.69022	1.40769	1.45372
	H	-3.89921	-2.17340	2.13578	H	4.99287	0.19593	-0.26480
	H	3.50293	-1.45736	-1.70918	H	5.07081	1.97038	1.48741

	N	1.44254	-1.45517	-1.36604	H	2.97280	2.73520	2.57415
	C	1.16515	-2.49767	-2.28987	H	0.78027	1.75707	1.93789
	C	1.99281	-3.63084	-2.39181	C	2.65960	-1.04807	-1.14652
	C	0.02258	-2.39383	-3.09952	H	-2.94291	3.27688	-2.43964
	C	1.69374	-4.62889	-3.32298	C	-2.87150	3.18415	-1.35211
	H	2.84793	-3.74406	-1.72962	C	-2.31740	1.83054	-0.98672
	C	-0.26449	-3.39289	-4.03178	H	-2.23465	3.97065	-0.94824
	H	-0.62692	-1.52914	-2.99698	H	-3.88383	3.28410	-0.94798
	C	0.56975	-4.51197	-4.14992	O	-1.34363	1.67076	-0.24925
	H	2.33418	-5.50525	-3.39242	O	-2.99589	0.82368	-1.54391
	H	-1.14477	-3.29966	-4.66363	Pd	-0.01269	-0.47531	-0.11988
	H	0.33788	-5.29330	-4.86987	H	-2.62894	-0.05389	-1.22250
INT5-4I	C	1.09745	4.68315	0.20542	H	-6.10051	-0.46130	-0.01753
	H	0.32810	5.25627	-0.31655	C	1.82593	-0.84798	-0.02395
	H	1.08395	4.97969	1.26019	C	1.22935	-2.13341	-0.08586
	H	2.08512	4.90938	-0.20139	C	2.02410	-3.29313	-0.12186
	N	-0.81193	-0.97678	-0.07007	C	3.41562	-3.16903	-0.09292
	H	-0.78868	-3.06227	-0.17557	C	4.00249	-1.89728	-0.02905
	C	-2.22805	-0.86226	-0.03653	C	3.21209	-0.73285	0.00662
	C	-3.02782	-1.77124	0.67999	H	1.55767	-4.27577	-0.16947
	C	-2.82953	0.20797	-0.71916	H	4.04317	-4.05643	-0.11976
	C	-4.41723	-1.62549	0.67851	H	5.08695	-1.80641	-0.00757
	H	-2.56747	-2.56909	1.25781	H	3.68672	0.24491	0.05533
	C	-4.21961	0.34262	-0.71841	C	-0.21549	-2.13393	-0.10996
	H	-2.20645	0.92137	-1.25206	Pd	0.52351	0.65954	0.01131
	C	-5.01893	-0.57377	-0.02387	C	0.80337	3.20565	0.11188
	H	-5.02926	-2.32780	1.23983	O	1.78771	2.37243	0.09833
	H	-4.67828	1.16767	-1.25840	O	-0.39038	2.77557	0.07044

Table S2. Cartesian coordinates of proton-transfer transition states and palladation products for all the 16 studied reactants with Pd(OAc)₂ as the catalyst, optimized at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent.

Names	Cartesian Coordinates							
1B	C	-1.82327	1.28188	-0.00019	H	-2.57549	-2.04595	0.00037
	C	-0.42776	1.19500	-0.00019	H	-3.68385	0.18503	0.00003
	C	0.20750	-0.06066	-0.00000	C	1.69952	-0.20030	-0.00004
	C	-0.58220	-1.22674	0.00018	O	2.22661	-1.31366	-0.00043
	C	-1.97411	-1.13961	0.00021	C	2.55900	1.05076	0.00038
	C	-2.59810	0.11632	0.00002	H	2.35388	1.66740	0.88222
	H	-2.30521	2.25679	-0.00037	H	3.61087	0.76126	0.00090
	H	0.15574	2.11128	-0.00038	H	2.35477	1.66722	-0.88180
	H	-0.08704	-2.19371	0.00029				
TS5-3B	Pd	-0.60135	0.01373	-0.09201	C	3.47665	-1.13359	0.23847

	O	0.13353	-1.79186	-0.88844	C	4.13100	-0.23326	1.08416
	H	0.88133	1.24550	-0.68440	C	3.48008	0.93481	1.48952
	C	-3.01342	-1.31787	0.69072	C	2.19416	1.22839	1.01393
	O	-2.33372	-1.66468	1.67080	H	3.96895	-2.06532	-0.02745
	O	-2.58048	-0.56168	-0.28379	H	5.13381	-0.45493	1.44079
	C	-4.46732	-1.74410	0.52854	H	3.97565	1.62781	2.16587
	H	-5.11527	-0.86317	0.57895	H	1.72727	2.16649	1.30478
	H	-4.62027	-2.20625	-0.45098	C	1.38496	-1.90214	-0.88053
	H	-4.74521	-2.44444	1.31788	H	-0.21603	4.91511	-0.44858
	C	1.99481	-3.12931	-1.49562	C	-1.05194	4.22697	-0.59557
	H	2.38014	-3.78740	-0.70834	C	-0.56013	2.80130	-0.50296
	H	1.23483	-3.66999	-2.06104	H	-1.83799	4.41660	0.13513
	H	2.83322	-2.86601	-2.14716	H	-1.44595	4.39297	-1.60332
	C	1.52576	0.36799	0.12956	O	-1.21987	1.98549	0.22814
	C	2.17842	-0.85880	-0.21974	O	0.48422	2.47259	-1.15953
INT5-4B	C	-4.61273	0.76188	0.02697	C	0.94381	0.69087	-0.00213
	C	-3.19722	0.24234	-0.00554	C	2.13465	-0.08392	0.00343
	H	-4.72854	1.58845	-0.67893	C	3.39449	0.54756	0.00675
	H	-4.82876	1.14885	1.02859	C	3.46455	1.93985	0.00433
	O	-2.22704	1.09701	-0.00927	C	2.28367	2.69931	-0.00126
	O	-2.94015	-0.99866	-0.01164	C	1.02240	2.08140	-0.00442
	Pd	-0.72118	-0.38008	-0.00620	H	4.30906	-0.04173	0.01101
	O	0.73025	-1.94066	0.00032	H	4.43080	2.43782	0.00672
	C	3.03899	-2.52694	0.01094	H	2.34521	3.78608	-0.00318
	H	3.67191	-2.38380	0.89345	H	0.11845	2.68649	-0.00870
	H	2.63243	-3.53898	0.01370	C	1.92119	-1.52471	0.00479
	H	3.67527	-2.39023	-0.87021	H	-5.31896	-0.03673	-0.20556
	1C	C	0.70755	0.73827	-0.00030	C	-0.98128	-1.15421
O		1.00051	1.92803	0.00039	C	-0.69318	0.22176	-0.00023
O		1.62904	-0.24698	-0.00095	C	-1.74494	1.15356	0.00001
C		3.02473	0.16851	-0.00028	C	-3.07058	0.71509	0.00025
H		3.20289	0.78499	0.88542	C	-3.35474	-0.65702	0.00027
H		3.20405	0.78424	-0.88623	H	-2.52954	-2.65429	0.00007
C		3.87740	-1.08750	0.00079	H	-0.17031	-1.87573	-0.00054
H		3.68413	-1.69588	-0.88794	H	-1.51153	2.21460	0.00001
H		3.68283	-1.69526	0.88966	H	-3.88146	1.43985	0.00042
H		4.93588	-0.80766	0.00147	H	-4.38764	-0.99856	0.00049
C		-2.30927	-1.58925	0.00002				
T55-3C		O	1.47617	-2.10270	-1.56633	H	-5.34739	3.09799
	Pd	0.78715	0.25326	-0.03151	C	-0.43224	-1.52964	0.21602
	O	-1.12996	1.11569	-0.36952	C	-1.79014	-1.09570	0.19456
	H	0.45801	-1.59159	-0.80982	C	-2.80874	-1.85400	0.78439
	C	1.92220	2.70231	0.92324	C	-2.49465	-3.04922	1.43848
	O	1.53477	2.28461	2.02687	C	-1.16253	-3.46522	1.52411

	O	1.76254	2.06891	-0.20911	C	-0.14711	-2.71184	0.92083
	C	2.65860	4.02850	0.77927	H	-3.83262	-1.49099	0.76246
	H	3.70575	3.83530	0.52385	H	-3.28346	-3.63859	1.89957
	H	2.22767	4.62136	-0.03219	H	-0.91123	-4.38174	2.05335
	H	2.61497	4.58711	1.71575	H	0.87637	-3.07662	0.96452
	O	-3.30847	0.58972	-0.53388	C	-2.05594	0.27596	-0.27444
	C	-3.60289	1.97880	-0.91958	H	3.77545	-3.41492	-1.38280
	H	-3.02509	2.20487	-1.81884	C	3.86205	-2.32927	-1.47487
	H	-3.26359	2.62868	-0.10938	C	2.56510	-1.68158	-1.04959
	C	-5.09746	2.07291	-1.15231	H	4.69632	-1.96133	-0.87805
	H	-5.65486	1.82837	-0.24359	H	4.03757	-2.09911	-2.53033
	H	-5.41512	1.40084	-1.95457	O	2.61932	-0.73766	-0.18902
INT5-4C	O	2.83180	-1.76997	-0.00949	C	-1.52058	1.00017	0.00128
	C	5.03897	-0.75751	0.02163	C	-2.45393	2.05047	0.00373
	H	5.38586	-0.49108	1.02584	C	-1.99137	3.36655	0.00361
	H	5.39686	-1.75879	-0.22333	C	-0.61104	3.62429	0.00099
	H	5.45228	-0.02496	-0.67647	C	0.32344	2.57642	-0.00152
	O	-3.13659	-0.75605	0.00307	H	-3.51916	1.83188	0.00569
	C	-3.47046	-2.18585	0.00253	H	-2.69789	4.19279	0.00551
	H	-3.01937	-2.63721	0.88959	H	-0.25747	4.65376	0.00090
	H	-3.02216	-2.63587	-0.88663	H	1.38911	2.79420	-0.00359
	C	-4.98258	-2.29530	0.00482	C	-1.85885	-0.42320	0.00106
	H	-5.41349	-1.82505	-0.88379	Pd	1.00320	-0.36844	-0.00450
	H	-5.41071	-1.82640	0.89548	O	-0.94556	-1.28668	-0.00105
	H	-5.26370	-3.35316	0.00446	C	3.53182	-0.71363	-0.00624
	C	-0.13152	1.25846	-0.00134	O	2.94903	0.44055	-0.00876
1D	H	3.66497	-0.07441	0.00000	C	-0.22213	0.03104	0.00000
	H	2.47975	2.11515	0.00005	C	0.44841	-1.20458	-0.00003
	C	-1.70912	0.11734	0.00000	C	1.84530	-1.23897	-0.00003
	O	-2.34303	1.16550	-0.00007	C	2.57749	-0.04482	0.00000
	O	-2.31730	-1.09180	0.00006	C	1.91116	1.18811	0.00003
	H	-3.29179	-0.93254	0.00003	H	-0.12064	-2.12913	-0.00004
	H	-0.01359	2.17582	0.00004	H	2.36294	-2.19539	-0.00005
	C	0.51571	1.22703	0.00002				
TS5-3D	O	-1.15085	1.99810	0.25986	C	2.16459	-0.91540	-0.23948
	O	0.54763	2.45579	-1.14457	C	3.44752	-1.24977	0.21173
	Pd	-0.59861	0.01469	-0.09124	C	4.13519	-0.37391	1.05717
	O	0.08155	-1.82580	-0.92815	C	3.52591	0.81531	1.46835
	H	0.92077	1.22068	-0.68435	C	2.24813	1.15390	1.00311
	C	-3.04595	-1.25189	0.68107	H	3.88596	-2.20420	-0.06692
	O	-2.37165	-1.64191	1.64821	H	5.13029	-0.63115	1.41168
	O	-2.59400	-0.48928	-0.28044	H	4.04752	1.48795	2.14566
	C	-4.51383	-1.62633	0.51886	H	1.81338	2.10445	1.30289
	H	-5.13214	-0.72600	0.59281	C	1.32958	-1.92160	-0.91166

	H -4.68777 -2.06155 -0.46945	H -0.07666 4.90617 -0.37874
	H -4.80979 -2.33436 1.29469	C -0.93158 4.24447 -0.53778
	O 1.94278 -2.96208 -1.45198	C -0.47860 2.80454 -0.47036
	H 1.26687 -3.59315 -1.81292	H -1.71182 4.44288 0.19672
	C 1.54666 0.31981 0.11629	H -1.32009 4.43915 -1.54246
INT5-4D	H -4.66850 1.69328 -0.65939	C 3.51273 1.86400 0.00374
	H -4.79652 1.20832 1.03455	C 2.34635 2.64634 -0.00110
	O -2.18517 1.12739 -0.01001	C 1.07291 2.05486 -0.00384
	O -2.94478 -0.95160 -0.01145	H 4.30885 -0.14988 0.00952
	Pd -0.71646 -0.38256 -0.00515	H 4.48810 2.34395 0.00578
	O 0.71471 -1.99655 0.00163	H 2.42922 3.73168 -0.00278
	O 2.92967 -2.38351 0.00951	H 0.18102 2.67741 -0.00760
	H 2.60195 -3.31910 0.01030	C 1.89151 -1.55849 0.00432
	C 0.96840 0.66468 -0.00175	H -5.29890 0.06872 -0.23620
	C 2.14318 -0.12125 0.00299	C -4.57808 0.84543 0.02439
	C 3.41710 0.47263 0.00584	C -3.17466 0.29475 -0.00702
1E	H -4.77399 -0.00049 -0.00008	C -0.86774 0.00012 0.00016
	H -3.52385 -2.15531 -0.00005	C -1.58250 1.20909 0.00014
	C 0.65749 0.00044 0.00024	C -2.98176 1.21126 0.00006
	O 1.24311 -1.12845 0.00024	C -3.68572 -0.00035 -0.00001
	O 1.24271 1.12929 0.00025	C -2.98141 -1.21170 0.00001
	H -1.02489 -2.14168 0.00011	H -1.02558 2.14188 0.00019
	K 3.79625 -0.00024 -0.00043	H -3.52454 2.15467 0.00004
	C -1.58209 -1.20907 0.00009	
TS5-3E	O -0.82916 -2.46747 -0.14417	C -1.29677 1.93610 0.09623
	O -2.12133 -1.39246 -1.63993	C -2.12452 2.93963 0.60981
	Pd 0.11847 -0.58508 0.01425	C -3.35110 2.60881 1.19525
	O 0.95841 1.28384 -0.26567	C -3.73741 1.26671 1.28774
	H -1.68214 -0.35786 -0.89194	C -2.91525 0.26359 0.76229
	C 2.48820 -1.86351 1.11162	H -1.78314 3.97133 0.57463
	O 1.94542 -1.65484 2.21192	H -3.99177 3.39065 1.59724
	O 2.00608 -1.50083 -0.04281	H -4.68017 1.00071 1.76116
	C 3.80942 -2.62350 1.02381	H -3.24921 -0.77053 0.81058
	H 3.59527 -3.67883 0.82079	C 0.10565 2.27928 -0.31164
	H 4.43128 -2.24816 0.20734	H -1.90028 -4.60381 -0.92093
	H 4.34759 -2.55760 1.97169	C -2.31450 -3.77650 -1.49701
	O 0.46007 3.43262 -0.61332	C -1.71127 -2.46034 -1.06358
	K 3.26758 2.73476 -0.98665	H -2.11271 -3.92809 -2.56153
	C -1.69644 0.57396 0.12630	H -3.40022 -3.73661 -1.37108
INT5-4E	H -5.19720 -1.71586 -0.24443	C 0.28662 1.46766 -0.00124
	C -4.87270 -0.70765 0.01881	C 1.67181 1.22319 0.00308
	C -3.36476 -0.60848 -0.00809	C 2.58160 2.28924 0.00486
	H -5.31373 0.02302 -0.66416	C 2.10433 3.60352 0.00241
	H -5.22847 -0.47383 1.02822	C 0.72184 3.84458 -0.00187

	O	-2.82776	0.56312	-0.01138	C	-0.19377	2.77949	-0.00376
	O	-2.63561	-1.64671	-0.00819	H	3.64897	2.07682	0.00812
	Pd	-0.82501	-0.17472	-0.00314	H	2.80088	4.43898	0.00378
	O	1.07652	-1.05963	0.00321	H	0.35239	4.86875	-0.00376
	O	3.26893	-0.59272	0.00866	H	-1.26332	2.97967	-0.00716
	K	2.68404	-3.38687	-0.00167	C	2.08123	-0.21193	0.00533
1F	H	-2.66281	-2.15529	-0.25234	C	-0.77275	-1.20856	0.18699
	C	1.39788	0.00010	0.66938	C	-0.07742	0.00005	0.34873
	H	1.66262	-0.88877	1.26238	C	-0.77283	1.20861	0.18693
	H	1.66262	0.88911	1.26215	C	-2.13554	1.21122	-0.13232
	C	3.55194	-0.00003	-0.31535	C	-2.81991	-0.00006	-0.29316
	H	4.04297	-0.00010	-1.29149	C	-2.13545	-1.21128	-0.13226
	H	3.86498	0.89359	0.24502	H	-0.24544	2.15272	0.31363
	H	3.86499	-0.89355	0.24516	H	-2.66295	2.15518	-0.25244
	O	2.14784	-0.00005	-0.55267	H	-3.87997	-0.00010	-0.53806
H	-0.24529	-2.15263	0.31376					
TS5-3F	H	0.79214	-2.51578	-2.43860	C	-1.68843	0.19347	0.08943
	H	5.02578	-1.14904	1.74322	C	-2.29743	-1.02345	-0.31883
	C	4.59438	-0.87815	0.77788	C	-3.53102	-1.40743	0.21081
	C	3.10479	-0.59208	0.92727	C	-4.17501	-0.59721	1.15676
	H	5.09589	0.02142	0.40476	C	-3.56689	0.57946	1.60605
	H	4.76717	-1.67550	0.05018	C	-2.32701	0.96136	1.08437
	O	2.46196	-0.54921	-0.21052	H	-1.17089	1.11012	-0.76717
	O	2.58642	-0.40828	2.04060	H	-3.98678	-2.34735	-0.09469
	Pd	0.44162	-0.06812	-0.06929	H	-5.13795	-0.90167	1.56082
	O	-0.84416	2.28379	-1.31474	H	-4.05429	1.19475	2.35891
	C	0.18914	2.70236	-0.68933	H	-1.86597	1.88585	1.42681
	O	0.89578	1.97148	0.08160	C	-1.52281	-1.93525	-1.22889
	C	0.59211	4.14814	-0.86699	H	-1.41472	-1.51801	-2.23942
	H	0.80319	4.32974	-1.92488	H	-1.97099	-2.93180	-1.29924
	H	-0.24433	4.79238	-0.58206	C	0.69172	-2.90757	-1.42052
	H	1.47088	4.38448	-0.26769	H	1.65833	-2.89077	-0.92074
O	-0.19356	-2.07194	-0.64044	H	0.28513	-3.92400	-1.44279	
INT5-4F	C	-0.21777	3.33444	0.03216	C	-1.16492	-0.61690	0.00901
	H	0.79330	3.42054	-0.36700	C	-2.26898	0.25284	0.06196
	H	-0.87777	4.04504	-0.47730	C	-3.56443	-0.28544	0.05139
	H	-0.21489	3.52925	1.11062	C	-3.75155	-1.67096	-0.00190
	Pd	0.61517	0.24998	-0.03581	C	-2.64494	-2.52778	-0.05118
	O	2.91058	0.56351	-0.03954	C	-1.34525	-2.00034	-0.04980
	C	2.99475	-0.69823	0.04575	H	-4.42802	0.37770	0.08559
	O	1.92076	-1.41404	0.09645	H	-4.75921	-2.08012	-0.00917
	C	4.32900	-1.40344	0.06977	H	-2.78994	-3.60539	-0.09516
	H	4.49811	-1.88275	-0.90050	H	-0.48402	-2.66360	-0.09189
	H	5.13454	-0.69220	0.25935	C	-2.03170	1.73419	0.17049

