Supporting information for "DFT Calculations on Kinetic Data for Some Diels-Alder Reactions in Solution"

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Table s1 The optimized geometries(in Å) for 9 transition states with different methods and solvents

CAM-B3LYP+IDSCRF/6-31G(d)

Species	Cartesian coordinates			Species	Cartesian coordinates		
TSaa $CHCl_3$	C	-4.17673	-0.04271 -1.46194	**TSaa** THF	C	-4.17429	-0.05043 -1.46335
	C	-3.05048	0.19883 -0.65807		C	-3.04912	0.19518 -0.65924
	C	-1.84554	0.80258 -1.14839		C	-1.84430	0.79828 -1.15104
	C	-3.03178	-0.25744 0.67522		C	-3.03160	-0.25508 0.67631
	C	-1.81126	-0.07053 1.40388		C	-1.81307	-0.06249 1.40660
	C	-0.96116	1.02760 1.09190		C	-0.96238	1.03350 1.08951
	C	-0.98397	1.49134 -0.24616		C	-0.98402	1.49126 -0.25056
	C	-5.27247	-0.68570 -0.92827		C	-5.27034	-0.69165 -0.92774
	C	-4.14011	-0.94982 1.19045		C	-4.14032	-0.94535 1.19377
	H	-1.71099	-0.54394 2.37656		H	-1.71509	-0.52951 2.38278
	C	-0.03533	1.58197 2.00576		C	-0.03928	1.59371 2.00260
	C	-0.08922	2.50951 -0.64709		C	-0.09092	2.50950 -0.65477
	C	0.76695	3.06539 0.27097		C	0.76239	3.07147 0.26251
	C	0.79651	2.59658 1.60356		C	0.79092	2.60855 1.59723
	H	-0.00501	1.20678 3.02413		H	-0.01118	1.22425 3.02324
	H	-0.10223	2.85241 -1.67718		H	-0.10380	2.84882 -1.68613
	H	1.43434	3.86804 -0.02733		H	1.42797	3.87490 -0.03800
	H	1.48926	3.04163 2.31087		H	1.48086	3.05911 2.30391
	C	-5.25396	-1.14060 0.40204		C	-5.25317	-1.14036 0.40475
	H	-4.17817	0.29182 -2.49524		H	-4.17505	0.28010 -2.49803
	H	-1.77756	1.03529 -2.20735		H	-1.77642	1.02859 -2.21063
	H	-6.15387	-0.85200 -1.53981		H	-6.15124	-0.86078 -1.53934
	H	-4.11317	-1.31806 2.21188		H	-4.11470	-1.30801 2.21733
	H	-6.12132	-1.65400 0.80536		H	-6.12103	-1.65184 0.80959
	N	1.38681	-0.86470 -0.31557		N	1.38759	-0.86371 -0.31055
	C	0.58089	-0.59231 -1.41641		C	0.58324	-0.59546 -1.41264
	C	0.57616	-1.36787 0.69757		C	0.57730	-1.36836 0.70179
	N	-0.74314	-1.48466 0.15604		N	-0.74101	-1.48603 0.16054
	N	-0.74053	-1.03276 -1.08199		N	-0.73783	-1.03614 -1.07870
	O	0.91610	-0.13021 -2.47968		O	0.92035	-0.13730 -2.47745
	O	0.90950	-1.70341 1.80813		O	0.91225	-1.70507 1.81196
	C	2.79089	-0.64878 -0.22864		C	2.79226	-0.65057 -0.22495
	C	3.58797	-1.58663 0.42317		C	3.59147	-1.60366 0.40137
	C	3.35693	0.48677 -0.80172		C	3.35569	0.49766 -0.77444
	C	4.95862	-1.37746 0.50626		C	4.96266	-1.39701 0.48313
	C	4.73113	0.67659 -0.72346		C	4.73040	0.68527 -0.69850