	H 4.32930 -2.18844 0.83049	H -2.15535 2.08165 1.20576
	O -0.66232 1.99198 -0.23885	H -2.70131 2.31708 -0.47378
1G	H 0.04304 2.27517 -0.05838	C -1.48089 -1.29614 -0.02101
	H -2.39630 1.97407 0.28820	C -0.10828 -1.12391 -0.21946
	H -3.38035 -0.31492 0.31447	C 0.45720 0.16347 -0.23703
	C 1.94786 0.34297 -0.44815	C -0.38117 1.27210 -0.05057
	H 2.25536 -0.09497 -1.40293	C -1.75903 1.10387 0.14550
	H 2.19370 1.41325 -0.47829	C -2.31160 -0.18087 0.16147
	O 2.74807 -0.33137 0.53785	H -1.90585 -2.29779 -0.01118
	H 2.48796 -0.00090 1.42024	H 0.53339 -1.99183 -0.35944
TS5-3G	H -1.27257 1.00151 0.69305	C -3.88883 -1.57837 -0.82179
	C 3.15609 -0.96969 -0.46662	C -3.57066 -0.36451 -1.43856
	O 2.52655 -1.98096 -0.83620	C -2.43282 0.34112 -1.03398
	O 2.61138 0.11558 0.00683	H -3.27916 -3.07147 0.61445
	C 4.67436 -0.90688 -0.56580	H -4.77079 -2.13392 -1.13284
	H 5.10370 -0.47118 0.34018	H -4.20335 0.03037 -2.23021
	H 5.08444 -1.90392 -0.73631	H -2.20090 1.29194 -1.50981
	H 4.95162 -0.25996 -1.40510	H -1.20118 4.71090 -0.13470
	C -0.93626 -1.99301 1.55857	C -0.22652 4.31537 0.16405
	H -1.11122 -3.05698 1.73860	C -0.30484 2.80917 0.25141
	H -0.93276 -1.46898 2.51848	H 0.54056 4.62538 -0.54506
	O 0.42248 -1.81782 1.04126	H 0.00223 4.71576 1.15613
	H 0.65663 -2.48704 0.35581	O 0.51630 2.12237 -0.44421
	C -1.61093 -0.13281 0.00894	O -1.19321 2.29381 1.01279
	C -1.92198 -1.39524 0.58996	Pd 0.52741 0.09715 0.07612
	C -3.05360 -2.10103 0.17582	
INT5-4G	H 2.69116 -2.54904 -0.47451	C 2.27889 -0.48570 0.06512
	Pd -0.61141 -0.46027 -0.02854	C 3.57670 0.04704 0.04930
	O -2.91684 -0.74057 -0.02638	C 3.77102 1.43134 -0.00778
	C -2.97904 0.52311 0.04402	C 2.66844 2.29345 -0.05714
	O -1.89308 1.22115 0.08864	C 1.36635 1.77225 -0.05244
	C -4.30075 1.25220 0.05662	H 4.43707 -0.62042 0.08234
	H -4.45878 1.72383 -0.91927	H 4.78070 1.83550 -0.01795
	H -5.11943 0.55763 0.25167	H 2.81849 3.37028 -0.10386
	H -4.28912 2.04541 0.80871	H 0.50853 2.43985 -0.09542
	O 0.65004 -2.20887 -0.22614	C 2.03316 -1.96475 0.17748
	H 0.31555 -3.04692 0.16164	H 2.16457 -2.30904 1.21023
	C 1.17772 0.38971 0.01156	
	1H	H 0.12889 -2.15517 0.00009
H 0.12889 2.15517 -0.00001		C -0.42963 -1.22517 0.00005
H -2.36918 2.15716 -0.00008		C 0.24547 -0.00000 0.00004
H -3.60983 0.00000 -0.00005		C -0.42963 1.22517 -0.00000
N 1.71414 0.00000 0.00009		C -1.82554 1.21566 -0.00004
O 2.30085 1.09105 0.00002		C -2.52215 -0.00000 -0.00002

	O	2.30085	-1.09105	-0.00013	H	-2.36917	-2.15717	0.00004
TS5-3H	Pd	-0.57411	-0.10543	-0.14007	C	4.12936	-0.10948	1.15354
	H	0.84671	1.22279	-0.68242	C	3.41649	1.03111	1.53861
	C	-3.00963	-1.28144	0.73227	C	2.13781	1.27837	1.02250
	O	-2.44163	-1.26240	1.83418	H	4.05303	-1.95244	0.01014
	O	-2.47404	-0.84874	-0.38328	H	5.12367	-0.29741	1.55014
	C	-4.42686	-1.80822	0.55707	H	3.85944	1.73787	2.23650
	H	-4.48113	-2.49110	-0.29493	H	1.62596	2.19743	1.29635
	H	-4.75195	-2.31551	1.46679	H	-2.14092	4.17327	0.15182
	H	-5.10074	-0.97025	0.35075	C	-1.33814	4.06262	-0.57679
	N	1.61205	-1.83148	-0.94259	C	-0.73401	2.67881	-0.51183
	O	2.25146	-2.71626	-1.49011	H	-1.73979	4.21553	-1.58368
	O	0.33551	-1.84008	-0.95687	H	-0.56004	4.81128	-0.41106
	C	1.52527	0.39923	0.11300	O	-1.35518	1.79424	0.17790
	C	2.26424	-0.76794	-0.20381	O	0.34874	2.45071	-1.14158
	C	3.54738	-1.02992	0.28027				
INT5-4H	O	2.92217	-0.92550	-0.01016	C	-2.13335	-0.16740	0.00302
	C	3.16452	0.31973	-0.00626	C	-3.43835	0.34857	0.00583
	O	2.17461	1.15325	-0.00967	C	-3.58146	1.73154	0.00372
	C	4.56861	0.86149	0.02255	C	-2.44122	2.55736	-0.00107
	H	4.78105	1.24923	1.02460	C	-1.14660	2.01786	-0.00373
	H	5.28583	0.07406	-0.21412	H	-4.29456	-0.32052	0.00944
	H	4.66770	1.69116	-0.68211	H	-4.57381	2.17420	0.00569
	N	-1.90691	-1.58037	0.00465	H	-2.56651	3.63834	-0.00275
	O	-2.81845	-2.39737	0.00884	H	-0.28101	2.67617	-0.00742
	O	-0.68168	-1.96503	0.00135	Pd	0.72772	-0.36642	-0.00485
	C	-0.97856	0.63293	-0.00165				
	1J	C	0.76519	0.02142	-0.00299	C	-0.72562	0.01965
C		1.50502	1.18978	0.26297	C	-1.46635	1.19287	-0.24456
C		2.89884	1.13714	0.24968	C	-2.86438	1.17067	-0.23852
H		1.00134	2.12256	0.49841	C	-3.55033	-0.02417	0.00946
C		2.71580	-1.19474	-0.25893	C	-2.82392	-1.19875	0.24384
C		3.52752	-0.08143	-0.02107	H	-0.86418	-2.08873	0.41082
H		3.48333	2.03120	0.45617	H	-0.95788	2.12892	-0.46126
H		3.16503	-2.16604	-0.46701	H	-3.41763	2.08663	-0.43440
H		4.61034	-0.17334	-0.04232	H	-4.63801	-0.04058	0.01607
N		1.37679	-1.15665	-0.25325	H	-3.34739	-2.13271	0.43744
C		-1.42719	-1.17766	0.23197				
TS5-3J	C	-1.16337	-1.21715	0.17166	H	-0.37264	-1.55462	-0.88718
	C	-2.29271	-0.34440	0.16613	C	2.88197	1.46057	1.04704
	C	-3.50241	-0.75910	0.74240	O	2.62179	0.85847	2.10174
	C	-3.60474	-2.01149	1.35516	O	2.19015	1.36318	-0.05787
	C	-2.48746	-2.84972	1.42855	C	4.08555	2.39021	0.93624
	C	-1.28140	-2.44717	0.84720	H	4.49406	2.60145	1.92604

	H	-4.35971	-0.09093	0.76146	H	4.85748	1.90752	0.32728
	H	-4.54842	-2.31698	1.80119	H	3.81044	3.32286	0.43611
	H	-2.55573	-3.81242	1.92999	C	-2.10276	1.04472	-0.28888
	H	-0.42807	-3.12064	0.88128	C	-3.12955	1.92375	-0.65661
	H	2.64998	-3.38836	-2.69818	C	-2.82061	3.23819	-1.00337
	C	2.49348	-3.50135	-1.62157	H	-4.15843	1.57775	-0.67780
	C	1.54677	-2.42458	-1.14246	C	-0.50570	2.74008	-0.61426
	H	2.03629	-4.48154	-1.45733	C	-1.48771	3.65924	-0.97579
	H	3.44784	-3.44247	-1.09861	H	-3.61112	3.92560	-1.29517
	O	1.93757	-1.64137	-0.21502	H	0.54996	2.99341	-0.58793
	O	0.38941	-2.35667	-1.68508	H	-1.20428	4.67422	-1.23889
	Pd	0.61255	-0.00663	0.00815	N	-0.81038	1.47292	-0.28512
INT5-4J	C	-4.92357	-0.15850	0.02115	C	0.47868	1.31599	-0.00107
	H	-5.36836	-1.12371	-0.22652	C	1.83673	0.91942	0.00186
	H	-5.24639	0.13389	1.02626	C	2.84566	1.89828	0.00408
	H	-5.27239	0.60961	-0.67400	C	2.50298	3.25297	0.00343
	C	2.07051	-0.52926	0.00224	C	1.15542	3.63773	0.00056
	C	3.31450	-1.17336	0.00509	C	0.13953	2.66819	-0.00172
	C	3.37034	-2.56659	0.00506	H	3.89557	1.61292	0.00627
	H	4.22899	-0.58795	0.00731	H	3.28499	4.00854	0.00513
	C	0.97343	-2.60786	-0.00064	H	0.89256	4.69386	0.00005
	C	2.18100	-3.30263	0.00214	H	-0.90495	2.97273	-0.00402
	H	4.33234	-3.07387	0.00729	Pd	-0.85281	-0.16158	-0.00442
	H	0.01842	-3.12768	-0.00302	C	-3.41642	-0.24336	-0.00684
	H	2.18004	-4.38863	0.00200	O	-2.73506	0.85062	-0.00874
	N	0.92028	-1.26536	-0.00057	O	-2.81823	-1.36384	-0.01019
1K	C	-2.30361	1.12319	0.00010	C	2.30363	-1.12320	0.00000
	C	-2.64152	-1.28888	-0.00005	C	1.77393	0.18342	-0.00008
	C	-3.68523	1.30589	0.00012	C	2.64150	1.28888	-0.00010
	H	-1.62850	1.97337	0.00019	C	4.02640	1.09798	-0.00002
	C	-4.02641	-1.09797	-0.00006	C	4.55111	-0.19925	0.00010
	H	-2.21364	-2.28872	-0.00011	C	3.68524	-1.30588	0.00011
	C	-4.55111	0.19928	0.00003	H	2.21361	2.28872	-0.00019
	H	-4.09642	2.31308	0.00019	H	4.69276	1.95743	-0.00006
	H	-4.69280	-1.95739	-0.00011	H	5.62805	-0.35226	0.00021
	H	-5.62805	0.35227	0.00005	H	4.09648	-2.31305	0.00020
	N	0.38830	0.49851	-0.00017	N	-0.38830	-0.49854	0.00001
	H	1.62851	-1.97338	-0.00001	C	-1.77393	-0.18342	-0.00001
TS5-3K	O	0.76139	-1.66432	2.51841	C	-1.00443	2.28080	0.02530
	O	0.99822	-2.03207	0.30437	C	-1.51356	3.52065	0.44341
	C	2.28047	-3.39166	1.76324	C	-2.82182	3.60284	0.92454
	H	1.90011	-4.32141	1.32902	C	-3.61008	2.44864	0.99646
	H	3.21354	-3.14767	1.24636	C	-3.11141	1.21949	0.54107
	H	2.47567	-3.53691	2.82698	H	-0.86064	4.38958	0.43378

	N	0.86576	1.07522	-0.26901	H	-3.21714	4.55778	1.26182
	C	2.27587	1.01438	-0.47700	H	-4.62323	2.50518	1.38784
	C	3.11022	2.06010	-0.03907	H	-3.76273	0.34891	0.55842
	C	2.81168	-0.10074	-1.13931	H	-3.26744	-3.25121	-2.59189
	C	4.48097	1.98433	-0.27634	C	-3.59967	-2.90508	-1.60801
	H	2.68130	2.90564	0.48936	C	-2.67076	-1.80604	-1.14459
	C	4.18489	-0.15349	-1.38791	H	-4.61145	-2.50793	-1.72190
	H	2.16048	-0.90509	-1.46068	H	-3.59400	-3.74123	-0.90893
	C	5.02142	0.88212	-0.95584	O	-1.90748	-2.04215	-0.14793
	H	5.13156	2.78292	0.07198	O	-2.68874	-0.69406	-1.77442
	H	4.60111	-1.00785	-1.91600	Pd	-0.43244	-0.53920	0.04787
	H	6.09201	0.82961	-1.14002	H	-2.00237	0.21902	-1.00070
	N	0.36056	2.23982	-0.24925	C	1.26701	-2.27268	1.55975
	C	-1.82015	1.10619	0.00046				
INT5-4K	H	1.77848	4.87665	1.05177	C	0.97468	-2.17309	0.00335
	H	2.37991	4.76770	-0.60658	C	1.61277	-3.42674	0.00694
	N	-0.84290	-0.90173	0.00095	C	3.00764	-3.47562	0.00582
	C	-2.25415	-0.72156	0.00126	C	3.75101	-2.28600	0.00111
	C	-3.14765	-1.81191	0.00389	C	3.11433	-1.02938	-0.00252
	C	-2.74520	0.59476	-0.00131	H	1.01354	-4.33423	0.01049
	C	-4.51909	-1.57282	0.00396	H	3.51826	-4.43521	0.00857
	H	-2.76044	-2.82499	0.00576	H	4.83832	-2.33172	0.00027
	C	-4.12439	0.82011	-0.00116	H	3.70893	-0.11824	-0.00620
	H	-2.05754	1.43472	-0.00344	Pd	0.58513	0.65015	-0.00542
	C	-5.01409	-0.25843	0.00145	C	1.08052	3.16412	-0.00838
	H	-5.20946	-2.41313	0.00594	O	1.99069	2.25066	-0.01236
	H	-4.50032	1.84027	-0.00315	O	-0.14570	2.83280	-0.01116
	H	-6.08710	-0.08131	0.00150	C	1.50218	4.61167	0.02525
N	-0.41023	-2.10044	0.00435	H	0.68239	5.25731	-0.29431	
C	1.72666	-0.96799	-0.00137					
1L	C	1.37872	0.36786	0.56267	C	-0.65148	-1.12107	0.24408
	H	1.63197	-0.07761	1.53439	C	-0.09867	0.17120	0.28255
	H	1.59173	1.44825	0.65049	C	-0.94243	1.26892	0.05872
	C	3.64952	-0.07709	-0.20714	C	-2.30939	1.08601	-0.19387
	H	4.22727	-0.52354	-1.02270	C	-2.84895	-0.20389	-0.22740
	H	3.93756	0.98555	-0.11972	C	-2.01374	-1.30875	-0.00758
	H	3.94088	-0.57897	0.72279	H	-0.53029	2.27665	0.08238
	N	2.21919	-0.28912	-0.44947	H	-2.94869	1.94975	-0.36478
	H	-0.00523	-1.98047	0.40986	H	-3.90939	-0.34947	-0.42241
	H	1.97521	0.08988	-1.36554	H	-2.42682	-2.31528	-0.03077
TSS5-3L	H	0.99046	-2.23768	-2.41402	C	-1.70368	0.15180	0.08818
	H	5.03999	-1.09811	1.74549	C	-2.29601	-1.06797	-0.33567
	C	4.62073	-0.74646	0.80091	C	-3.53508	-1.47012	0.16800
	C	3.10928	-0.57708	0.92077	C	-4.20331	-0.67345	1.10857

	H	5.06934	0.22238	0.55523	C	-3.61380	0.50637	1.57563
	H	4.87379	-1.43909	-0.00611	C	-2.36981	0.90577	1.07654
	O	2.49632	-0.47880	-0.22548	H	-1.18156	1.09783	-0.75425
	O	2.55352	-0.52764	2.03311	H	-3.97436	-2.41354	-0.15116
	Pd	0.44197	-0.06782	-0.09249	H	-5.17085	-0.98867	1.49317
	O	-0.89340	2.28727	-1.27492	H	-4.12116	1.11219	2.32316
	C	0.13106	2.72540	-0.64127	H	-1.92738	1.83476	1.43138
	O	0.85542	1.99950	0.11261	C	-1.46431	-1.95864	-1.22024
	C	0.48160	4.18775	-0.79299	H	-1.34204	-1.52450	-2.21887
	H	-0.34865	4.79578	-0.42145	H	-1.89759	-2.95954	-1.33551
	H	1.39274	4.42850	-0.24558	C	0.86268	-2.78414	-1.47776
	H	0.60939	4.41983	-1.85405	H	1.82633	-2.84024	-0.97310
	N	-0.09814	-2.05422	-0.61311	H	0.49006	-3.79308	-1.69298
	H	-0.18329	-2.55549	0.27830				
INT5-4L	H	0.99521	3.38761	-0.47885	C	-2.28617	0.32055	0.12809
	H	-0.60182	4.11447	-0.15252	C	-3.60392	-0.15502	0.14586
	H	0.26946	3.24067	1.13621	C	-3.85302	-1.52897	0.03438
	Pd	0.60372	0.22080	-0.06610	C	-2.78680	-2.42710	-0.09996
	O	2.90224	0.50242	-0.04595	C	-1.46437	-1.95682	-0.12777
	C	2.97858	-0.75841	0.08235	H	-4.43531	0.54164	0.24599
	O	1.90599	-1.46969	0.14115	H	-4.87661	-1.89679	0.04867
	C	4.31530	-1.45967	0.14803	H	-2.98186	-3.49437	-0.18693
	H	4.49732	-1.97342	-0.80216	H	-0.63851	-2.65740	-0.23359
	H	5.11884	-0.74219	0.32235	C	-1.91791	1.77176	0.29162
	H	4.30682	-2.21755	0.93585	H	-1.81592	2.02241	1.35359
	N	-0.57529	1.98418	-0.33710	H	-2.65810	2.45784	-0.14031
	C	-0.71467	2.00440	-1.35284	C	0.05666	3.26397	0.06549
	C	-1.21752	-0.58617	-0.01090				
1M	H	1.24327	-0.07944	-1.79639	C	-0.85841	1.12183	-0.23988
	H	1.28346	-1.51598	-0.77173	C	-0.36766	-0.18644	-0.39075
	C	3.38311	0.26035	-0.49283	C	-1.25503	-1.25927	-0.22453
	H	4.06726	0.84141	0.13441	C	-2.60483	-1.03596	0.08066
	H	3.79260	-0.76411	-0.58397	C	-3.08325	0.27014	0.22837
	H	3.37169	0.71177	-1.49056	C	-2.20297	1.34971	0.06830
	N	2.03948	0.29376	0.08442	H	-0.89015	-2.27976	-0.33145
	C	2.04742	-0.22625	1.45240	H	-3.27810	-1.88140	0.20708
	H	2.37205	-1.28343	1.50668	H	-4.12972	0.44708	0.46784
	H	2.72845	0.37043	2.06813	H	-2.56701	2.36894	0.18255
	H	1.04651	-0.15493	1.88707	C	1.08466	-0.42694	-0.76751
	H	-0.17496	1.96005	-0.35598				
TS5-3M	H	0.83529	-1.78980	-2.60227	H	0.83627	-2.88350	0.89925
	H	5.02807	-1.07122	1.72179	H	-0.86361	-2.46999	1.19803
	C	4.61121	-0.72326	0.77476	C	-1.69504	0.31751	0.07140
	C	3.10419	-0.52163	0.89970	C	-2.31499	-0.87573	-0.38470

	H	5.07803	0.23305	0.51432	C	-3.56359	-1.26226	0.10679
	H	4.84621	-1.43123	-0.02440	C	-4.21336	-0.47648	1.06943
	O	2.48800	-0.42549	-0.24598	C	-3.59587	0.67516	1.56930
	O	2.55402	-0.44733	2.01264	C	-2.34261	1.05914	1.08066
	Pd	0.44411	0.04154	-0.11482	H	-1.14514	1.27306	-0.74328
	O	-0.82550	2.46877	-1.22635	H	-4.02430	-2.18615	-0.23830
	C	0.20853	2.85921	-0.57711	H	-5.18833	-0.77906	1.44530
	O	0.91022	2.09101	0.15564	H	-4.08853	1.27135	2.33419
	C	0.59846	4.31584	-0.68180	H	-1.87838	1.96695	1.46149
	H	-0.21174	4.93268	-0.28142	C	-1.50467	-1.75100	-1.30300
	H	1.51991	4.51246	-0.13403	H	-1.37847	-1.27114	-2.27946
	H	0.72383	4.58153	-1.73516	H	-1.96601	-2.73392	-1.46520
	N	-0.12862	-1.92858	-0.72083	C	0.79384	-2.47264	-1.75173
	C	-0.15884	-2.84256	0.45426	H	1.79336	-2.56367	-1.32806
	H	-0.46126	-3.85065	0.13922	H	0.43871	-3.45528	-2.09005
	H	0.58800	3.91668	-0.59722	C	1.15408	-0.75642	-0.03962
	H	-0.25217	2.76005	-1.66831	C	2.24176	0.10412	-0.28147
	Pd	-0.63672	0.11670	-0.02003	C	3.54663	-0.40414	-0.27404
	O	-2.92169	0.48355	-0.01790	C	3.76374	-1.76782	-0.03552
	C	-3.04630	-0.77972	-0.04773	C	2.67839	-2.62068	0.19970
	O	-2.00152	-1.53355	-0.06749	C	1.36806	-2.11542	0.20236
	C	-4.40819	-1.43360	-0.04073	H	4.39273	0.25794	-0.45399
	H	-4.59294	-1.86592	0.94865	H	4.77754	-2.16202	-0.02971
	H	-5.18802	-0.70204	-0.25880	H	2.84850	-3.67950	0.38585
	H	-4.44005	-2.24925	-0.76790	H	0.52743	-2.78115	0.38757
	N	0.59428	1.88546	0.06495	C	1.90162	1.53836	-0.59221
	C	0.82067	2.24038	1.49407	H	1.75993	1.66103	-1.67145
	H	1.42118	3.15821	1.56638	H	2.68106	2.24687	-0.27961
	H	-0.13983	2.40272	1.98752	C	-0.05545	3.02621	-0.62801
	H	1.34474	1.42621	1.99588	H	-1.00313	3.25591	-0.13590
	H	-4.20975	-0.00437	-0.60595	C	-1.13174	-1.20751	0.24545
	H	-2.99997	-2.15738	-0.26676	C	-0.44413	0.00252	0.43615
	C	1.01303	0.00511	0.82836	C	-1.13485	1.20998	0.24079
	H	1.25830	-0.87961	1.42412	C	-2.48359	1.20922	-0.13214
	H	1.25787	0.89682	1.41374	C	-3.16071	-0.00246	-0.31790
	S	2.08026	-0.00357	-0.68321	C	-2.48041	-1.21168	-0.12752
	C	3.72711	0.00118	0.11107	H	-0.60893	-2.15114	0.39249
	H	4.47048	-0.00239	-0.69024	H	-0.61453	2.15554	0.38422
	H	3.86939	0.89857	0.72008	H	-3.00560	2.15303	-0.27492
	H	3.87028	-0.89004	0.72888				
	H	-1.59477	-1.49653	2.45782	C	2.10243	-1.35607	0.39186
	H	-4.70638	1.06576	-1.67414	C	3.25936	-1.99164	-0.06607
	C	-4.71771	0.28489	-0.90698	C	4.07215	-1.37078	-1.02468
	C	-3.30950	-0.27852	-0.73334	C	3.71554	-0.12459	-1.55272

	H	-5.05617	0.74904	0.02400	C	2.55767	0.51196	-1.09879
	H	-5.41044	-0.50473	-1.20277	H	1.42763	0.92802	0.74118
	O	-2.46063	0.59596	-0.27333	H	3.52150	-2.98017	0.30585
	O	-3.05130	-1.46236	-1.01597	H	4.97254	-1.87236	-1.37275
	Pd	-0.40374	0.25003	-0.13161	H	4.33699	0.34666	-2.31076
	O	1.38903	2.13680	1.33339	H	2.29548	1.49039	-1.49677
	C	0.59970	2.85467	0.62419	C	1.13068	-2.05639	1.30038
	O	-0.18983	2.37933	-0.25352	H	0.97219	-1.50728	2.23454
	C	0.62430	4.35145	0.84228	H	1.41784	-3.08630	1.52684
	H	0.40254	4.56454	1.89197	S	-0.47416	-2.06776	0.36689
	H	1.63040	4.72832	0.63625	C	-1.66748	-2.30584	1.72975
	H	-0.10091	4.85095	0.20015	H	-2.65501	-2.32108	1.27049
	C	1.74343	-0.06948	-0.10179	H	-1.45657	-3.26841	2.20296
INT5-4N	S	-0.63135	2.06991	-0.54582	C	-1.16516	-0.71204	0.00912
	C	-0.03965	3.42279	0.53326	C	-2.33202	0.06907	0.14198
	H	0.93899	3.72590	0.15574	C	-3.58704	-0.55953	0.16267
	H	-0.73284	4.26426	0.45918	C	-3.68096	-1.95207	0.07231
	H	0.04947	3.08569	1.56725	C	-2.51931	-2.72434	-0.04930
	Pd	0.65074	0.13486	-0.09605	C	-1.26196	-2.10512	-0.08762
	O	2.90784	0.43843	-0.08613	H	-4.49153	0.04036	0.25245
	C	3.03047	-0.81448	0.10094	H	-4.65709	-2.43141	0.09287
	O	1.98503	-1.55646	0.19748	H	-2.58886	-3.80813	-0.11970
	C	4.39401	-1.45672	0.19205	H	-0.36292	-2.70938	-0.18673
	H	4.59410	-2.00360	-0.73574	C	-2.20080	1.56134	0.29565
	H	5.16864	-0.70076	0.33139	H	-2.10256	1.84739	1.34817
H	4.41740	-2.17900	1.01228	H	-3.03381	2.11747	-0.14274	
10	H	-2.97271	2.19319	-0.30958	C	-1.12853	1.21321	0.23187
	C	0.99674	-0.02598	0.84250	C	-0.46209	-0.00527	0.44902
	H	1.26556	0.88596	1.38576	C	-1.18020	-1.20036	0.26591
	H	1.20358	-0.87684	1.50138	C	-2.52561	-1.17886	-0.11802
	P	2.12408	-0.22798	-0.65811	C	-3.17894	0.04183	-0.32938
	C	3.77840	0.17002	0.11232	C	-2.47438	1.23875	-0.15226
	H	4.09894	-0.67112	0.73535	H	-0.59140	2.15037	0.37046
	H	4.52240	0.29719	-0.68077	H	-0.68285	-2.15520	0.42931
	H	3.76026	1.07594	0.72643	H	-3.06446	-2.11507	-0.24912
	H	1.87261	1.05530	-1.22398	H	-4.22556	0.05985	-0.62544
TS5-30	H	-5.01105	1.08562	-0.22697	C	2.00783	-1.51067	0.36100
	C	-4.67309	0.45348	-1.05250	C	3.11942	-2.19990	-0.13291
	C	-3.29003	-0.11794	-0.75590	C	3.94136	-1.61695	-1.10731
	H	-5.38915	-0.35070	-1.22907	C	3.64548	-0.34579	-1.61205
	H	-4.61557	1.08507	-1.94529	C	2.53977	0.34994	-1.11746
	O	-2.44165	0.76482	-0.31928	H	1.46847	0.81612	0.74220
	O	-3.04671	-1.32662	-0.94091	H	3.33793	-3.20422	0.22474
	Pd	-0.40485	0.32154	-0.11196	H	4.80258	-2.16570	-1.48273

	O	1.55179	2.02838	1.34794	H	4.27342	0.09922	-2.38056
	C	0.84045	2.83928	0.65188	H	2.32660	1.34853	-1.49390
	O	0.01236	2.46703	-0.23672	C	1.01991	-2.17398	1.29151
	C	1.03185	4.32059	0.89885	H	1.01292	-1.68976	2.27691
	H	2.00622	4.62122	0.49969	H	1.21918	-3.24003	1.43745
	H	0.24755	4.90016	0.41134	C	-1.89470	-2.40264	1.74214
	H	1.04078	4.51987	1.97330	H	-2.87807	-2.39086	1.27239
	P	-0.63929	-1.87493	0.51688	H	-1.65997	-3.41187	2.09525
	H	-0.69534	-2.82924	-0.51543	H	-1.88586	-1.71372	2.59049
	C	1.71271	-0.19803	-0.11078				
INT5-4O	H	0.83993	3.92989	-0.11738	C	-2.38324	0.05282	0.14854
	H	-0.86540	4.38098	0.13892	C	-3.61921	-0.61257	0.17054
	H	0.04253	3.52574	1.41713	C	-3.67839	-2.00503	0.05411
	Pd	0.66023	0.12111	-0.07205	C	-2.49774	-2.74435	-0.08786
	O	2.89754	0.44323	-0.06359	C	-1.25855	-2.09031	-0.11909
	C	3.06663	-0.81189	0.09460	H	-4.53832	-0.03895	0.28111
	O	2.05693	-1.59634	0.17127	H	-4.64160	-2.51025	0.07370
	C	4.46073	-1.39094	0.17440	H	-2.53855	-3.82825	-0.17733
	H	4.68008	-1.92485	-0.75659	H	-0.34555	-2.67166	-0.22980
	H	5.20268	-0.60296	0.31437	C	-2.28159	1.55491	0.30322
	H	4.52050	-2.11567	0.99081	H	-2.30304	1.84478	1.36163
	P	-0.61244	1.99889	-0.35729	H	-3.08143	2.10237	-0.20559
	H	-0.85613	2.30643	-1.71436	C	-0.10445	3.62032	0.33839
	C	-1.19342	-0.69416	-0.00420				
1P	C	0.74365	-0.42656	0.91662	C	-1.35746	0.98327	0.71307
	H	1.02305	0.30956	1.68008	C	-0.69513	-0.23686	0.49474
	H	0.88172	-1.42196	1.35579	C	-1.40215	-1.27268	-0.14334
	P	1.95765	-0.32684	-0.52358	C	-2.72964	-1.09582	-0.54672
	C	3.54961	-0.44962	0.43818	C	-3.37829	0.12576	-0.32289
	H	3.66121	-1.46234	0.83968	C	-2.68615	1.16498	0.30923
	H	4.39496	-0.26354	-0.23272	H	-0.83230	1.79722	1.21020
	H	3.59854	0.26531	1.26827	H	-0.90839	-2.22651	-0.32226
	C	1.93476	1.50646	-0.85186	H	-3.25911	-1.91226	-1.03377
	H	2.10696	2.09924	0.05460	H	-4.41135	0.26381	-0.63460
	H	2.71362	1.74936	-1.58256	H	-3.18017	2.11710	0.49236
	H	0.97133	1.79405	-1.28345				
		C	-4.68567	0.77570	-0.84607	C	1.74993	-0.09716
TS5-3P	C	-3.32228	0.11341	-0.66482	C	2.04466	-1.37173	0.48098
	H	-4.63565	1.48680	-1.67716	C	3.16460	-2.08931	0.05119
	H	-4.95507	1.34180	0.05011	C	3.99556	-1.57160	-0.95242
	O	-2.39886	0.93273	-0.25815	C	3.70021	-0.34070	-1.54946
	O	-3.16451	-1.09889	-0.90246	C	2.58691	0.38390	-1.11680
	Pd	-0.36933	0.43113	-0.11228	H	1.51064	0.95641	0.71166
	O	1.60679	2.19296	1.27081	H	3.38346	-3.06470	0.48148

	C	0.90020	2.97773	0.54067	H	4.86401	-2.14045	-1.27803
	O	0.06598	2.57196	-0.32626	H	4.33570	0.05147	-2.34023
	C	1.10693	4.46722	0.71818	H	2.37563	1.35418	-1.56229
	H	2.07637	4.74161	0.28908	C	1.03562	-1.96880	1.43336
	H	0.31915	5.03082	0.21756	H	0.99447	-1.40532	2.37485
	H	1.13563	4.71504	1.78207	H	1.23954	-3.01799	1.67198
	P	-0.60052	-1.75207	0.58481	C	-1.88273	-2.14942	1.82937
	C	-0.66459	-3.08130	-0.67308	H	-2.86109	-2.13756	1.34715
	H	-0.61079	-4.06032	-0.18464	H	-1.68907	-3.14008	2.25520
	H	-1.60070	-2.98647	-1.22416	H	-1.86318	-1.40419	2.62875
	H	0.17628	-2.97595	-1.36285	H	-5.44988	0.02627	-1.05872
INT5-4P	H	0.99786	4.10745	-0.85360	C	1.10004	-0.89455	-0.03932
	H	0.04678	3.07834	-1.96008	C	2.32281	-0.23711	-0.30215
	Pd	-0.70260	0.03039	-0.01926	C	3.52063	-0.96882	-0.28586
	O	-2.91939	0.49023	-0.01746	C	3.50983	-2.34253	-0.02248
	C	-3.16874	-0.76131	-0.04506	C	2.29657	-2.99527	0.22811
	O	-2.21284	-1.61303	-0.06174	C	1.09544	-2.27280	0.22118
	C	-4.59790	-1.25584	-0.03883	H	4.46479	-0.46278	-0.48248
	H	-4.82626	-1.67666	0.94643	H	4.44374	-2.90038	-0.01294
	H	-5.29390	-0.44108	-0.24583	H	2.28282	-4.06430	0.43205
	H	-4.72226	-2.05509	-0.77438	H	0.15693	-2.78755	0.41667
	P	0.67627	1.85624	0.04672	C	2.29090	1.24330	-0.61565
	C	1.03227	2.48997	1.73476	H	2.29015	1.41477	-1.69992
	H	1.74819	3.31776	1.69124	H	3.13947	1.79603	-0.19686
	H	0.10687	2.83974	2.20056	C	0.20984	3.34902	-0.91368
H	1.44636	1.68356	2.34520	H	-0.71836	3.76681	-0.51352	

Table S3. Cartesian coordinates of proton-transfer transition states and palladation products for designed open complex systems during ring-opening, optimized at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent.

Names	Cartesian Coordinates							
TS5-3AA	O	-2.82955	-0.16470	1.61972	C	1.78358	0.44554	0.09732
	Pd	-0.32388	0.02021	-0.17183	C	2.30873	0.09150	1.36304
	O	0.95177	2.93665	0.12034	C	3.57875	-0.47710	1.48418
	C	-0.28583	2.99447	-0.19155	C	4.34816	-0.71209	0.33538
	O	-1.01593	1.97587	-0.39833	C	3.85324	-0.36678	-0.93036
	C	-0.91987	4.36231	-0.30879	C	2.58415	0.20639	-1.04513
	H	-0.97849	4.80665	0.68991	H	1.28876	1.69535	0.11459
	H	-0.28882	5.00908	-0.92320	H	5.33670	-1.15795	0.42735
	H	-1.92126	4.29050	-0.73279	H	4.45823	-0.54023	-1.81800
	H	1.71967	0.27828	2.25978	H	2.21367	0.48748	-2.02990
	H	3.97148	-0.73546	2.46550	H	-5.13457	-1.12107	1.01724
	C	-0.42912	-2.94444	-0.47539	C	-4.55666	-0.92430	0.11222

	O 0.27472 -2.02152 0.00130	C -3.12549 -0.53486 0.47137
	H -1.38401 -2.73663 -0.97056	H -4.57357 -1.79820 -0.54438
	N -0.06814 -4.22511 -0.40675	H -5.02484 -0.09604 -0.43108
	H -0.66242 -4.95189 -0.79655	O -2.29163 -0.61796 -0.53054
	H 0.80206 -4.49416 0.04991	
INT5-4AA	C -4.37726 -1.23259 0.02290	C 1.08253 -0.75468 -0.07245
	C -3.02640 -0.55604 -0.00952	C 2.15523 -0.44500 -0.91997
	H -4.38598 -2.02808 0.77269	C 3.31843 -1.23049 -0.88710
	H -4.56995 -1.69476 -0.95133	C 3.41541 -2.31404 -0.00640
	O -1.97225 -1.30174 0.02841	C 2.33968 -2.61988 0.83675
	O -2.91868 0.70298 -0.08896	C 1.16896 -1.84751 0.80077
	Pd -0.59941 0.31144 -0.10246	H 4.14561 -0.99117 -1.55316
	O 0.45028 2.17596 -0.22613	H 4.31946 -2.91869 0.01934
	H 2.09549 0.39299 -1.61108	H 2.40457 -3.46430 1.52075
	H 1.87146 1.88484 1.22973	H 0.33163 -2.10859 1.44413
	N 1.87606 3.79791 0.47521	C 1.38920 2.55736 0.51026
	H 1.48423 4.48912 -0.16273	H -5.16480 -0.50673 0.23240
	H 2.63933 4.07325 1.08779	
T55-3BB	Pd -0.33255 0.03376 -0.16899	C 1.76464 0.50136 0.09777
	O 0.89448 2.97937 0.06916	C 2.28567 0.17460 1.37277
	C -0.35269 3.00816 -0.20176	C 3.55901 -0.38282 1.50910
	O -1.07073 1.97285 -0.36944	C 4.33465 -0.63319 0.36779
	C -1.01519 4.36165 -0.33044	C 3.84330 -0.31507 -0.90649
	H -2.06658 4.25588 -0.59631	C 2.57073 0.24622 -1.03771
	H -0.92360 4.89377 0.62095	H 1.25642 1.74153 0.08497
	H -0.49082 4.94863 -1.08953	H 5.32556 -1.07086 0.47209
	H 1.69154 0.37463 2.26331	H 4.45351 -0.50062 -1.78800
	H 3.94934 -0.62077 2.49642	H 2.20190 0.50622 -2.02889
	C -0.33407 -2.95270 -0.51187	H -5.02809 -0.20450 -0.39351
	O 0.30643 -2.01375 -0.02762	C -4.53155 -1.03399 0.12193
	H -1.28422 -2.74735 -1.02827	C -3.11016 -0.61278 0.48117
	C 0.13304 -4.36423 -0.41475	H -5.09525 -1.27268 1.02583
	H -0.64016 -4.95833 0.08888	H -4.52855 -1.88927 -0.55878
	H 0.22739 -4.77652 -1.42738	O -2.27913 -0.65443 -0.52715
	H 1.08116 -4.44073 0.11931	O -2.81560 -0.25593 1.63347
INT5-4BB	C -3.04386 -0.50194 -0.01627	C 1.05726 -0.79092 -0.06944
	H -4.44241 -1.94485 0.74832	C 2.11549 -0.52433 -0.94849
	H -4.61198 -1.59195 -0.97330	C 3.26657 -1.32766 -0.91361
	O -2.00858 -1.27461 0.01256	C 3.36280 -2.38506 -0.00194
	O -2.90180 0.75497 -0.07802	C 2.29944 -2.64779 0.87087
	Pd -0.60303 0.31013 -0.09547	C 1.14077 -1.85753 0.83474
	O 0.49818 2.15793 -0.17773	H 4.08361 -1.12295 -1.60313
	C 2.02231 3.90118 0.42393	H 4.25722 -3.00372 0.02477
	H 3.08061 3.84939 0.13822	H 2.36431 -3.47216 1.57876