	C 5.53508 -0.24981 -0.06853 H 3.13498 -2.46368 0.86871 H 2.72645 1.20688 -1.30666 H 5.57854 -2.10697 1.01837 H 5.17305 1.55962 -1.17497 H 6.60774 -0.09398 -0.00664		C 5.53670 -0.25644 -0.06847 H 3.13997 -2.49139 0.82743 H 2.72270 1.23024 -1.25837 H 5.58486 -2.13826 0.97534 H 5.17074 1.57848 -1.13124 H 6.60973 -0.10233 -0.00781
TSaa **1,4-dioxane**	C -4.18024 -0.02894 -1.45784 C -3.05201 0.20375 -0.65448 C -1.84476 0.80572 -1.14215 C -3.03214 -0.26277 0.67496 C -1.80883 -0.08585 1.40155 C -0.95896 1.01468 1.09854 C -0.98315 1.48912 -0.23573 C -5.27693 -0.67253 -0.92761 C -4.14167 -0.95597 1.18633 H -1.70490 -0.57026 2.36804 C -0.02754 1.55766 2.01379 C -0.08436 2.50618 -0.63060 C 0.77694 3.05061 0.28891 C 0.80784 2.57122 1.61768 H 0.00675 1.17147 3.02765 H -0.09616 2.85446 -1.65866 H 1.44848 3.85105 -0.00539 H 1.50609 3.00551 2.32596 C -5.25745 -1.13746 0.39902 H -4.18192 0.31173 -2.48894 H -1.77559 1.04382 -2.19948 H -6.15930 -0.83238 -1.53919 H -4.11344 -1.33352 2.20411 H -6.12506 -1.65208 0.79981 N 1.38495 -0.86467 -0.32863 C 0.57668 -0.57706 -1.42496 C 0.57347 -1.37446 0.68224 N -0.74757 -1.48524 0.13990 N -0.74604 -1.02109 -1.09244 O 0.90636 -0.09798 -2.48134 O 0.90431 -1.71691 1.79040 C 2.78789 -0.64408 -0.23782 C 3.57967 -1.54986 0.46450 C 3.36017 0.46424 -0.85709 C 4.94911 -1.33560 0.55081 C 4.73321 0.65836 -0.77344 C 5.53148 -0.23556 -0.06898 H 3.12303 -2.40372 0.94836	**TSaa** **$PhCH_3$**	C -4.18009 -0.02954 -1.45792 C -3.05192 0.20345 -0.65456 C -1.84470 0.80544 -1.14238 C -3.03217 -0.26257 0.67510 C -1.80908 -0.08514 1.40192 C -0.95894 1.01506 1.09833 C -0.98300 1.48900 -0.23611 C -5.27684 -0.67293 -0.92747 C -4.14173 -0.95557 1.18670 H -1.70551 -0.56886 2.36884 C -0.02764 1.55838 2.01351 C -0.08415 2.50588 -0.63132 C 0.77710 3.05065 0.28810 C 0.80781 2.57181 1.61708 H 0.00629 1.17279 3.02764 H -0.09601 2.85397 -1.65947 H 1.44859 3.85108 -0.00641 H 1.50587 3.00654 2.32532 C -5.25747 -1.13736 0.39934 H -4.18176 0.31089 -2.48912 H -1.77551 1.04331 -2.19982 H -6.15924 -0.83292 -1.53901 H -4.11362 -1.33259 2.20470 H -6.12517 -1.65175 0.80029 N 1.38490 -0.86467 -0.32859 C 0.57662 -0.57774 -1.42505 C 0.57357 -1.37445 0.68235 N -0.74738 -1.48553 0.14029 N -0.74590 -1.02164 -1.09221 O 0.90651 -0.09992 -2.48205 O 0.90480 -1.71710 1.79041 C 2.78787 -0.64406 -0.23783 C 3.57980 -1.55113 0.46266 C 3.35994 0.46558 -0.85495 C 4.94927 -1.33701 0.54912 C 4.73300 0.65964 -0.77115 C 5.53145 -0.23570 -0.06866 H 3.12335 -2.40615 0.94473