	H	1.46623	4.52221	-0.27983	H	0.31249	-2.08431	1.50240
	H	1.99564	4.34234	1.42852	C	1.47205	2.51777	0.49054
	H	2.05484	0.28993	-1.66795	H	-5.18010	-0.39919	0.21925
	H	1.96587	1.80088	1.16579	C	-4.41107	-1.14337	0.00556
TS5-3CC	O	-3.62099	0.03868	0.30210	H	5.32480	-0.61622	-0.55941
	C	-3.34943	-1.20209	0.18272	C	-1.43731	1.47378	0.03086
	O	-2.18593	-1.66048	-0.04933	C	-1.09631	2.08865	1.26020
	C	-4.48363	-2.19113	0.33550	C	-0.85193	3.46165	1.33492
	H	-4.14422	-3.20653	0.13278	C	-0.94008	4.24754	0.17652
	H	-4.87246	-2.12732	1.35628	C	-1.28141	3.66382	-1.05196
	H	-5.29488	-1.91937	-0.34506	C	-1.52379	2.29029	-1.12256
	H	-1.03958	1.48563	2.16540	H	-2.51100	0.69153	0.15489
	H	-0.59777	3.92136	2.28772	H	-0.74764	5.31718	0.23253
	C	2.30712	0.54149	0.04490	H	-1.35827	4.27985	-1.94542
	O	1.28674	0.69150	-0.63536	H	-1.79903	1.84473	-2.07730
	H	2.36802	-0.20031	0.85288	H	2.06547	-4.21486	-1.16337
	O	3.36673	1.28300	-0.19998	C	1.80465	-4.13331	-0.10535
	C	4.57606	1.05661	0.60212	C	1.25435	-2.74876	0.21893
	H	4.88176	2.05262	0.92743	H	1.02847	-4.87809	0.10291
	H	4.31322	0.46264	1.48235	H	2.67343	-4.35245	0.51851
	C	5.64005	0.38385	-0.24661	O	0.50406	-2.24304	-0.71362
	H	5.86294	0.97860	-1.13686	O	1.51701	-2.19374	1.30619
H	6.55829	0.28655	0.34197	Pd	-0.50788	-0.45059	-0.29064	
INT5-4CC	H	5.35467	-0.96870	-0.76724	C	0.07446	1.39028	-0.08753
	O	2.92309	0.17052	0.14452	C	-0.90768	1.76377	-1.01455
	O	2.61766	-2.01372	-0.10247	C	-1.46543	3.05095	-0.95436
	Pd	0.90634	-0.41772	-0.15320	C	-1.05123	3.95537	0.03017
	O	-1.00648	-1.39443	-0.44696	C	-0.06743	3.57545	0.95177
	H	-1.23798	1.07370	-1.78839	C	0.50385	2.29538	0.89161
	H	-2.11685	-0.48377	1.01399	H	-2.22223	3.34116	-1.68097
	O	-3.07611	-2.01285	0.01882	H	-1.48753	4.95086	0.07595
	C	-4.28485	-1.79374	0.82419	H	0.26427	4.27525	1.71674
	H	-4.04289	-1.12382	1.65483	H	1.28306	2.01854	1.59834
	H	-4.53239	-2.77787	1.22612	C	-2.02821	-1.24467	0.22542
	C	-5.39311	-1.24129	-0.05385	H	5.12695	-2.25380	0.43905
	H	-6.30781	-1.15028	0.54110	C	4.88947	-1.21732	0.19298
	H	-5.13575	-0.25162	-0.44309	C	3.39514	-1.03049	0.07707
H	-5.59477	-1.91061	-0.89478	H	5.30255	-0.54254	0.94683	
TS5-3DD	Pd	-0.35947	0.14287	-0.27251	C	2.23428	-0.13224	1.28170
	O	1.12986	2.92378	0.30243	C	3.44836	-0.81854	1.35695
	C	-0.12336	3.08294	0.12571	C	4.21543	-1.00359	0.19734
	O	-0.93678	2.13712	-0.12300	C	3.77492	-0.49455	-1.03295
	C	-0.67941	4.48596	0.22660	C	2.56033	0.19137	-1.10377
	H	-1.73720	4.50456	-0.03423	H	1.37928	1.65845	0.17098

	H	-0.54498	4.84525	1.25140	H	5.16081	-1.53967	0.25393
	H	-0.11342	5.14860	-0.43335	H	4.37967	-0.63073	-1.92709
	H	1.64867	0.01906	2.18744	H	2.23010	0.59598	-2.05936
	H	3.80016	-1.20530	2.31109	H	-4.75248	-1.06966	-1.14031
	C	-0.39036	-2.84542	0.16370	C	-4.60074	-0.79947	-0.09245
	O	0.11643	-1.95015	-0.51962	C	-3.11616	-0.72154	0.24516
	O	-0.08233	-4.11980	0.01332	H	-5.04946	0.18783	0.06385
	H	-1.13805	-2.66149	0.94156	H	-5.10101	-1.51650	0.56140
	H	0.59191	-4.22691	-0.70801	O	-2.37979	-0.22996	-0.70726
	C	1.76449	0.38694	0.05083	O	-2.69050	-1.09509	1.35704
INT5-4DD	C	4.35998	-1.27374	-0.00703	C	-1.09363	-0.74532	0.07144
	C	3.01390	-0.58919	0.01802	C	-2.15365	-0.42158	0.92835
	H	4.36481	-2.07541	-0.75016	C	-3.33051	-1.18677	0.89542
	H	4.54844	-1.72871	0.97139	C	-3.44970	-2.26192	0.00751
	O	1.95438	-1.32814	-0.01747	C	-2.38408	-2.58084	-0.84351
	O	2.91203	0.67103	0.08931	C	-1.19998	-1.82911	-0.80926
	Pd	0.60046	0.30027	0.09940	H	-4.15012	-0.93764	1.56701
	O	-0.45030	2.20042	0.19049	H	-4.36422	-2.85049	-0.01797
	H	-2.07564	0.40859	1.62750	H	-2.46713	-3.41915	-1.53288
	H	-1.87060	1.96325	-1.27886	H	-0.37055	-2.09852	-1.45935
	O	-1.84330	3.81974	-0.51013	C	-1.36376	2.59084	-0.53842
H	-1.36158	4.36110	0.16947	H	5.15173	-0.55397	-0.22144	
TS5-3EE	O	-1.60373	1.92715	2.05794	C	1.77474	-0.85711	-0.07373
	Pd	0.07102	0.48624	-0.11995	C	2.30358	-1.06051	1.22402
	O	2.96257	1.26219	-1.08266	C	2.80235	-2.30563	1.61809
	C	2.33615	2.30415	-0.68095	C	2.79250	-3.37635	0.71329
	O	1.18077	2.27295	-0.15718	C	2.28920	-3.19854	-0.58368
	C	3.03003	3.64111	-0.80944	C	1.78172	-1.95472	-0.96711
	H	3.67725	3.77785	0.06372	H	2.28776	0.25261	-0.65823
	H	3.65848	3.65787	-1.70175	H	3.18094	-4.34669	1.01639
	H	2.30118	4.45200	-0.83387	H	2.29218	-4.02874	-1.28715
	H	2.33312	-0.22970	1.92771	H	1.39285	-1.82627	-1.97574
	H	3.20060	-2.44281	2.62136	H	-3.85084	2.94880	-0.08841
	C	-1.21670	-2.14518	0.64300	C	-3.25109	3.15615	0.80089
	O	-1.21188	-1.15688	-0.19615	C	-2.08324	2.17940	0.93665
	O	-2.08948	-3.03214	0.64525	H	-2.84809	4.17100	0.70710
H	-0.39879	-2.17216	1.38398	H	-3.87592	3.12264	1.69647	
K	-3.82131	-1.67028	-1.20394	O	-1.65929	1.69362	-0.19286	
INT5-4EE	C	-0.34919	4.64965	-0.07993	C	-1.57254	-0.72874	-0.09760
	C	-0.13479	3.15373	-0.01768	C	-1.44719	-1.97057	-0.73742
	H	-1.19273	4.93897	0.55238	C	-2.55525	-2.82699	-0.83105
	H	-0.59541	4.93411	-1.10879	C	-3.78672	-2.45514	-0.27881
	O	-1.17040	2.38838	-0.07870	C	-3.90996	-1.21523	0.36057
	O	1.02929	2.65972	0.07404	C	-2.80920	-0.34954	0.44615

	Pd -0.05864 0.56524 0.02735	H -2.45052 -3.78627 -1.33540
	O 1.41299 -0.93204 0.14036	H -4.64269 -3.12321 -0.34843
	H -0.49638 -2.27754 -1.16535	H -4.86425 -0.91473 0.79011
	H 0.60240 -1.95963 1.70902	H -2.92478 0.61957 0.92628
	O 2.49167 -2.55735 1.24291	C 1.49104 -1.83891 1.06227
	K 4.16016 -1.08385 -0.60490	H 0.55296 5.18149 0.22741
TS5-3FF	Pd -0.33803 -0.00046 -0.21012	H 0.43990 -3.74199 -1.52430
	O 0.91896 2.92732 0.05848	C 1.76243 0.44049 0.07866
	C -0.34722 2.96944 -0.09611	C 2.26142 0.10215 1.35931
	O -1.08570 1.94285 -0.22560	C 3.52510 -0.47380 1.51135
	C -1.00950 4.32890 -0.12245	C 4.31539 -0.72537 0.38059
	H -0.84505 4.82183 0.84027	C 3.84788 -0.39087 -0.89842
	H -0.53883 4.94431 -0.89396	C 2.58362 0.18478 -1.04541
	H -2.07829 4.23692 -0.31351	H 1.26600 1.68512 0.05664
	H 1.65968 0.31073 2.24311	H 5.29966 -1.17474 0.49707
	H 3.89753 -0.72185 2.50312	H 4.47041 -0.57500 -1.77159
	O 0.28934 -2.09378 -0.27139	H 2.23424 0.45767 -2.04035
	C -0.09684 -2.88019 0.87726	H -5.02026 -0.15740 -0.34650
	H 0.23677 -2.33722 1.76111	C -4.53433 -1.05124 0.05988
	H -1.18245 -3.01315 0.90759	C -3.09425 -0.70743 0.42794
	H 0.40599 -3.85201 0.82362	H -5.08389 -1.37794 0.94480
	C -0.02765 -2.75136 -1.51784	H -4.56799 -1.82368 -0.71285
H -1.11171 -2.83621 -1.64044	O -2.29178 -0.64287 -0.59945	
H 0.39457 -2.13962 -2.31574	O -2.76125 -0.50321 1.60782	
INT5-4FF	H 1.26957 2.10035 1.67703	C 1.37425 -0.44521 -0.06556
	H 0.96406 3.78679 1.16265	C 2.38318 0.34362 -0.63231
	H -0.32375 2.85672 1.99775	C 3.70562 -0.12740 -0.64348
	Pd -0.52620 0.15931 -0.04209	C 4.01827 -1.37336 -0.08766
	O -2.84646 -0.00306 -0.04523	C 3.00262 -2.15624 0.47486
	C -2.66877 -1.25794 -0.05384	C 1.67637 -1.69846 0.48158
	O -1.47225 -1.74445 -0.06372	H 4.48801 0.48468 -1.08880
	C -3.83166 -2.22077 -0.03083	H 5.04484 -1.73340 -0.09607
	H -3.91664 -2.65513 0.97117	H 3.23651 -3.12828 0.90549
	H -4.76177 -1.70358 -0.27227	H 0.89113 -2.32221 0.90213
	H -3.66003 -3.04076 -0.73295	C -0.85366 3.17585 -0.62893
	O 0.08192 2.28850 0.02024	H -1.78011 3.25393 -0.04882
	H -1.06438 2.75502 -1.61257	H -0.39558 4.16494 -0.73872
H 2.15431 1.31507 -1.06291	C 0.51938 2.79486 1.29993	
TS5-3GG	Pd -0.35616 -0.10643 -0.17080	C 2.24488 0.04620 1.39654
	O 1.01665 2.76781 -0.19690	C 3.48061 -0.56760 1.62284
	C -0.25550 2.85697 -0.23256	C 4.26605 -0.97329 0.53427
	O -1.04241 1.85808 -0.20634	C 3.82469 -0.75266 -0.77870
	C -0.86482 4.23820 -0.32351	C 2.58837 -0.13982 -1.00109
	H -1.95118 4.18970 -0.25639	H 1.31022 1.50867 -0.08607

	H	-0.46104	4.86647	0.47463	H	5.22692	-1.45324	0.70891
	H	-0.57295	4.68818	-1.27749	H	4.44473	-1.05468	-1.62018
	H	1.64495	0.36917	2.24602	H	2.25847	0.04175	-2.02299
	H	3.83301	-0.72837	2.63946	H	-4.58082	-1.93922	-0.50471
	C	-0.31635	-3.05283	-1.25136	C	-4.52351	-1.17710	0.27681
	H	-1.35685	-2.78712	-1.42774	C	-3.07434	-0.80494	0.57347
	H	0.28201	-2.86056	-2.14701	H	-5.05195	-0.28973	-0.08849
	H	-0.23809	-4.10356	-0.95768	H	-5.01551	-1.53040	1.18499
	O	0.12975	-2.22174	-0.14492	O	-2.33393	-0.68887	-0.49640
	H	1.06683	-2.41051	0.06405	O	-2.68106	-0.62125	1.73735
	C	1.76865	0.26637	0.08079				
INT5-4GG	O	-2.81889	0.05058	0.04974	C	4.10435	-1.01164	0.02861
	C	-3.72202	-2.19467	0.23190	C	3.14894	-1.78091	-0.64757
	H	-3.76552	-2.57331	1.25878	C	1.80072	-1.39341	-0.65106
	H	-4.67611	-1.72547	-0.01393	C	1.41467	-0.22272	0.01443
	H	-3.53829	-3.04763	-0.42667	C	2.36332	0.54996	0.69672
	H	1.06338	-2.00839	-1.16229	C	3.70916	0.14933	0.70288
	H	5.14820	-1.31797	0.03379	H	3.44780	-2.68785	-1.17016
	C	-1.00352	3.37128	-0.33709	H	2.07001	1.45389	1.22608
	H	-1.70175	3.21249	0.48409	H	4.44397	0.74781	1.23847
	H	-1.51291	3.21837	-1.29282	Pd	-0.50880	0.29643	-0.00247
	H	-0.59053	4.38247	-0.28129	C	-2.59525	-1.19537	0.12164
	O	0.06871	2.40672	-0.15728	O	-1.38281	-1.63892	0.11986
	H	0.75847	2.53155	-0.84181				
TS5-3HH	O	-2.34104	-0.64894	-0.44205	C	1.72496	0.41723	0.16587
	O	-2.65369	-0.66887	1.79604	C	2.20465	0.16878	1.47476
	Pd	-0.38024	-0.01549	-0.10297	C	3.45483	-0.41812	1.68260
	O	0.91889	2.90645	-0.07349	C	4.24693	-0.77628	0.58204
	C	-0.33367	2.95019	-0.30831	C	3.79547	-0.53829	-0.72427
	O	-1.08462	1.92587	-0.38466	C	2.54572	0.05158	-0.92890
	C	-0.96855	4.30895	-0.50579	H	1.25049	1.65575	0.04132
	H	-2.02517	4.21250	-0.75353	H	5.21992	-1.23642	0.74268
	H	-0.85387	4.88966	0.41428	H	4.41874	-0.80789	-1.57428
	H	-0.43989	4.84108	-1.30124	H	2.20683	0.24854	-1.94478
	H	1.59705	0.45261	2.33284	H	-5.07105	-0.31453	0.07203
	H	3.81425	-0.59542	2.69399	C	-4.50765	-1.21381	0.34438
	N	0.20194	-2.89511	-0.70619	C	-3.06248	-0.82105	0.63220
	O	0.15779	-2.10182	0.25768	H	-4.96233	-1.65497	1.23348
	O	0.06632	-2.62316	-1.88256	H	-4.56728	-1.90860	-0.49705
		H	0.37942	-3.89530	-0.43486			
INT5-4HH	O	-1.57773	-1.60499	0.05991	C	3.90685	-1.50848	0.11930
	O	-2.86789	0.17151	-0.25075	C	2.86055	-2.06362	0.86614
	C	-3.95812	-1.96352	0.12043	C	1.56093	-1.54557	0.75996
	H	-4.11383	-2.16178	1.18656	C	1.32015	-0.45937	-0.08913

	H	-4.84875	-1.47549	-0.27922	C	2.35825	0.10241	-0.84144
	H	-3.79456	-2.92339	-0.37565	C	3.65301	-0.43031	-0.73611
	H	0.75069	-1.99567	1.32868	H	3.04900	-2.90528	1.53015
	H	4.91222	-1.91592	0.20065	H	2.17827	0.94050	-1.51091
	N	0.27632	3.08250	0.34882	H	4.45924	0.00279	-1.32537
	O	0.19018	2.26947	-0.59600	Pd	-0.54568	0.23610	-0.21925
	O	0.04028	2.86381	1.52127	C	-2.74999	-1.07299	-0.04141
	H	0.58608	4.04640	0.06713				
TS5-3II	Pd	-0.74090	-0.26720	-0.00446	C	4.49618	-0.95670	-1.77279
	O	-2.60332	1.91911	-1.39127	H	3.22969	-2.33929	-2.84905
	C	-3.17841	0.77731	-1.36332	H	5.50117	0.48017	-0.50853
	O	-2.67412	-0.25601	-0.82480	H	5.34418	-1.08467	-2.44144
	C	-4.54882	0.66443	-1.99263	C	-0.44313	1.89337	0.10696
	H	-5.26657	1.20368	-1.36591	C	-0.75313	2.43517	1.37909
	H	-4.54437	1.14213	-2.97539	C	0.00255	3.47313	1.92991
	H	-4.85271	-0.37890	-2.07587	C	1.08755	3.99951	1.21361
	H	-1.60607	2.04700	1.93438	C	1.40967	3.49108	-0.05246
	H	-0.25301	3.87695	2.90745	C	0.65517	2.44711	-0.59389
	C	1.34695	-0.52293	2.08638	H	-1.52597	1.81654	-0.68822
	H	0.48884	-0.39646	2.73966	H	1.67656	4.80971	1.63908
	H	2.32934	-0.71532	2.52418	H	2.24523	3.90795	-0.61101
	N	1.18384	-0.47473	0.81729	H	0.90935	2.06426	-1.58096
	C	2.31311	-0.62527	-0.05730	H	-1.49037	-4.88029	1.99379
	C	2.20854	-1.48941	-1.15701	C	-1.26126	-4.45829	1.01370
	C	3.49772	0.08906	0.17586	C	-1.17210	-2.93678	1.09510
	C	3.30582	-1.65809	-2.00474	H	-0.31551	-4.86954	0.64728
	H	1.28443	-2.03560	-1.32233	H	-2.03898	-4.74709	0.29969
	C	4.58656	-0.08118	-0.68478	O	-0.88178	-2.36948	-0.04113
H	3.55738	0.79372	1.00165	O	-1.36527	-2.33481	2.16787	
INT5-4II	H	-0.99373	5.00132	-0.59694	C	-1.94838	-0.69975	0.08401
	H	-1.01063	4.82728	1.15974	C	-3.18462	-0.26678	-0.41751
	N	0.88421	-1.06872	-0.73516	C	-4.32882	-1.05996	-0.24600
	H	1.29625	-2.72648	-1.91383	C	-4.24830	-2.27877	0.43888
	C	2.23293	-1.00352	-0.24152	C	-3.01672	-2.70320	0.95009
	C	3.32861	-1.10737	-1.11204	C	-1.86523	-1.92090	0.76918
	C	2.43705	-0.80994	1.13249	H	-5.28293	-0.71848	-0.64376
	C	4.62740	-1.04660	-0.59769	H	-5.13796	-2.88984	0.57571
	H	3.16912	-1.20307	-2.18355	H	-2.94458	-3.64514	1.49112
	C	3.73784	-0.76349	1.63832	H	-0.91836	-2.27156	1.17261
	H	1.58047	-0.71059	1.79488	C	0.57278	-1.97581	-1.58765
	C	4.83575	-0.88239	0.77646	Pd	-0.38422	0.52851	-0.16549
	H	5.47531	-1.11626	-1.27500	C	-0.32366	3.09260	0.09131
	H	3.89349	-0.62778	2.70591	O	-1.37528	2.36992	0.27925
	H	5.84741	-0.83282	1.17218	O	0.77429	2.55125	-0.24000

	H	-0.43734	-2.00947	-1.98606	C	-0.44329	4.58964	0.25597
	H	-3.26821	0.68844	-0.93112	H	0.54424	5.05230	0.29711
TS5-3JJ	O	1.72295	-2.75811	0.72623	H	-2.03697	0.31996	-1.82572
	C	2.62782	-2.07337	0.13585	C	-0.64083	-1.74503	0.17791
	O	2.41557	-0.94880	-0.41425	C	-1.47208	-1.70973	1.32380
	C	4.02335	-2.65214	0.07741	C	-2.74346	-2.28847	1.31654
	H	4.73010	-1.92126	-0.31519	C	-3.21933	-2.90937	0.15275
	H	4.32746	-2.97711	1.07564	C	-2.41673	-2.96477	-0.99571
	H	4.01197	-3.53562	-0.56875	C	-1.14215	-2.39198	-0.97847
	H	-1.10856	-1.23508	2.23399	H	0.59965	-2.16831	0.49202
	H	-3.36376	-2.25709	2.20995	H	-4.21153	-3.35633	0.14324
	C	-1.32941	2.05295	0.88066	H	-2.78282	-3.45902	-1.89331
	C	-2.44996	2.87396	0.99534	H	-0.51692	-2.46171	-1.86775
	C	-3.46622	2.77463	0.04202	H	2.48408	4.14171	-1.22246
	C	-3.32387	1.85057	-0.99611	C	2.92723	3.67540	-0.33889
	C	-2.18030	1.05575	-1.04104	C	2.08426	2.49697	0.14095
	N	-1.20177	1.15542	-0.11906	H	3.92027	3.30861	-0.62150
	H	-4.35004	3.40527	0.10541	H	3.04158	4.41063	0.46009
	H	-0.50227	2.11057	1.58113	O	1.58777	1.77573	-0.82082
	H	-2.51092	3.57911	1.81964	O	1.92894	2.27653	1.35796
H	-4.08312	1.73679	-1.76479	Pd	0.56201	0.02687	-0.24694	
INT5-4JJ	H	4.27969	-3.14796	-0.26794	C	-0.26300	4.35958	0.19273
	H	4.91966	-1.52341	-0.67374	C	0.69269	3.82357	-0.67932
	H	1.67089	2.03911	-1.39461	C	0.90935	2.43824	-0.72791
	H	-0.42586	5.43454	0.23282	C	0.15702	1.58068	0.08824
	C	-2.38066	-0.29673	-0.86347	C	-0.80166	2.11557	0.96118
	C	-3.69632	-0.74545	-0.96837	C	-1.00423	3.50345	1.01539
	C	-4.09814	-1.85295	-0.21810	H	1.27737	4.48116	-1.32037
	C	-3.16019	-2.47702	0.60878	H	-1.39133	1.46713	1.60515
	C	-1.86141	-1.97521	0.65362	H	-1.74453	3.91052	1.70205
	N	-1.47325	-0.89961	-0.06617	Pd	0.57755	-0.37536	0.00499
	H	-5.11910	-2.22303	-0.27700	C	2.87384	-1.53678	-0.01192
	H	-2.03386	0.56437	-1.42479	O	2.71712	-0.25800	0.01133
	H	-4.38514	-0.22741	-1.62989	O	1.86390	-2.30638	-0.03165
	H	-3.42028	-3.34189	1.21268	C	4.27915	-2.09155	0.00593
	H	-1.10193	-2.44035	1.27634	H	4.69279	-1.98623	1.01480
TS5-3KK	C	-2.98723	1.88051	-0.62056	H	5.43318	-1.25054	-2.01334
	O	-2.62289	0.69105	-0.87958	C	0.15541	1.75934	0.34922
	C	-4.34476	2.33824	-1.10538	C	0.59202	1.91464	1.68897
	H	-4.96400	2.59163	-0.23959	C	1.78765	2.56928	1.99098
	H	-4.22902	3.24595	-1.70398	C	2.58208	3.07962	0.95393
	H	-4.83144	1.55897	-1.69145	C	2.17408	2.94527	-0.38041
	H	-0.02564	1.53390	2.50129	C	0.97576	2.29178	-0.67609
	H	2.10147	2.68528	3.02625	H	-1.11096	2.16176	0.21251

	N	0.84141	-1.12152	0.65334	H	3.51572	3.58790	1.18673
	N	0.79600	-1.73300	1.74091	H	2.78762	3.35178	-1.18163
	H	-0.17589	-1.67225	2.09702	H	0.65668	2.21128	-1.71405
	C	2.10160	-1.13756	-0.04244	H	-2.96405	-4.61660	0.93758
	C	2.09060	-0.94708	-1.42961	C	-2.93124	-3.93716	0.08363
	C	3.30452	-1.35863	0.64716	C	-2.17609	-2.66554	0.44760
	C	3.29216	-1.00285	-2.13936	H	-2.47665	-4.43094	-0.77849
	H	1.15002	-0.78071	-1.94824	H	-3.95863	-3.67054	-0.18832
	C	4.50023	-1.39141	-0.06863	O	-1.70318	-2.00956	-0.56741
	H	3.29238	-1.48917	1.72474	O	-2.06358	-2.31196	1.64274
	C	4.49670	-1.22011	-1.46112	Pd	-0.84271	-0.13098	-0.11843
	H	3.28676	-0.87231	-3.21858	O	-2.27338	2.71788	0.02850
	H	5.43839	-1.54760	0.45844				
INT5-4KK	H	1.12400	4.65054	1.57476	C	3.76307	-2.72751	0.91196
	H	1.48100	-0.53913	2.19706	C	3.00323	-2.02953	1.85906
	H	4.49938	-3.46064	1.23418	C	2.05523	-1.08063	1.44807
	N	-1.54195	-1.44697	-1.51450	C	1.86406	-0.83322	0.08202
	C	-2.51782	-1.11426	-0.54815	C	2.61845	-1.53201	-0.86843
	C	-2.65190	0.13612	0.08917	C	3.57155	-2.47482	-0.45081
	C	-3.44276	-2.14451	-0.29074	H	3.14649	-2.21883	2.92143
	C	-3.69034	0.32564	1.00047	H	2.49065	-1.34746	-1.93454
	H	-1.99429	0.96427	-0.15362	H	4.16123	-3.00740	-1.19477
	C	-4.45765	-1.95304	0.64655	Pd	0.56502	0.61091	-0.44403
	H	-3.33807	-3.08704	-0.82231	C	0.57166	3.11186	0.17330
	C	-4.58230	-0.71680	1.29313	O	1.46307	2.27726	0.57801
	H	-3.81109	1.29404	1.48013	O	-0.38191	2.71974	-0.57185
	H	-5.15777	-2.75674	0.86038	C	0.69470	4.56270	0.57412
	H	-5.38433	-0.55737	2.01031	H	1.36912	5.06713	-0.12686
N	-0.43793	-0.85037	-1.54200	H	-0.27835	5.05584	0.53093	
H	0.11567	-1.23386	-2.32377					
TS5-3LL	C	-0.36532	2.93413	-0.09439	C	2.32525	0.07104	1.34997
	O	-1.09450	1.91028	-0.26374	C	3.60799	-0.46930	1.47931
	C	-1.01380	4.29971	-0.14035	C	4.39723	-0.67044	0.33746
	H	-0.51541	4.91234	-0.89686	C	3.90742	-0.31967	-0.92891
	H	-2.07725	4.21756	-0.36380	C	2.62305	0.21924	-1.05117
	H	-0.87420	4.79297	0.82622	H	1.24267	1.64439	0.09209
	H	1.72667	0.23979	2.24424	H	5.39586	-1.09143	0.43561
	H	3.99588	-0.72848	2.46233	H	4.52723	-0.46324	-1.81161
	N	0.27589	-2.09550	-0.22525	H	2.25866	0.50460	-2.03709
	C	-0.25004	-2.84367	0.94665	H	-4.99624	-0.03973	-0.47512
	H	0.10808	-2.37546	1.86499	C	-4.57732	-0.93059	0.00589
	H	-1.33901	-2.81023	0.93469	C	-3.13384	-0.64098	0.40957
	H	0.08582	-3.88790	0.91331	H	-5.17795	-1.16839	0.88602
	C	-0.10320	-2.74354	-1.50864	H	-4.62636	-1.74827	-0.71794

	H -1.18365 -2.66917 -1.63580	O -2.29083 -0.69867 -0.58452
	H 0.39241 -2.22704 -2.33327	O -2.83893 -0.36909 1.58615
	H 0.19874 -3.79855 -1.50785	Pd -0.32658 -0.05039 -0.20235
	H 1.29605 -2.10080 -0.16295	O 0.89568 2.88576 0.11729
	C 1.79625 0.42026 0.08234	
INT5-4LL	Pd 0.53360 0.13730 -0.04239	C -4.09535 -1.20403 -0.07799
	H -1.38804 -1.08011 1.99529	C -3.52385 -0.63983 -1.22411
	N -0.08081 2.19668 -0.01349	C -2.18266 -0.22412 -1.21534
	C 0.89822 3.03462 -0.75386	H -3.75413 -1.79517 1.97383
	H 1.88451 2.92416 -0.29795	H -5.13505 -1.52428 -0.08522
	H 0.95097 2.69995 -1.79181	H -4.11676 -0.52173 -2.12948
	H 0.60670 4.09259 -0.72729	H -1.75594 0.20712 -2.11994
	C -0.29138 2.69784 1.37022	H 4.77415 -1.70556 -0.24127
	H -1.06325 2.09913 1.85652	C 3.85295 -2.23598 0.00601
	H 0.63976 2.60408 1.93364	C 2.66932 -1.29689 -0.03162
	H -0.59750 3.75216 1.36120	H 3.69825 -3.06933 -0.68427
	H -0.97845 2.25266 -0.50090	H 3.94511 -2.65479 1.01407
	C -1.40361 -0.37850 -0.05852	O 1.48475 -1.79912 -0.04306
	C -1.97722 -0.94591 1.08976	O 2.83349 -0.03621 -0.03276
C -3.31909 -1.35566 1.07783		
TS5-3MM	O -1.14373 1.86404 -0.44551	C 1.74681 0.58787 0.10181
	C -1.28869 4.24106 -0.22804	C 2.41045 0.32228 1.32531
	H -1.55432 4.58909 0.77550	C 3.77452 0.02363 1.36386
	H -0.63844 4.99366 -0.68012	C 4.50837 -0.02947 0.17017
	H -2.19781 4.11598 -0.81627	C 3.88231 0.23692 -1.05656
	H 1.85132 0.38016 2.25840	C 2.52131 0.55123 -1.08547
	H 4.26753 -0.16434 2.31546	H 1.09831 1.72770 0.24247
	N 0.16324 -2.21474 -0.10197	H 5.57028 -0.26598 0.19661
	C 1.57748 -2.60249 0.14202	H 4.45861 0.21079 -1.97910
	H 2.22936 -2.13375 -0.59405	H 2.05272 0.79197 -2.03871
	H 1.88064 -2.28952 1.13979	H -5.31224 -0.74551 0.78010
	H 1.67517 -3.69408 0.06572	C -4.64693 -0.67836 -0.08292
	C -0.67541 -2.85151 0.95304	C -3.20966 -0.43817 0.37184
	H -0.40743 -2.44017 1.92807	H -4.72072 -1.58551 -0.68858
	H -1.72593 -2.65166 0.75615	H -4.96596 0.16183 -0.70960
	H -0.50349 -3.93691 0.95978	O -2.32123 -0.68612 -0.55260
	C -0.24083 -2.73492 -1.43957	O -2.95771 -0.04062 1.52130
	H -1.27726 -2.46362 -1.63796	Pd -0.34481 -0.06664 -0.16423
H 0.40414 -2.29948 -2.20623	O 0.64534 2.95684 0.35862	
H -0.13421 -3.82853 -1.46414	C -0.54524 2.92919 -0.10038	
INT5-4MM	O 1.49387 -1.90116 -0.01388	H -0.88580 3.65368 -1.21219
	O 2.87542 -0.16311 -0.01186	C -1.35450 -0.53312 -0.00113
	Pd 0.56504 0.04247 -0.00443	C -2.01061 -0.78816 1.21195
	H -1.50881 -0.61562 2.16263	C -3.32676 -1.27593 1.21176

	N	0.04165	2.16688	0.00504	C	-3.99268	-1.51334	0.00334
	C	1.35508	2.86722	0.00361	C	-3.33533	-1.26386	-1.20734
	H	1.92725	2.57899	0.88742	C	-2.01923	-0.77599	-1.21201
	H	1.92165	2.58586	-0.88600	H	-3.82675	-1.47076	2.15903
	H	1.20695	3.95630	0.00830	H	-5.01275	-1.89157	0.00506
	C	-0.71771	2.55627	1.22206	H	-3.84201	-1.44928	-2.15294
	H	-1.68324	2.04998	1.22860	H	-1.52416	-0.59387	-2.16442
	H	-0.15722	2.26363	2.11259	H	4.78254	-1.86865	-0.23774
	H	-0.87780	3.64393	1.24013	C	3.85308	-2.38201	0.01467
	C	-0.72544	2.56595	-1.20397	C	2.68782	-1.41941	-0.01133
	H	-0.17048	2.28070	-2.10034	H	3.67729	-3.20979	-0.67731
	H	-1.69091	2.05952	-1.20855	H	3.94436	-2.80631	1.02050
TS5-3NN	O	1.03167	2.98671	0.15562	C	1.82736	0.48356	0.08576
	C	-0.21404	3.08534	-0.11825	C	2.35082	0.10791	1.34824
	O	-0.97423	2.09325	-0.33145	C	3.61879	-0.46595	1.46572
	C	-0.80983	4.47548	-0.17329	C	4.39272	-0.68333	0.31635
	H	-0.85439	4.87684	0.84433	C	3.90428	-0.31457	-0.94538
	H	-0.16432	5.13252	-0.76112	C	2.63613	0.26072	-1.05629
	H	-1.81480	4.44965	-0.59461	H	1.34071	1.72804	0.11835
	H	1.76085	0.28683	2.24628	H	5.37952	-1.13350	0.40500
	H	4.00702	-0.74103	2.44423	H	4.51341	-0.47343	-1.83285
	C	-0.64186	-2.96566	1.19907	H	2.27053	0.55887	-2.03791
	H	-0.19913	-2.59479	2.12492	H	-5.19745	-0.68959	0.93096
	H	-1.68813	-2.66631	1.14547	C	-4.58973	-0.51690	0.04061
	H	-0.54140	-4.05327	1.15366	C	-3.12595	-0.32593	0.42632
	C	-0.61260	-2.93051	-1.60328	H	-4.70629	-1.34480	-0.66360
	H	-1.64054	-2.56572	-1.59305	H	-4.94604	0.39152	-0.45752
	H	-0.10329	-2.59694	-2.50956	O	-2.29668	-0.47157	-0.57180
H	-0.57504	-4.02142	-1.54469	O	-2.79794	-0.04964	1.59261	
S	0.30904	-2.24217	-0.18386	Pd	-0.30228	0.07826	-0.19891	
INT5-4NN	C	1.43623	3.18699	-0.13195	C	-1.39906	-0.51719	-0.08682
	H	2.04270	2.96667	-1.01203	C	-1.89475	-1.17284	1.04921
	H	1.21105	4.25602	-0.09984	C	-3.22311	-1.62374	1.07271
	H	1.97206	2.87942	0.76786	C	-4.05692	-1.42482	-0.03483
	Pd	0.54794	-0.02062	-0.10185	C	-3.55876	-0.77054	-1.16712
	O	2.82080	-0.20631	-0.05915	C	-2.23271	-0.30966	-1.19425
	C	2.67289	-1.46823	0.03244	H	-3.60113	-2.13312	1.95738
	O	1.49723	-1.98381	0.06592	H	-5.08592	-1.77731	-0.01489
	C	3.87399	-2.38395	0.07846	H	-4.19865	-0.61277	-2.03353
	H	4.01887	-2.83035	-0.91153	H	-1.86459	0.20190	-2.08129
	H	4.77390	-1.82740	0.34646	C	-0.95430	2.71312	1.26053
	H	3.70500	-3.19827	0.78747	H	-0.33032	2.45082	2.11685
	H	-1.25651	-1.34616	1.91380	H	-1.16098	3.78623	1.24990
	H	-1.89129	2.15653	1.30137	S	-0.12903	2.25765	-0.30796

TS5-300	O	1.68909	2.71249	0.48891	C	1.86879	0.12394	0.04715
	C	0.53635	3.17225	0.17025	C	2.38845	-0.51686	1.20095
	O	-0.44073	2.44567	-0.17799	C	3.50981	-1.34705	1.13231
	C	0.35551	4.67556	0.19674	C	4.14107	-1.56241	-0.10140
	H	0.78591	5.08683	1.11305	C	3.66108	-0.93231	-1.25914
	H	0.89980	5.10951	-0.64855	C	2.54265	-0.09987	-1.18176
	H	-0.69941	4.93959	0.11872	H	1.66663	1.41791	0.28294
	H	1.91693	-0.33883	2.16654	H	5.01212	-2.21217	-0.15880
	H	3.89530	-1.82242	2.03195	H	4.16266	-1.08896	-2.21190
	C	-0.45342	-2.86699	1.45397	H	2.18868	0.39827	-2.08307
	H	0.38046	-2.55828	2.08770	H	-4.84131	1.32652	0.03078
	H	-1.39365	-2.56685	1.91843	C	-4.69103	0.25340	-0.12710
	H	-0.42229	-3.95328	1.32302	C	-3.25107	-0.11098	0.22524
	C	-1.62019	-2.81915	-1.22801	H	-5.39011	-0.30284	0.49976
	H	-2.60299	-2.62612	-0.79624	H	-4.88958	0.04934	-1.18308
	H	-1.58315	-2.39776	-2.23528	O	-2.37416	0.37623	-0.60164
	H	-1.44911	-3.89898	-1.27926	O	-2.99120	-0.81409	1.21976
	P	-0.33336	-2.03663	-0.17863	Pd	-0.31484	0.28234	-0.17805
H	0.85389	-2.57896	-0.71434					
INT5-400	H	4.15567	-2.53861	1.22913	C	-1.39233	-0.51861	-0.07240
	O	1.63355	-1.99928	0.08635	C	-2.00596	-0.88237	1.13684
	O	2.82473	-0.12777	-0.01432	C	-3.30615	-1.40920	1.13773
	Pd	0.56937	-0.03237	-0.06401	C	-4.00613	-1.56616	-0.06480
	H	-1.47789	-0.76985	2.08216	C	-3.40038	-1.19199	-1.26985
	C	1.17901	3.34435	-0.52162	C	-2.10097	-0.66150	-1.27514
	H	1.90577	3.30130	0.29377	H	-3.76873	-1.69526	2.08077
	H	1.68964	3.08245	-1.45178	H	-5.01489	-1.97358	-0.06201
	H	0.78115	4.36079	-0.59977	H	-3.93653	-1.30795	-2.21017
	C	-1.08795	2.81550	1.24108	H	-1.64901	-0.37311	-2.22235
	H	-1.97885	2.21040	1.42255	H	4.90379	-1.62340	-0.09915
	H	-0.44966	2.77244	2.12768	C	4.03330	-2.21523	0.18956
	H	-1.38216	3.85339	1.05849	C	2.76403	-1.40088	0.07402
	P	-0.17294	2.13668	-0.20244	H	3.96364	-3.11369	-0.42910
	H	-1.06395	2.38652	-1.26804				
	TS5-3PP	C	-0.06340	3.22900	0.12241	H	1.26807	-3.91863
O		-0.82509	2.36011	-0.39773	C	1.79466	0.48256	0.10716
C		-0.48188	4.68397	0.08384	C	2.42706	-0.04883	1.25971
H		0.12915	5.20521	-0.66057	C	3.72764	-0.55678	1.21110
H		-1.53400	4.77719	-0.18655	C	4.43126	-0.55228	-0.00224
H		-0.29339	5.15222	1.05291	C	3.83691	-0.02808	-1.15925
H		1.90182	-0.02403	2.21342	C	2.53923	0.48551	-1.10067
H		4.19708	-0.94715	2.11173	H	1.30214	1.67149	0.40412
C		-0.09449	-2.67709	1.67770	H	5.44420	-0.94767	-0.04364
H		0.80843	-2.31556	2.17407	H	4.38931	-0.01459	-2.09650