	H 2.73560 1.15728 -1.40454		H 2.73523 1.16000 -1.40052
	H 5.56361 -2.04036 1.10236		H 5.56391 -2.04286 1.09913
	H 5.17888 1.51949 -1.26185		H 5.17849 1.52191 -1.25773
	H 6.60335 -0.07638 -0.00402		H 6.60333 -0.07657 -0.00353
TSaa $ClCH_2CH_2Cl$	C -4.17519 -0.04981 -1.46275	**TSab** $CHCl_3$	C -4.19817 -0.04753 -1.42797
	C -3.04963 0.19603 -0.65910		C -3.06703 0.19968 -0.63355
	C -1.84617 0.80080 -1.15149		C -1.85629 0.78547 -1.13807
	C -3.03119 -0.25443 0.67635		C -3.04001 -0.24586 0.70599
	C -1.81195 -0.06213 1.40567		C -1.81212 -0.05483 1.42089
	C -0.96154 1.03432 1.08830		C -0.97359 1.06291 1.10027
	C -0.98401 1.49216 -0.25176		C -0.99968 1.50805 -0.23942
	C -5.27068 -0.69167 -0.92659		C -5.29031 -0.68554 -0.87801
	C -4.13938 -0.94497 1.19448		C -4.14396 -0.93539 1.23534
	H -1.71355 -0.52914 2.38185		H -1.73253 -0.48120 2.41934
	C -0.03864 1.59501 2.00113		C -0.07524 1.64280 2.01183
	C -0.09147 2.51067 -0.65654		C -0.12809 2.52867 -0.65220
	C 0.76200 3.07301 0.26051		C 0.71504 3.11727 0.26702
	C 0.79099 2.61032 1.59528		C 0.74180 2.67400 1.59951
	H -0.01061 1.22621 3.02206		H -0.04377 1.28412 3.03598
	H -0.10536 2.85046 -1.68778		H -0.13586 2.85542 -1.68741
	H 1.42702 3.87688 -0.04020		H 1.37256 3.92327 -0.04285
	H 1.48054 3.06173 2.30186		H 1.41995 3.14129 2.30640
	C -5.25261 -1.14037 0.40591		C -5.26312 -1.13015 0.45403
	H -4.17679 0.28134 -2.49728		H -4.20878 0.27838 -2.46342
	H -1.77963 1.03126 -2.21125		H -1.82553 1.05513 -2.19230
	H -6.15195 -0.86095 -1.53767		H -6.17578 -0.85640 -1.48196
	H -4.11329 -1.30731 2.21818		H -4.11151 -1.29454 2.25930
	H -6.12021 -1.65192 0.81131		H -6.12746 -1.64075 0.86651
	N 1.38758 -0.86426 -0.30936		C -0.63537 -1.55075 0.21930
	C 0.58349 -0.59944 -1.41237		C -0.67919 -1.07313 -1.15367
	C 0.57741 -1.36634 0.70390		C 0.59904 -1.43368 0.94058
	N -0.74052 -1.48574 0.16279		N 1.57650 -1.31179 1.54743
	N -0.73715 -1.03856 -1.07787		C -1.40880 -2.70962 0.56095
	O 0.92181 -0.14453 -2.47849		N -2.05463 -3.62188 0.85961
	O 0.91262 -1.70021 1.81507		C -1.47799 -1.80823 -2.09580
	C 2.79239 -0.65162 -0.22433		N -2.14204 -2.36783 -2.85960
	C 3.59246 -1.61005 0.39259		C 0.52882 -0.53647 -1.71811
	C 3.35469 0.50133 -0.76483		N 1.48198 -0.06922 -2.17713
	C 4.96380 -1.40405 0.47418		
	C 4.72955 0.68847 -0.68947		
	C 5.53676 -0.25863 -0.06862		
	H 3.14157 -2.50189 0.81100		
	H 2.72069 1.23836 -1.24087		