	H	-0.97176	-2.29877	2.20748	H	2.09915	0.91614	-1.99879
	H	-0.09651	-3.77247	1.69191	H	-4.95289	0.92104	-0.37754
	C	-1.56744	-2.98399	-0.79021	C	-4.71110	-0.12956	-0.18512
	H	-2.47058	-2.79343	-0.20920	C	-3.24866	-0.23964	0.23814
	H	-1.73360	-2.65480	-1.81830	H	-5.36571	-0.50922	0.60137
	H	-1.35063	-4.05765	-0.78077	H	-4.88392	-0.67856	-1.11513
	P	-0.15528	-2.07026	-0.05399	O	-2.40838	0.00804	-0.72428
	C	1.29929	-2.83123	-0.87721	O	-2.93680	-0.54560	1.40402
	H	1.28009	-2.59864	-1.94529	Pd	-0.38101	0.24348	-0.22436
	H	2.22747	-2.44602	-0.45297	O	1.06120	2.95075	0.66736
INT5-4PP	Pd	0.61412	-0.12583	-0.00149	C	-1.95509	-1.03631	1.21192
	H	-1.47897	-0.80591	2.16342	C	-3.21455	-1.65495	1.21075
	C	1.21773	3.21817	0.01112	C	-3.84887	-1.96460	0.00174
	H	1.83159	3.05247	0.90032	C	-3.21637	-1.65378	-1.20791
	H	1.84244	3.05381	-0.87074	C	-1.95687	-1.03518	-1.21036
	H	0.85331	4.25110	0.00970	H	-3.69684	-1.89258	2.15742
	C	-1.20699	2.53900	1.44602	H	-4.82636	-2.44225	0.00224
	H	-2.12456	1.94711	1.47619	H	-3.70004	-1.89053	-2.15409
	H	-0.64816	2.36193	2.36914	H	-1.48205	-0.80411	-2.16235
	H	-1.46281	3.60191	1.37988	H	5.04093	-1.41561	-0.25412
	P	-0.19035	2.03291	0.00161	C	4.22233	-2.08693	0.01163
	C	-1.19141	2.54336	-1.45216	C	2.89673	-1.35779	-0.01000
	H	-0.62209	2.37038	-2.36963	H	4.19551	-2.94043	-0.67079
	H	-2.10791	1.95051	-1.49468	H	4.39875	-2.47621	1.02039
	H	-1.44940	3.60569	-1.38501	O	1.81088	-2.03306	-0.01018
	C	-1.31380	-0.73203	0.00045	O	2.86977	-0.08023	-0.00882

Table S4. Frequencies (cm^{-1}) of some stationary points, computed at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent.

Names	Frequencies													
CAT	34	35	54	76	121	174	200	236	278	368	383	471		
	539	601	606	683	699	952	954	1012	1013	1065	1065	1387	1389	
	1436	1438	1472	1473	1506	1509	1510	1515	3059	3059	3147	3147	3180	3180
HOAc	46	428	541	582	650	870	1008	1066	1212	1346	1421	1483	1487	
	1780	3065	3145	3194	3484									
TS-1	95i	15	23	33	39	48	55	60	69	78	115	131		
	152	236	290	292	341	411	414	488	509	606	610	613		
	614	685	695	698	707	859	878	937	943	986	990	1001		
	1011	1015	1016	1018	1048	1057	1065	1065	1166	1184	1186	1358	1367	1370
	1381	1417	1429	1477	1478	1487	1493	1497	1501	1555	1589	1623	1632	3058
	3058	3144	3145	3175	3176	3180	3188	3190	3202	3203	3211			
INT-1	25	33	41	43	53	62	66	93	106	111	128	171		
	202	213	274	315	335	418	421	487	520	606	607	611		

	611 683 690 695 716 859 902 929 948 983 988 991 1014 1014 1020 1021 1039 1056 1061 1065 1169 1183 1187 1317 1367 1375 1386 1397 1439 1475 1482 1488 1489 1490 1500 1524 1602 1631 1671 3057 3058 3142 3146 3174 3177 3188 3196 3198 3208 3210 3216
TS-2	1212i 9 22 30 54 54 83 97 112 121 154 193 207 231 242 290 321 336 400 468 482 556 606 614 624 662 679 689 706 771 853 938 948 954 993 1002 1012 1017 1017 1043 1052 1065 1067 1081 1171 1191 1195 1274 1346 1359 1384 1392 1448 1449 1458 1473 1485 1490 1492 1497 1528 1601 1614 1619 3058 3066 3144 3151 3175 3177 3178 3186 3191 3195 3203
INT-2	29 33 37 48 53 54 61 91 120 148 164 190 196 217 226 277 328 410 466 467 486 550 609 614 619 653 675 678 692 736 832 898 908 944 976 992 1003 1021 1031 1034 1065 1068 1078 1087 1169 1189 1234 1311 1340 1377 1379 1435 1442 1452 1475 1476 1484 1491 1492 1564 1605 1614 1709 3056 3067 3141 3148 3171 3174 3177 3191 3196 3201 3202 3392
1A	52 150 216 335 375 411 413 504 559 615 627 699 717 764 809 855 944 990 1007 1013 1045 1084 1110 1146 1174 1195 1333 1360 1380 1474 1522 1622 1629 1650 1704 3180 3187 3196 3205 3213 3519 3644
TS5-1A	104i 12 23 32 34 37 51 52 63 69 79 127 131 155 174 218 224 286 321 342 346 378 409 413 480 510 516 577 603 608 618 627 680 698 701 720 768 807 856 938 948 948 992 1009 1013 1014 1015 1046 1064 1065 1090 1113 1153 1175 1198 1335 1362 1367 1386 1397 1418 1437 1474 1475 1479 1488 1500 1524 1524 1596 1614 1628 1650 1674 3057 3058 3144 3146 3174 3177 3181 3187 3196 3206 3224 3513 3639
INT5-1A	9 25 31 35 42 58 66 71 83 102 123 143 158 181 199 212 253 270 336 341 385 397 411 414 492 520 541 606 606 611 626 643 683 689 701 726 776 804 853 927 946 951 989 1010 1013 1014 1022 1046 1059 1065 1102 1114 1163 1177 1198 1317 1335 1363 1387 1395 1439 1444 1473 1474 1483 1490 1506 1514 1525 1579 1627 1649 1653 1674 3056 3059 3141 3146 3172 3178 3184 3190 3198 3206 3211 3495 3623
TS5-2A	53i 26 30 35 37 39 61 62 69 77 118 126 145 181 190 212 218 247 282 312 388 393 416 428 497 512 542 602 609 613 624 653 669 696 711 727 776 799 861 924 933 943 990 1010 1017 1020 1022 1044 1057 1062 1097 1109 1163 1178 1194 1306 1331 1348 1366 1389 1406 1456 1470 1480 1482 1488 1491 1525 1575 1622 1638 1640 1656 1666 3057 3058 3139 3142 3145 3173 3174 3188 3197 3208 3217 3487 3613
INT5-2A	22 28 33 36 41 46 54 65 75 92 116 125 152 180 199 208 225 245 284 306 380 402 420 430 499 517 541 601 611 614 623 649 670 691 713 731

	771 794 858 924 929 934 990 1009 1020 1022 1022 1043 1058 1060 1094 1105 1159 1180 1194 1310 1328 1332 1370 1391 1397 1457 1468 1482 1482 1489 1491 1524 1579 1615 1634 1654 1658 1672 3057 3057 3142 3143 3159 3173 3173 3190 3199 3209 3219 3481 3606
TS5-3A	1379i 19 24 29 43 56 62 85 100 120 128 146 176 192 200 225 252 265 282 313 323 350 406 432 458 503 519 547 586 613 632 651 658 675 692 714 743 787 799 889 927 942 972 1009 1024 1027 1041 1059 1061 1068 1092 1124 1168 1184 1220 1273 1333 1336 1363 1390 1399 1443 1449 1464 1482 1482 1490 1490 1504 1562 1587 1607 1628 1651 1659 3055 3065 3138 3150 3170 3182 3188 3190 3199 3209 3496 3621
INT5-3A	27 30 41 43 56 72 83 89 102 122 130 151 182 196 212 220 246 258 292 305 313 407 437 479 486 492 518 570 602 608 644 656 670 681 697 734 786 798 876 927 931 960 1003 1026 1040 1044 1051 1060 1068 1087 1112 1138 1168 1181 1280 1294 1341 1375 1402 1428 1448 1457 1473 1483 1486 1494 1497 1547 1552 1608 1629 1652 1659 1697 2212 3051 3065 3130 3146 3169 3171 3181 3194 3203 3209 3506 3633
TS5-4A	66i 30 39 48 49 54 64 70 79 106 117 118 148 159 189 208 233 245 267 268 307 406 420 449 461 484 514 564 596 613 620 638 656 675 693 734 781 792 864 892 916 936 954 998 1023 1026 1045 1053 1067 1069 1085 1138 1164 1181 1277 1284 1340 1361 1387 1421 1440 1442 1456 1474 1480 1487 1489 1492 1556 1598 1608 1628 1653 1726 3055 3063 3135 3145 3169 3171 3176 3177 3190 3193 3206 3510 3636
INT5-4A	21 42 59 85 108 125 183 199 202 227 267 298 315 340 407 437 476 483 518 571 610 654 673 678 697 733 785 797 873 945 957 1001 1020 1044 1050 1065 1087 1137 1166 1181 1279 1341 1379 1446 1450 1456 1472 1490 1495 1551 1564 1609 1628 1656 3057 3141 3168 3175 3180 3193 3205 3506 3632
1B	49 151 160 219 365 409 428 465 591 601 626 696 742 771 856 946 963 995 1010 1013 1042 1044 1094 1106 1174 1194 1286 1336 1363 1399 1475 1483 1491 1520 1625 1645 1724 3048 3125 3171 3182 3191 3201 3212 3214
TS5-3B	1351i 20 29 30 41 56 69 84 100 119 124 135 161 178 194 202 221 250 261 277 314 320 410 423 456 504 512 539 611 613 631 641 651 675 694 737 765 773 890 928 943 977 990 1013 1023 1026 1041 1044 1053 1061 1068 1104 1137 1184 1224 1268 1327 1335 1338 1359 1390 1399 1405 1441 1464 1472 1479 1482 1483 1489 1491 1492 1582 1593 1619 1623 1653 3053 3056 3065 3134 3139 3151 3171 3180 3187 3190 3197 3203 3212
INT5-4B	19 41 57 88 99 112 127 196 197 199 221 250 308 340 414 422 466 484 505 609 612 634 669 680 722 762 767 878 945 966 984 1006 1019 1041 1045 1047 1066

	1104 1147 1177 1276 1341 1354 1379 1409 1449 1456 1470 1472 1478 1483 1489 1563 1578 1611 1623 3051 3058 3128 3142 3176 3178 3179 3187 3194 3207
1C	39 78 99 111 187 265 267 327 388 412 451 496 626 683 696 717 809 821 858 860 887 956 996 1010 1014 1035 1046 1098 1130 1146 1174 1176 1188 1292 1303 1337 1362 1401 1435 1477 1499 1505 1519 1524 1628 1649 1734 3051 3080 3130 3139 3151 3183 3193 3203 3214 3222
TS5-3C	1358i 8 24 27 31 45 57 64 79 92 102 105 124 145 164 180 192 195 226 233 263 275 289 308 336 356 426 457 465 504 522 551 613 631 651 673 688 709 714 746 804 817 869 880 897 927 943 981 1013 1020 1024 1026 1041 1060 1061 1068 1116 1133 1174 1178 1181 1222 1266 1306 1332 1335 1360 1364 1390 1398 1418 1440 1444 1466 1481 1482 1489 1490 1494 1498 1503 1519 1583 1595 1613 1629 1654 3056 3056 3066 3094 3139 3143 3145 3151 3167 3171 3187 3190 3197 3205 3214
INT5-4C	21 35 52 55 86 97 103 117 151 189 193 208 215 268 278 310 325 372 424 449 482 487 530 610 667 679 696 701 742 802 816 867 880 882 946 970 1005 1020 1023 1039 1052 1066 1126 1134 1171 1174 1181 1273 1305 1345 1365 1380 1418 1442 1448 1461 1472 1484 1489 1498 1504 1520 1563 1579 1614 1628 3055 3058 3092 3141 3142 3144 3164 3176 3179 3192 3197 3208
II	37 58 71 129 186 246 281 338 413 418 460 517 537 548 625 628 661 699 702 760 778 832 839 854 884 918 936 976 991 992 999 1007 1011 1011 1043 1043 1098 1098 1169 1173 1184 1186 1212 1266 1317 1335 1355 1361 1408 1476 1478 1512 1525 1619 1622 1636 1650 1686 3037 3173 3176 3182 3182 3191 3192 3197 3203 3205 3210
TS5-II	107i 12 18 27 32 37 40 49 51 59 66 71 81 112 128 149 159 177 226 262 286 289 322 350 373 414 418 450 479 510 527 534 553 604 610 626 628 662 682 697 701 702 763 771 829 837 857 888 921 942 943 947 975 993 994 996 1009 1010 1014 1014 1016 1045 1046 1064 1065 1102 1105 1171 1175 1190 1195 1208 1264 1321 1341 1356 1365 1376 1386 1413 1425 1436 1476 1476 1478 1478 1489 1500 1513 1526 1528 1574 1620 1621 1635 1650 1672 3054 3058 3058 3145 3145 3174 3175 3177 3178 3183 3184 3192 3194 3198 3204 3206 3231
INT5-II	16 24 32 36 39 43 50 52 60 70 86 94 116 144 163 175 179 202 208 264 269 318 333 354 409 414 421 483 496 516 530 552 575 606 612 626 630 667 683 686 698 701 766 770 833 840 856 909 929 934 949 950 980 987 995 1000 1009 1012 1015 1017 1025 1046 1048 1059 1065 1104 1113 1173 1178 1191 1203 1209 1262 1327 1328 1349 1357 1370 1386 1397 1418 1448 1473 1477 1480 1483 1491 1503 1513

	1519 1526 1616 1627 1632 1647 1656 1663 3056 3058 3113 3142 3145 3173 3178 3179 3183 3184 3189 3190 3195 3200 3202 3208 3209
TS5-2I	57i 9 31 32 34 36 43 49 58 69 73 77 93 126 150 168 184 190 212 216 273 289 304 330 405 414 417 493 497 507 520 553 574 611 613 624 629 666 671 691 698 713 756 776 834 841 859 910 924 931 935 939 980 982 990 1001 1009 1013 1014 1021 1022 1043 1045 1058 1063 1103 1110 1173 1176 1189 1191 1215 1265 1309 1321 1334 1357 1358 1362 1390 1392 1411 1471 1480 1481 1482 1489 1491 1512 1521 1614 1624 1628 1633 1642 1659 1664 3056 3058 3074 3127 3142 3145 3172 3174 3184 3186 3190 3194 3196 3203 3206 3210 3213
INT5-2I	23 31 34 36 39 42 47 52 63 70 79 89 106 126 155 173 187 194 216 226 279 292 298 328 398 414 422 495 500 513 520 554 571 612 614 625 629 665 672 687 697 723 757 777 834 841 866 909 926 930 931 937 979 981 991 1002 1010 1013 1018 1022 1024 1043 1045 1059 1061 1104 1110 1174 1176 1186 1190 1217 1263 1313 1316 1333 1340 1359 1362 1390 1392 1400 1468 1481 1481 1482 1489 1490 1510 1519 1609 1626 1630 1637 1647 1658 1663 2977 3056 3058 3133 3141 3143 3172 3174 3185 3188 3191 3197 3199 3207 3208 3213 3218
TS5-3I	1384i 20 24 26 38 45 50 63 70 72 89 107 119 155 166 181 194 205 223 255 271 285 303 328 341 405 416 442 502 506 519 533 563 581 613 627 632 651 668 674 691 699 739 762 777 836 847 886 913 928 934 940 969 979 989 1000 1008 1012 1022 1025 1040 1045 1061 1061 1069 1103 1124 1173 1180 1190 1209 1220 1260 1270 1326 1337 1340 1358 1364 1389 1390 1400 1448 1468 1479 1482 1483 1489 1490 1492 1515 1587 1595 1623 1625 1633 1649 1655 3055 3064 3135 3138 3148 3169 3182 3184 3187 3188 3190 3198 3198 3207 3208 3220
INT5-3I	24 33 37 47 48 57 58 69 78 88 90 111 135 158 170 182 194 216 229 247 267 306 331 350 391 419 433 483 486 509 536 554 577 605 611 628 644 662 665 672 699 724 760 774 835 845 881 910 919 924 932 959 977 991 996 1000 1012 1026 1034 1038 1046 1055 1056 1068 1088 1102 1133 1172 1173 1190 1219 1263 1274 1303 1325 1344 1358 1360 1385 1403 1413 1465 1472 1475 1481 1483 1486 1492 1506 1517 1591 1622 1624 1632 1652 1665 1687 2532 3052 3065 3131 3134 3147 3169 3176 3181 3181 3188 3195 3197 3201 3205 3206 3217
TS5-4I	56i 31 33 43 46 49 53 59 70 72 84 92 115 133 152 160 178 189 212 230 256 286 327 346 380 416 434 449 461 505 536 551 568 596 614 620 628 656 664 675 698 722 754 772 835 843 868 892 908 924 928 940 953 978 982 996 998 1011 1023 1027 1037 1045 1058 1067 1069 1104 1133 1172 1173 1190 1220 1259 1270 1285 1324