	H 5.58695 -2.14941 0.95899		

	H 5.16921 1.58552 -1.11495 H 6.60988 -0.10485 -0.00813		
TSab **THF**	C -4.20156 -0.04212 -1.42906 C -3.06854 0.20209 -0.63585 C -1.86239 0.79487 -1.14040 C -3.03824 -0.24803 0.70209 C -1.80662 -0.06161 1.41408 C -0.97166 1.06099 1.09591 C -1.00158 1.51095 -0.24209 C -5.29278 -0.68121 -0.87854 C -4.14127 -0.93788 1.23195 H -1.72815 -0.48627 2.41352 C -0.07279 1.63950 2.00731 C -0.13262 2.53462 -0.65393 C 0.71148 3.12164 0.26540 C 0.74149 2.67390 1.59640 H -0.03920 1.27823 3.03060 H -0.14502 2.86559 -1.68788 H 1.36624 3.93066 -0.04277 H 1.41922 3.14110 2.30391 C -5.26260 -1.12936 0.45232 H -4.21441 0.28888 -2.46300 H -1.83117 1.06305 -2.19520 H -6.18030 -0.84895 -1.48051 H -4.10717 -1.29918 2.25521 H -6.12699 -1.63920 0.86593 C -0.63809 -1.54818 0.22696 C -0.67423 -1.07964 -1.14997 C 0.59905 -1.43692 0.94613 N 1.58021 -1.32192 1.54805 C -1.40905 -2.71052 0.56563 N -2.05270 -3.62563 0.85969 C -1.47385 -1.81386 -2.09025 N -2.14058 -2.37641 -2.84982 C 0.53385 -0.54193 -1.71036 N 1.49086 -0.07560 -2.16268	**TSab** **1,4-dixoane**	C -4.20313 -0.04182 -1.42995 C -3.07102 0.20632 -0.63622 C -1.86501 0.79872 -1.13958 C -3.03888 -0.24654 0.70054 C -1.80261 -0.06586 1.40718 C -0.97233 1.06249 1.09435 C -1.00424 1.51506 -0.24251 C -5.29140 -0.68646 -0.88164 C -4.13930 -0.94204 1.22798 H -1.72309 -0.49180 2.40539 C -0.06885 1.63661 2.00369 C -0.13202 2.53623 -0.65447 C 0.71642 3.11858 0.26290 C 0.74792 2.66856 1.59286 H -0.02940 1.27075 3.02473 H -0.14185 2.86586 -1.68849 H 1.37601 3.92269 -0.04663 H 1.43152 3.12924 2.29851 C -5.25948 -1.13679 0.44822 H -4.21582 0.28636 -2.46440 H -1.83180 1.06380 -2.19446 H -6.17614 -0.86038 -1.48534 H -4.10282 -1.31016 2.24832 H -6.11992 -1.65436 0.85961 C -0.64310 -1.54195 0.23234 C -0.67472 -1.08013 -1.14568 C 0.59263 -1.43055 0.95669 N 1.56618 -1.31486 1.57037 C -1.41504 -2.70386 0.57617 N -2.05933 -3.61400 0.88330 C -1.47879 -1.80785 -2.08739 N -2.14946 -2.35671 -2.85350 C 0.52975 -0.53529 -1.70722 N 1.47794 -0.05821 -2.16690
TSab **$PhCH_3$**	C -4.20305 -0.04176 -1.42988 C -3.07083 0.20600 -0.63622 C -1.86482 0.79845 -1.13968 C -3.03881 -0.24668 0.70063 C -1.80285 -0.06562 1.40764 C -0.97226 1.06235 1.09442 C -1.00405 1.51475 -0.24252 C -5.29157 -0.68592 -0.88137	**TSab** **$ClCH_2CH_2Cl$**	C -4.20172 -0.04167 -1.42907 C -3.06850 0.20212 -0.63594 C -1.86328 0.79631 -1.14060 C -3.03803 -0.24825 0.70199 C -1.80687 -0.06137 1.41454 C -0.97154 1.06073 1.09577 C -1.00160 1.51094 -0.24221 C -5.29305 -0.68051 -0.87834

	C -4.13943 -0.94172 1.22827 H -1.72336 -0.49153 2.40591 C -0.06915 1.63682 2.00393 C -0.13214 2.53618 -0.65444 C 0.71592 3.11893 0.26310 C 0.74734 2.66903 1.59312 H -0.03012 1.27131 3.02514 H -0.14219 2.86597 -1.68844 H 1.37510 3.92346 -0.04630 H 1.43048 3.13023 2.29892 C -5.25975 -1.13612 0.44855 H -4.21580 0.28667 -2.46428 H -1.83176 1.06372 -2.19456 H -6.17656 -0.85930 -1.48490 H -4.10315 -1.30934 2.24883 H -6.12050 -1.65308 0.86012 C -0.64270 -1.54246 0.23198 C -0.67457 -1.08024 -1.14598 C 0.59311 -1.43120 0.95602 N 1.56722 -1.31577 1.56889 C -1.41451 -2.70443 0.57551 N -2.05862 -3.61500 0.88178 C -1.47828 -1.80837 -2.08765 N -2.14855 -2.35811 -2.85348 C 0.53013 -0.53591 -1.70747 N 1.47890 -0.05965 -2.16682		C -4.14122 -0.93767 1.23209 H -1.72859 -0.48576 2.41419 C -0.07305 1.63950 2.00738 C -0.13295 2.53496 -0.65398 C 0.71091 3.12214 0.26555 C 0.74092 2.67429 1.59656 H -0.04009 1.27857 3.03086 H -0.14607 2.86649 -1.68780 H 1.36519 3.93173 -0.04235 H 1.41810 3.14204 2.30432 C -5.26279 -1.12871 0.45255 H -4.21481 0.29020 -2.46278 H -1.83203 1.06440 -2.19547 H -6.18095 -0.84760 -1.48002 H -4.10725 -1.29830 2.25565 H -6.12752 -1.63785 0.86644 C -0.63760 -1.54900 0.22717 C -0.67342 -1.08087 -1.14999 C 0.59981 -1.43772 0.94557 N 1.58241 -1.32220 1.54506 C -1.40850 -2.71142 0.56505 N -2.05247 -3.62716 0.85654 C -1.47303 -1.81537 -2.08970 N -2.13906 -2.37939 -2.84884 C 0.53477 -0.54342 -1.70977 N 1.49274 -0.07850 -2.16159
TSac **$CHCl_3$**	C -4.20645 -0.05895 -1.44249 C -3.06377 0.18105 -0.65238 C -1.86248 0.77373 -1.15990 C -3.03300 -0.27413 0.68354 C -1.80345 -0.09745 1.39702 C -0.96559 1.01483 1.07597 C -0.99645 1.47075 -0.26190 C -5.29499 -0.70088 -0.90026 C -4.14519 -0.96279 1.20918 H -1.72455 -0.52157 2.39578 C -0.04975 1.58752 1.98520 C -0.11102 2.49225 -0.66936 C 0.74423 3.06198 0.24208 C 0.77511 2.60704 1.57668 H -0.01697 1.22142 3.00714 H -0.12576 2.82675 -1.70249 H 1.40884 3.86321 -0.06592 H 1.46317 3.06289 2.28189	**TSac** **THF**	C -4.20632 -0.05876 -1.44274 C -3.06368 0.18102 -0.65249 C -1.86246 0.77373 -1.16019 C -3.03290 -0.27419 0.68354 C -1.80327 -0.09790 1.39709 C -0.96521 1.01435 1.07587 C -0.99613 1.47038 -0.26203 C -5.29493 -0.70048 -0.90025 C -4.14512 -0.96263 1.20945 H -1.72469 -0.52192 2.39602 C -0.04936 1.58712 1.98520 C -0.11074 2.49206 -0.66953 C 0.74445 3.06202 0.24203 C 0.77538 2.60698 1.57674 H -0.01758 1.22182 3.00758 H -0.12657 2.82748 -1.70247 H 1.40811 3.86431 -0.06561 H 1.46250 3.06384 2.28235