	1343 1358 1360 1384 1388 1421 1440 1463 1474 1475 1481 1482 1487 1490 1516 1590 1601 1621 1622 1630 1650 1728 3054 3063 3133 3135 3144 3159 3172 3175 3180 3182 3189 3190 3192 3197 3205 3205 3212
INT5-4I	21 31 43 50 54 80 97 122 169 181 188 211 245 268 323 334 358 387 415 431 480 512 536 554 575 609 628 665 672 679 698 721 759 773 835 845 877 911 931 945 956 979 987 999 999 1011 1021 1036 1046 1055 1065 1105 1132 1172 1173 1193 1220 1262 1274 1325 1344 1360 1381 1386 1446 1464 1474 1477 1484 1495 1517 1556 1590 1621 1623 1630 1651 3056 3137 3142 3174 3175 3180 3183 3190 3191 3197 3204 3204 3210
1D	62 158 218 382 411 433 497 577 626 634 697 720 777 818 858 957 996 1011 1014 1043 1095 1120 1175 1182 1207 1336 1363 1376 1477 1521 1629 1650 1748 3184 3194 3203 3214 3221 3488
TS5-3D	1355i 18 27 30 39 52 63 83 100 121 135 152 174 193 197 220 248 264 277 312 324 409 431 460 505 522 554 585 612 631 651 668 680 692 717 746 802 809 898 927 942 982 1014 1023 1026 1041 1059 1061 1068 1114 1164 1182 1213 1224 1267 1332 1336 1361 1390 1398 1437 1441 1466 1480 1482 1489 1491 1501 1583 1599 1618 1638 1654 3056 3065 3139 3151 3171 3188 3191 3198 3205 3214 3407
INT5-4D	21 43 56 90 112 130 185 197 201 218 255 304 338 412 428 477 485 535 577 609 659 675 680 699 742 797 806 882 945 971 1006 1019 1038 1050 1066 1124 1161 1174 1215 1274 1349 1379 1438 1447 1462 1472 1489 1493 1562 1585 1618 1636 3058 3142 3176 3180 3192 3197 3209 3428
1E	21 72 74 133 170 238 390 418 449 505 626 679 700 719 829 830 862 951 995 1001 1012 1039 1083 1143 1167 1179 1318 1354 1390 1468 1511 1587 1637 1644 3171 3180 3194 3209 3211
TS5-3E	1402i 21 25 30 39 41 46 59 63 84 98 112 121 127 153 174 193 206 223 255 273 284 313 335 422 447 464 496 523 566 611 631 653 670 685 713 715 750 814 848 896 925 940 977 1006 1024 1025 1040 1054 1058 1068 1108 1157 1174 1201 1260 1328 1340 1353 1357 1389 1399 1450 1467 1482 1483 1485 1489 1492 1590 1602 1625 1642 1654 3052 3064 3136 3147 3165 3179 3187 3189 3198 3206
INT5-4E	16 20 43 46 67 91 112 120 132 188 195 205 229 270 317 338 423 444 477 485 551 611 669 675 696 707 743 814 845 881 943 965 995 1021 1036 1050 1065 1119 1157 1171 1256 1341 1344 1380 1455 1465 1472 1474 1491 1564 1607 1621 1639 3056 3139 3171 3173 3182 3188 3199
1F	10 89 106 226 294 332 341 411 504 615 630 706 760 844 852 921 971 983 996 1000 1014 1047 1105 1116 1172 1173 1192 1213 1238 1253 1352 1358 1415 1479 1481 1498 1513 1526 1527 1633 1655 2992 3000 3040 3062 3145 3171 3173 3183 3192 3202

TS5-3F	1345i 28 32 39 45 61 66 72 89 106 128 138 160 174 181 200 211 238 252 274 301 313 326 377 413 453 504 510 537 610 611 632 657 675 690 741 761 842 881 925 927 940 970 1006 1010 1022 1024 1042 1059 1060 1064 1068 1124 1174 1179 1189 1214 1224 1243 1279 1330 1336 1373 1391 1399 1406 1445 1469 1476 1482 1483 1489 1490 1492 1496 1503 1511 1590 1605 1631 1656 3034 3047 3054 3066 3112 3136 3137 3150 3169 3178 3182 3191 3193 3205 3209
INT5-4F	20 47 58 66 88 117 141 164 184 202 225 237 249 283 337 389 424 442 482 501 610 613 673 677 704 748 834 864 942 945 950 990 1020 1026 1042 1054 1065 1093 1135 1171 1176 1219 1226 1251 1281 1328 1380 1407 1450 1463 1472 1479 1484 1490 1497 1504 1515 1564 1603 1629 3025 3041 3057 3086 3129 3141 3166 3175 3178 3183 3191 3201
1G	48 148 282 308 388 411 484 600 629 706 754 819 852 921 974 982 999 1012 1029 1048 1102 1171 1191 1202 1228 1331 1357 1378 1417 1479 1512 1523 1632 1652 3033 3106 3169 3175 3184 3192 3202 3626
TS5-3G	1377i 26 26 40 55 63 67 89 105 126 159 172 184 195 215 238 256 293 304 321 378 415 459 501 506 538 610 613 631 654 665 677 693 743 759 833 882 929 940 961 964 979 1005 1019 1025 1042 1060 1061 1068 1117 1158 1179 1190 1222 1272 1316 1336 1349 1373 1389 1392 1403 1446 1472 1481 1483 1489 1490 1491 1495 1588 1604 1629 1635 3055 3066 3082 3139 3149 3150 3170 3176 3181 3191 3193 3205 3504
INT5-4G	21 49 58 86 104 149 162 202 221 238 281 328 358 410 430 476 483 498 610 624 671 677 704 748 816 863 945 947 987 989 1020 1021 1042 1056 1065 1134 1171 1212 1243 1248 1289 1332 1379 1426 1450 1466 1472 1485 1490 1509 1565 1603 1629 3050 3057 3109 3141 3166 3175 3177 3190 3201 3558
1H	43 168 254 398 412 442 521 620 681 690 715 810 846 855 958 996 1014 1014 1039 1101 1124 1176 1189 1332 1370 1373 1483 1504 1566 1634 1652 3191 3202 3210 3234 3234
TS5-3H	1257i 26 28 30 42 59 68 83 98 123 136 151 175 190 197 227 247 276 289 313 346 416 434 462 508 529 574 611 631 649 677 689 704 721 729 797 865 891 928 944 984 1016 1022 1030 1041 1058 1061 1067 1111 1150 1180 1243 1253 1282 1325 1341 1372 1390 1397 1429 1459 1479 1482 1482 1488 1491 1564 1587 1603 1631 1660 3058 3066 3142 3152 3174 3192 3195 3206 3212 3222
INT5-4H	19 43 59 89 113 135 188 206 208 222 284 334 344 416 439 479 489 569 609 665 682 684 713 729 795 859 877 947 975 1010 1018 1037 1054 1066 1119 1156 1178

	1253 1283 1366 1380 1446 1451 1471 1477 1488 1556 1558 1609 1622 3059 3143 3178 3186 3199 3207 3218
1J	42 94 147 243 323 394 412 414 476 558 620 631 646 702 752 754 766 812 851 898 935 977 986 1001 1002 1006 1011 1034 1059 1082 1101 1115 1170 1174 1198 1290 1302 1320 1342 1360 1450 1478 1501 1529 1609 1629 1636 1650 3163 3177 3184 3188 3195 3203 3207 3213 3215
TS5-3J	1372i 23 26 34 42 57 65 81 84 106 120 126 163 177 188 204 225 244 258 288 309 324 360 419 439 453 498 503 533 564 612 632 637 656 672 673 691 739 747 764 774 802 885 901 927 939 972 994 1005 1015 1022 1025 1028 1040 1048 1060 1068 1073 1086 1121 1135 1176 1184 1193 1258 1300 1312 1329 1332 1342 1369 1389 1400 1446 1455 1473 1482 1482 1489 1490 1491 1521 1589 1600 1614 1627 1648 1656 3054 3064 3137 3148 3169 3183 3188 3190 3198 3199 3207 3214 3218 3226
INT5-4J	21 44 51 82 84 116 139 168 197 203 235 259 301 338 370 420 433 472 474 488 566 611 635 660 677 682 718 745 759 773 800 873 893 945 957 976 994 1011 1021 1023 1036 1047 1065 1071 1085 1125 1139 1172 1179 1258 1304 1313 1337 1345 1380 1451 1457 1468 1470 1486 1491 1517 1559 1602 1612 1625 1650 3057 3140 3174 3175 3181 3191 3196 3202 3203 3215 3222
1K	18 63 83 92 221 249 304 306 415 417 484 525 543 555 621 626 679 693 697 772 793 834 849 850 932 941 945 990 990 1004 1004 1010 1010 1037 1037 1093 1096 1160 1168 1172 1172 1204 1256 1326 1334 1362 1365 1474 1479 1498 1513 1545 1625 1631 1643 1646 3181 3181 3190 3190 3198 3198 3207 3207 3219 3219
TS5-3K	1331i 14 24 25 27 44 51 67 70 83 89 112 120 155 172 182 196 207 232 258 275 291 304 329 352 413 425 447 501 519 532 542 568 595 613 627 632 650 672 681 689 694 733 769 783 833 849 888 928 931 939 963 978 982 1004 1008 1012 1023 1024 1040 1044 1059 1061 1068 1107 1121 1175 1176 1186 1210 1219 1255 1282 1333 1338 1344 1364 1365 1389 1400 1442 1463 1472 1477 1480 1482 1489 1491 1498 1516 1585 1595 1622 1628 1640 1650 3056 3064 3138 3149 3171 3188 3189 3189 3198 3198 3205 3208 3214 3223 3243
INT5-4K	21 22 47 52 59 96 97 119 164 187 188 217 261 286 313 333 375 404 417 436 480 536 553 557 595 609 627 667 679 686 692 715 768 782 846 847 876 946 946 963 964 993 998 1007 1009 1021 1035 1044 1057 1066 1108 1128 1170 1174 1188 1223 1268 1297 1344 1355 1367 1381 1448 1454 1464 1471 1472 1492 1496 1517 1555 1596 1619 1629 1641 3057 3142 3176 3180 3187 3191 3197 3197 3207 3210 3222 3230

1L	33 97 114 249 273 322 359 412 495 609 629 707 750 813 837 852 921 967 981 990 997 1013 1046 1098 1124 1151 1170 1181 1191 1228 1272 1344 1356 1393 1462 1479 1494 1503 1519 1524 1528 1631 1652 2959 2965 3046 3074 3125 3168 3175 3184 3192 3201 3466
TS5-3L	1368i 26 33 38 49 63 67 72 91 106 124 159 175 182 199 207 224 239 255 296 300 328 363 418 440 453 499 513 536 609 613 631 655 672 688 745 759 840 882 926 937 939 961 974 1004 1022 1025 1040 1045 1060 1060 1068 1078 1119 1158 1177 1183 1201 1221 1270 1300 1330 1344 1373 1387 1392 1401 1453 1456 1471 1474 1481 1482 1489 1491 1493 1498 1506 1510 1594 1605 1632 1647 3047 3050 3053 3064 3108 3136 3148 3149 3168 3175 3179 3188 3191 3197 3203 3409
INT5-4L	18 47 54 74 93 134 161 180 200 225 231 253 295 327 366 420 427 447 477 507 611 612 672 674 713 748 833 867 935 943 948 978 989 1021 1040 1046 1054 1065 1090 1132 1165 1171 1187 1225 1269 1311 1327 1380 1386 1455 1458 1468 1470 1476 1483 1491 1504 1507 1515 1562 1607 1626 3038 3040 3056 3095 3136 3139 3166 3172 3174 3174 3187 3198 3417
1M	34 77 109 238 256 260 335 346 380 413 445 497 617 629 707 746 833 854 860 922 983 991 998 1013 1041 1050 1061 1098 1121 1169 1174 1190 1204 1224 1291 1299 1351 1356 1404 1449 1474 1483 1497 1501 1513 1513 1522 1524 1631 1652 2933 2937 2946 3056 3075 3084 3125 3136 3167 3175 3184 3193 3200
TS5-3M	1370i 26 34 40 46 60 68 72 88 105 122 151 169 179 190 214 227 237 245 254 280 295 303 314 361 405 440 459 494 499 522 536 612 617 630 655 672 689 741 759 841 852 889 926 939 967 975 994 1005 1023 1025 1037 1040 1060 1060 1068 1120 1123 1165 1177 1197 1208 1223 1269 1273 1302 1338 1343 1374 1390 1395 1400 1446 1453 1470 1476 1481 1482 1489 1489 1491 1494 1499 1504 1512 1522 1594 1606 1631 1650 3032 3035 3042 3053 3064 3106 3136 3144 3145 3148 3167 3175 3179 3187 3188 3191 3194 3203
INT5-4M	15 46 56 70 96 131 147 178 201 215 226 250 258 285 297 326 364 399 429 477 478 492 513 611 619 672 675 712 747 836 852 873 944 946 985 989 1001 1021 1037 1040 1055 1065 1123 1131 1167 1171 1205 1225 1267 1274 1312 1332 1380 1392 1446 1457 1463 1470 1475 1483 1491 1495 1499 1511 1515 1520 1561 1608 1626 3024 3026 3033 3056 3094 3130 3134 3139 3165 3171 3173 3174 3180 3186 3198
1N	42 53 90 172 211 257 341 412 484 571 630 690 706 713 785 819 850 904 926 979 982 993 998 1013 1047 1093 1155 1172 1194 1225 1284 1349 1358 1370 1479 1482 1494 1498 1524 1631 1651 3044 3056 3119 3141 3155 3172 3174 3184 3192 3202

TS5-3N	1290i 23 30 43 49 64 77 84 93 104 125 144 161 170 176 185 204 215 230 258 275 296 303 319 392 449 497 507 531 574 616 629 652 667 679 690 705 758 769 826 882 919 931 937 973 992 1004 1007 1020 1028 1040 1060 1061 1068 1110 1144 1178 1179 1211 1258 1285 1340 1342 1360 1382 1393 1398 1449 1470 1473 1478 1481 1482 1489 1490 1490 1491 1593 1602 1627 1646 3055 3064 3064 3066 3138 3143 3148 3170 3173 3178 3182 3188 3193 3205 3205
INT5-4N	19 43 55 58 92 118 142 157 178 194 214 232 250 266 301 325 384 433 473 498 579 611 664 673 692 705 732 751 822 864 913 944 956 987 991 1004 1020 1039 1057 1065 1130 1165 1173 1217 1254 1308 1332 1370 1381 1457 1463 1467 1474 1481 1482 1484 1491 1552 1602 1622 3057 3060 3062 3132 3140 3169 3172 3174 3177 3184 3191 3200
1O	44 58 88 175 212 249 342 412 482 566 629 656 687 706 722 740 779 814 850 901 928 961 980 995 1012 1024 1047 1092 1158 1171 1194 1217 1250 1340 1348 1357 1478 1485 1485 1487 1522 1629 1650 2371 3039 3049 3111 3135 3136 3168 3170 3182 3190 3201
TS5-3O	1292i 30 35 42 49 61 72 88 92 103 125 143 154 168 173 178 210 214 223 256 270 293 306 342 388 447 495 506 525 573 617 625 650 670 679 694 732 751 758 763 767 824 881 925 934 934 946 972 1005 1016 1019 1031 1039 1059 1061 1067 1108 1145 1172 1178 1201 1239 1277 1334 1336 1349 1382 1392 1400 1450 1459 1467 1472 1475 1481 1487 1488 1491 1493 1596 1601 1626 1634 2488 3041 3056 3057 3062 3120 3139 3146 3153 3172 3176 3181 3184 3192 3192 3203
INT5-4O	14 44 55 58 93 117 146 158 178 194 211 222 248 270 297 349 387 435 467 498 578 611 660 671 694 720 738 757 763 764 817 867 920 940 943 961 991 1022 1028 1037 1057 1065 1126 1157 1173 1203 1238 1299 1325 1345 1381 1453 1462 1467 1472 1473 1477 1481 1492 1550 1601 1620 2449 3041 3052 3056 3111 3139 3153 3163 3167 3172 3175 3188 3198
1P	37 58 86 180 197 202 217 274 277 354 413 480 571 630 647 683 701 708 773 807 816 842 851 895 928 941 969 981 995 1012 1048 1090 1155 1171 1194 1216 1248 1331 1347 1349 1357 1474 1477 1479 1484 1486 1493 1522 1628 1650 3028 3029 3035 3096 3120 3121 3132 3138 3169 3171 3182 3189 3201
TS5-3P	1267i 28 34 44 47 58 73 78 94 100 121 142 148 158 169 174 184 195 201 214 225 240 258 282 293 316 352 388 446 497 507 524 575 616 624 651 666 672 681 725 746 758 767 810 834 874 885 921 933 934 953 973 984 1005 1019 1031 1038 1059 1060 1067 1105 1141 1175 1177 1199 1237 1275 1329 1336 1340 1350 1381 1391 1401 1450

	1458 1462 1472 1472 1475 1482 1483 1488 1491 1493 1494 1598 1602 1627 1643 3038 3049 3052 3055 3061 3113 3138 3146 3148 3151 3170 3175 3180 3182 3184 3189 3191 3203
INT5-4P	9 33 44 49 83 107 130 151 178 183 186 199 211 219 231 265 285 304 363 388 435 464 498 580 611 660 669 679 711 734 745 757 809 827 865 871 916 941 945 957 980 990 1021 1037 1057 1065 1125 1154 1173 1202 1237 1298 1325 1338 1352 1380 1453 1462 1465 1469 1473 1473 1477 1482 1486 1492 1552 1602 1620 3036 3044 3046 3056 3099 3138 3143 3146 3159 3162 3167 3172 3174 3187 3197

Table S5. The electron energies (E in hartree), solution entropies (S in cal/mol·K), solution Gibbs free-energies (G in hartree) for some stationary points of the 16 studied C–H activation reactions, calculated at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent at a temperature of 373K, and the electron energies (E_{LBS} in hartree) calculated at the B3LYP-IDSCRF/LBS level of theory in DCE solvent.

Species	E	S	G	E_{LBS}
CAT	-5396.77710	87.557	-5396.70993	-5396.86134
1A	-401.00798	66.072	-400.90779	-401.09462
TS5-1A	-5797.77831	136.890	-5797.59983	-5797.94758
INT5-1A	-5797.79265	138.019	-5797.61342	-5797.96218
TS5-2A	-5797.77729	134.269	-5797.59730	-5797.94736
INT5-2A	-5797.77780	138.185	-5797.59897	-5797.94834
TS5-3A	-5797.75297	133.571	-5797.57719	-5797.92690
INT5-3A	-5797.80276	135.131	-5797.62309	-5797.97570
TS5-4A	-5797.78783	134.030	-5797.60788	-5797.96099
INT5-4A	-5568.66054	104.847	-5568.53305	-5568.78761
HOAc	-229.13420	51.914	-229.09630	-229.18122
1B	-384.94014	70.162	-384.83119	-385.02118
TS5-3B	-5781.68103	135.812	-5781.49537	-5781.84981
INT5-4B	-5552.59007	107.833	-5552.45313	-5552.71185
1C	-499.51018	83.042	-499.37170	-499.61003
TS5-3C	-5896.24777	149.550	-5896.03309	-5896.43558
INT5-4C	-5667.15606	119.668	-5666.98895	-5667.29691
1D	-420.88563	63.810	-420.79700	-420.97178
TS5-3D	-5817.62203	131.929	-5817.45838	-5817.79597
INT5-4D	-5588.53063	102.076	-5588.41453	-5588.65773
1E	-1020.24953	74.246	-1020.17624	-1020.40735
TS5-3E	-6417.01205	143.054	-6416.86388	-6417.25558
INT5-4E	-6187.91506	113.289	-6187.81446	-6188.11211
1F	-386.12269	74.933	-385.99220	-386.20453
TS5-3F	-5782.86658	137.756	-5782.65736	-5783.03491

INT5-4F	-5553.76725	110.808	-5553.60743	-5553.88902
1G	-346.81836	63.718	-346.71164	-346.89575
TS5-3G	-5743.56468	128.315	-5743.38057	-5743.72852
INT5-4G	-5514.46305	101.248	-5514.32836	-5514.58050
1H	-436.81265	62.467	-436.73562	-436.89626
TS5-3H	-5833.54343	130.116	-5833.39116	-5833.71509
INT5-4H	-5604.45708	100.923	-5604.35274	-5604.58167
1I	-556.79837	88.093	-556.63039	-556.91881
TS5-1I	-5953.56836	155.622	-5953.31996	-5953.77192
INT5-1I	-5953.59511	155.789	-5953.34502	-5953.79902
TS5-2I	-5953.57726	153.307	-5953.32744	-5953.78196
INT5-2I	-5953.57867	155.226	-5953.32897	-5953.78359
TS5-3I	-5953.55628	151.773	-5953.30993	-5953.76362
INT5-3I	-5953.60334	152.166	-5953.35190	-5953.80980
TS5-4I	-5953.59013	150.833	-5953.33872	-5953.79668
INT5-4I	-5724.46265	123.736	-5724.26498	-5724.62324
1J	-479.38607	76.011	-479.24727	-479.48790
TS5-3J	-5876.15189	140.342	-5875.93513	-5876.34077
INT5-4J	-5647.05628	112.509	-5646.88834	-5647.19856
1K	-572.81176	88.053	-572.65625	-572.93213
TS5-3K	-5969.56890	151.576	-5969.33500	-5969.77587
INT5-4K	-5740.47891	122.542	-5740.29286	-5740.63908
1L	-366.25260	73.939	-366.10862	-366.33573
TS5-3L	-5763.02395	136.137	-5762.80006	-5763.19336
INT5-4L	-5533.92102	109.135	-5533.74653	-5534.04401
1M	-405.56254	80.672	-405.39285	-405.65241
TS5-3M	-5802.33068	142.609	-5802.08082	-5802.50734
INT5-4M	-5573.22737	115.759	-5573.02711	-5573.35778
1N	-709.06307	77.772	-708.93715	-709.19283
TS5-3N	-6105.82344	140.369	-6105.61885	-6106.04245
INT5-4N	-5876.72073	113.461	-5876.56554	-5876.89400
1O	-652.83066	78.386	-652.69641	-652.95688
TS5-3O	-6049.61050	140.853	-6049.39717	-6049.82581
INT5-4O	-5820.50560	115.014	-5820.34234	-5820.67563
1P	-692.15550	87.514	-691.99540	-692.29092
TS5-3P	-6088.94053	150.083	-6088.70132	-6089.16496
INT5-4P	-5859.83551	125.000	-5859.64691	-5860.01481
Benzene	-232.26848	48.383	-232.18914	-232.32245
TS-1	-5629.03417	120.573	-5628.87736	-5629.17147
INT-1	-5629.04539	121.241	-5628.88767	-5628.88767
TS-2	-5629.01709	120.071	-5628.86472	-5629.15712
INT-2	-5629.04480	121.996	-5628.88769	-5629.18553

Table S6. The electron energies (in kcal/mol) calculated at the B3LYP-IDSCRF level of theory using DGDZVP and LBS basis sets, respectively, in DCE solvent.

Species	E_{DZVP}	E_{LBS}	Species	E_{DZVP}	E_{LBS}
1AA	-169.93250	-169.97072	1II	-325.71554	-325.78691
INT5-4AA	-5569.84834	-5569.97945	INT5-4II	-5725.64087	-5725.80608
TS5-3AA	-5798.95745	-5799.13387	TS5-3II	-5954.75048	-5954.96060
1BB	-153.85984	-153.89229	1JJ	-248.31171	-248.36476
INT5-4BB	-5553.77062	-5553.89683	INT5-4JJ	-5648.24069	-5648.38760
TS5-3BB	-5782.87986	-5783.05130	TS5-3JJ	-5877.35053	-5877.54261
1CC	-268.42607	-268.47757	1KK	-341.73683	-341.81037
INT5-4CC	-5668.33573	-5668.48130	INT5-4KK	-5741.66210	-5741.82927
TS5-3CC	-5897.44544	-5897.63616	TS5-3KK	-5970.77183	-5970.98364
1DD	-189.80511	-189.84261	1LL	-135.18396	-135.21782
INT5-4DD	-5589.71388	-5589.84497	INT5-4LL	-5535.11739	-5535.24457
TS5-3DD	-5818.82332	-5818.99956	TS5-3LL	-5764.22862	-5764.40073
1EE	-789.17163	-789.28160	1MM	-174.49549	-174.53605
INT5-4EE	-6189.10028	-6189.30143	INT5-4MM	-5574.42289	-5574.55739
TS5-3EE	-6418.21292	-6418.45919	TS5-3MM	-5803.52777	-5803.70695
1FF	-155.05348	-155.08543	1NN	-477.99594	-478.07613
INT5-4FF	-5554.96324	-5555.08877	INT5-4NN	-5877.92044	-5878.09821
TS5-3FF	-5784.07103	-5784.24204	TS5-3NN	-6107.02913	-6107.25134
1GG	-115.74679	-115.77511	1OO	-421.76418	-421.84105
INT5-4GG	-5515.65980	-5515.78107	INT5-4OO	-5821.70922	-5821.88384
TS5-3GG	-5744.76759	-5744.93389	TS5-3OO	-6050.81836	-6051.03698
1HH	-205.74075	-205.77780	1PP	-461.08941	-461.17559
INT5-4HH	-5605.64596	-5605.77607	INT5-4PP	-5861.03815	-5861.22200
TS5-3HH	-5834.75315	5834.92847	TS5-3PP	-6090.14546	-6090.37345

Table S7. The free-energy (in kcal/mol) profiles for some selected C–H activation reactions directed by different functionalities, calculated at the B3LYP-IDSCRF/DGDZVP level of theory at 373K in DCE solvent.

1X	TS5-1X	INT5-1X	TS5-2X	INT5-2X	TS5-3X	INT5-3X	TS5-4X	INT5-4X
1A	11.2	2.6	12.7	11.7	25.4	-3.4	6.1	-7.4
1B	13.0	6.6	17.0	16.1	28.7	-1.5	7.8	-5.2
1C	14.0	8.1	19.2	18.1	30.5	2.0	10.5	-2.3
1D	12.6	6.7	18.8	18.0	30.5	1.1	9.9	-2.4
1E	8.5	-5.9	2.0	-2.7	14.0	-16.6	-1.8	-15.4
1F	13.0	6.7	17.6	14.5	28.1	3.2	10.9	-1.0
1I	12.7	-3.0	8.0	7.0	19.0	-7.3	0.9	-13.2
1L	8.6	-9.9	3.3	-2.9	11.6	-12.1	-1.7	-15.2
1N	9.6	-5.7	8.9	7.3	17.7	-7.3	2.1	-9.3

Table S8. Calculated thermodynamic parameters (ΔE , ΔS and ΔG ; difference between final palladacycle and starting materials), kinetic parameters (ΔE^\ddagger , ΔS^\ddagger and ΔG^\ddagger ; difference between proton-transfer transition state and starting materials), coordination parameters (ΔE_{coord} and ΔG_{coord} ; difference between encounter complex and starting materials) and predicted *Type A/B* for 16 directing group systems studied, determined at the B3LYP-IDSCRF/LBS level of theory in DCE. (Units: E and G in kcal·mol⁻¹; S in cal·mol⁻¹·K⁻¹)

Reactants	Coordination Parameters		Thermodynamic Parameters			Kinetic & Activation Parameters			D.G. Type
	ΔE_{Coord}	ΔG_{Coord}	ΔE	ΔS	ΔG	ΔE^\ddagger	ΔS^\ddagger	ΔG^\ddagger	A/B
Benzene	0.5	7.5	-1.0	-14.0	5.5	16.7	-15.8	20.4	Ref.
1A	-3.9	3.5	-8.1	3.2	-9.3	18.2	-20.1	23.5	A
1B	-0.5	7.2	-6.6	1.9	-7.4	20.5	-22.0	26.5	A
1C	0.4	8.6	-4.2	1.1	-4.7	22.5	-21.2	28.2	A
1D	0.1	7.4	-3.7	2.4	-4.7	23.3	-19.6	28.3	A
1E	-11.6	-4.2	-15.5	3.2	-16.6	8.2	-18.8	13.1	B
1F	-2.0	7.5	-2.7	0.3	-2.7	19.4	-24.7	26.7	A
1G	-2.9	5.2	-2.9	1.9	-3.7	17.9	-22.8	24.3	A
1H	6.5	12.9	-3.3	2.7	-4.5	26.7	-19.8	31.7	A
1I	-11.8	-2.5	-15.3	0.0	-15.0	10.4	-23.9	17.4	B
1J	-14.5	-5.4	-19.2	0.8	-19.2	5.3	-23.1	12.0	B
1K	-7.7	1.7	-16.8	-1.1	-16.0	11.0	-24.1	18.1	B
1L	-19.0	-8.9	-17.7	-0.5	-16.9	2.3	-25.5	10.3	B
1M	-16.7	-5.7	-15.8	-0.5	-15.0	4.0	-25.7	12.2	B
1N	-15.8	-7.0	-13.2	0.0	-13.2	7.4	-24.9	14.6	B
1O	-27.5	-18.8	-24.2	1.1	-24.4	-4.8	-25.2	2.8	B
1P	-31.4	-22.0	-27.5	1.9	-28.0	-8.0	-24.9	-0.5	B

From these data it can be observed that the B3LYP-IDSCRF/LBS results are very close to the B3LYP-IDSCRF/DGDZVP results reported in the article (see **Table 1**).

Table S9. Reaction free-energy (relative to initial materials, in kcal/mol) profiles for some selected model reactions, calculated with B3LYP, B3LYP+D3 and M06 density functional methods for comparison. It can be seen that both D3 and M06 predict 4~11 kcal/mol lower in relative free-energies in comparison to the B3LYP results for most stationary points.

1A+CAT	TS5-1A	INT5-1A	TS5-2A	INT5-2A	TS5-3A	INT5-3A
B3LYP	11.2	2.6	12.7	11.7	25.4	-3.4
B3LYP+D3	6	-3.4	5.6	3.3	18.3	-10.3
M06	7.1	-0.4	5.4	4.5	20.8	-7.4
1B+CAT	TS5-1B	INT5-1B	TS5-2B	INT5-2B	TS5-3B	INT5-3B
B3LYP	13.0	6.6	17.0	16.1	28.7	-1.5
B3LYP+D3	7.4	0.4	9.5	8.5	20.9	-8.5
M06	8.6	2.4	11.6	10.3	23.5	-4.8
1I+CAT	TS5-1I	INT5-1I	TS5-2I	INT5-2I	TS5-3I	INT5-3I

B3LYP	12.7	-3.0	8.0	7.0	19.0	-7.3
B3LYP+D3	not located	-12.8	-3.0	-4.7	7.8	-18.7
M06	5.2	-9.5	-0.3	-1.8	10.7	-14.3
1N+CAT	TS5-1N	INT5-1N	TS5-2N	INT5-2N	TS5-3N	INT5-3N
B3LYP	9.6	-5.7	8.9	7.3	17.7	-7.3
B3LYP+D3	2.7	-14.0	-2.6	-4.5	6.8	-17.1
M06	3.2	-12.1	-0.2	-2.6	8.6	-14.4

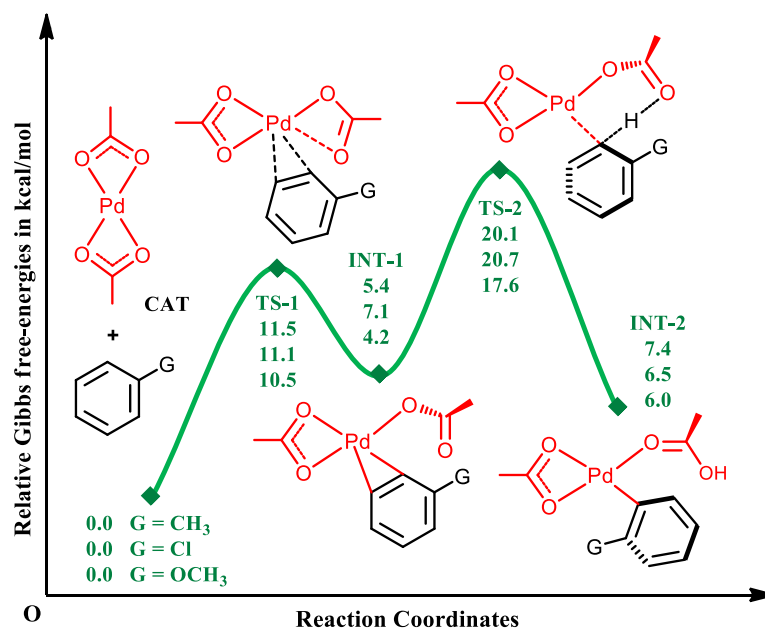


Figure S1. Free-energy profiles for the C-H activation reactions of some mono-substituted benzenes, calculated at the B3LYP-IDSCRF/DGDZVP level of theory in DCE solvent (373 K).

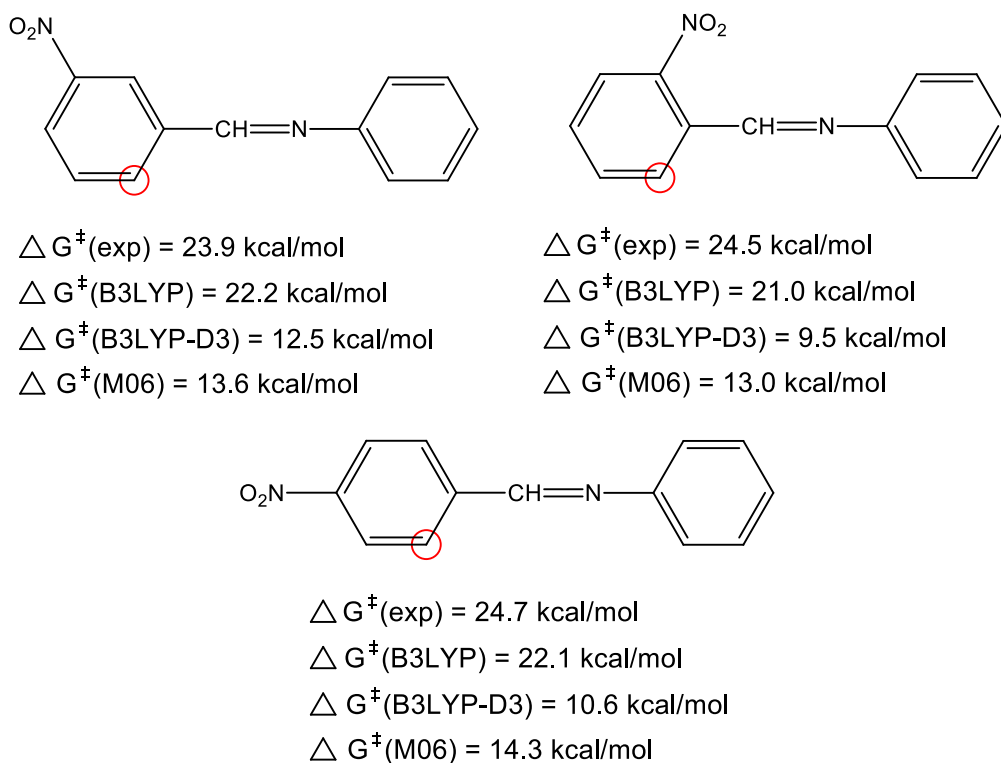
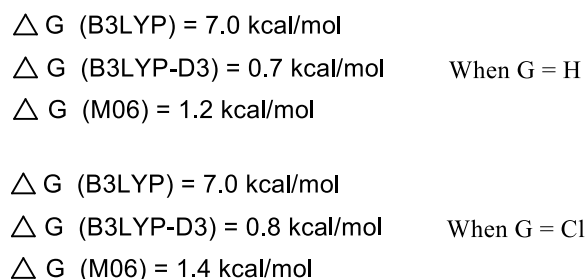
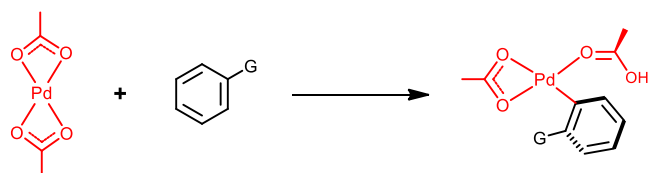


Figure S2. Cyclopalladation reactions of three substrates with $\text{Pd}(\text{OAc})_2$ under stoichiometric reaction conditions, along with experimentally determined free-energy barriers at 298.15 K in toluene. The B3LYP/DGDZVP results are closest to the experimental values, and substantial underestimation of free-energy barriers can be noticed for other two density functional methods. Experimental kinetic data are from Gómez, M.; Granell J.; Martínez, M. *Organometallics* **1997**, *16*, 2539-2546.

Besides, the B3LYP method predicts the instability of open palladation intermediate, being consistent with the fact that only cyclopalladation intermediates have been isolated so far under stoichiometric reaction conditions. But both B3LYP-D3 and M06 predict modest stability of open palladation intermediate (see below).



Estimation of Overall Kinetics Based on the Energetic Span Model

(Please see: S. Kozuch, S. Shaik, *J. Am. Chem. Soc.*, 2006, **128**, 3355; S. Kozuch, S. Shaik, *J. Phys. Chem. A*, 2008, **112**, 6032; S. Kozuch, S. E. Lee, S. Shaik, *Organometallics*, 2009, **28**, 1303.)

The turnover frequency (TOF) of a catalytic cycle can be computed from equation (1),

$$TOF = \frac{e^{-\Delta G} - 1}{\sum_{i,j=1}^N e^{T_i - I_j - \delta G'_{i,j}}} \quad (1)$$

in which $\delta G'_{i,j} = \Delta G$ if $i > j$ and $\delta G'_{i,j} = 0$ if $i \leq j$.

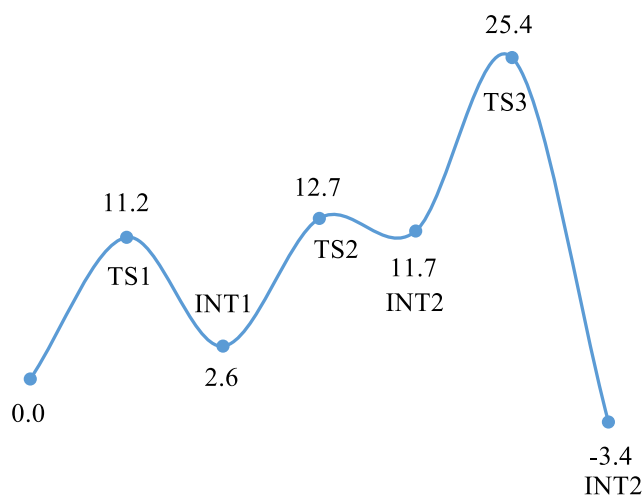
The free-energy terms in this equation should be in units of k_bT . If relative free-energies are measured in units of kcal/mol, equation (1) needs to be rewritten into (2),

$$TOF = \frac{e^{-\Delta G/aRT} - 1}{\sum_{i,j=1}^N e^{(T_i - I_j - \delta G'_{i,j})/aRT}} \quad (2)$$

in which $\delta G'_{i,j} = \Delta G$ if $i > j$ and $\delta G'_{i,j} = 0$ if $i \leq j$

$$a = \frac{1}{4.18 \times 1000}$$

Herein, we present a derivation of apparent rate-determining free-energy barrier based on the energetic span model, using the reaction of **1A** with Pd(OAc)₂ as an example. The studied free-energy profile is shown below, which involves three transition states and three intermeidates.



$$TOF = \frac{e^{3.4/aRT} - 1}{e^{8.6/aRT} + e^{-0.5/aRT} + e^{14.6/aRT} + e^{13.5/aRT} + e^{1.0/aRT} + e^{16.1/aRT} + e^{26.2/aRT} + e^{17.1/aRT} + e^{28.8/aRT}}$$

T1-I1
T1-I2
T1-I3
T2-I1
T2-I2
T2-I3
T3-I1
T3-I2
T3-I3

The largest term in the denominator is $e^{28.8/aRT}$ that comes from the T3-I3 pair. The second largest term in the denominator is $e^{26.2/aRT}$, being *ca.* 2/27 times of $e^{28.8/aRT}$. All the other 7 terms are completely negligible as compared to the magnitude of $e^{28.8/aRT}$.

And it is easily realized that the numerator is nearly equal to $e^{3.4/aRT}$. Therefore, the TOF can be roughly calculated by only considering the largest one term, as equation and result shown below, which means that the apparent rate-determining free-energy barrier is 25.4 kcal/mol.

$$TOF \approx \frac{e^{3.4/aRT}}{e^{28.8/aRT}} = e^{-25.4/aRT}$$

More accurately, the TOF should be calculated by considering the largest two terms in the denominator (see below). But the result is practically the same.

$$TOF \frac{e^{3.4/aRT}}{e^{28.8/aRT} + e^{26.2/aRT}} = e^{-25.5/aRT}$$