	C -5.26414 -1.15555 0.43340 H -4.22162 0.28246 -2.47387 H -1.83170 1.04860 -2.21211 H -6.18403 -0.86347 -1.50183 H -4.11284 -1.32232 2.23399 H -6.12968 -1.66423 0.84668 C -0.72700 -1.61756 0.16496 C -0.75470 -1.16632 -1.15576 C 0.64040 -1.39563 0.66968 O 1.14540 -1.68165 1.71893 C 0.59553 -0.66481 -1.47020 O 1.05710 -0.24327 -2.49343 H -1.32538 -2.41715 0.57766 H -1.37796 -1.55451 -1.94856 O 1.35715 -0.72446 -0.31131		C -5.26412 -1.15510 0.43356 H -4.22126 0.28246 -2.47425 H -1.83176 1.04860 -2.21250 H -6.18399 -0.86319 -1.50186 H -4.11260 -1.32227 2.23427 H -6.12973 -1.66378 0.84684 C -0.72716 -1.61795 0.16511 C -0.75495 -1.16678 -1.15595 C 0.63991 -1.39615 0.66927 O 1.14668 -1.68133 1.71825 C 0.59478 -0.66540 -1.47019 O 1.05804 -0.24342 -2.49284 H -1.32553 -2.41757 0.57806 H -1.37831 -1.55491 -1.94887 O 1.35697 -0.72467 -0.31147
TSac **1,4-dioxane**	C -4.20739 -0.05998 -1.44233 C -3.06510 0.18190 -0.65224 C -1.86403 0.77527 -1.15891 C -3.03425 -0.27337 0.68367 C -1.80441 -0.09666 1.39645 C -0.96777 1.01651 1.07662 C -0.99878 1.47274 -0.26117 C -5.29513 -0.70397 -0.90139 C -4.14620 -0.96321 1.20820 H -1.72468 -0.52051 2.39503 C -0.04965 1.58687 1.98475 C -0.11095 2.49172 -0.66922 C 0.74631 3.05908 0.24126 C 0.77711 2.60415 1.57563 H -0.01355 1.21787 3.00527 H -0.12240 2.82321 -1.70310 H 1.41436 3.85666 -0.06800 H 1.46848 3.05637 2.27959 C -5.26435 -1.15837 0.43216 H -4.22323 0.28213 -2.47336 H -1.83171 1.04975 -2.21095 H -6.18342 -0.86774 -1.50345 H -4.11463 -1.32179 2.23325 H -6.12924 -1.66799 0.84522 C -0.72731 -1.61472 0.16596 C -0.75521 -1.16462 -1.15415 C 0.64180 -1.39093 0.67165 O 1.14144 -1.67689 1.72220 C 0.59601 -0.66002 -1.46911	**TSac** **$PhCH_3$**	C -4.20730 -0.05989 -1.44238 C -3.06499 0.18182 -0.65227 C -1.86392 0.77519 -1.15901 C -3.03413 -0.27345 0.68364 C -1.80430 -0.09679 1.39648 C -0.96757 1.01633 1.07656 C -0.99857 1.47256 -0.26123 C -5.29512 -0.70367 -0.90130 C -4.14611 -0.96317 1.20829 H -1.72471 -0.52061 2.39510 C -0.04965 1.58690 1.98479 C -0.11097 2.49179 -0.66923 C 0.74613 3.05934 0.24133 C 0.77694 2.60439 1.57572 H -0.01390 1.21821 3.00546 H -0.12279 2.82362 -1.70302 H 1.41385 3.85728 -0.06779 H 1.46800 3.05695 2.27981 C -5.26434 -1.15809 0.43227 H -4.22306 0.28214 -2.47344 H -1.83173 1.04970 -2.21107 H -6.18348 -0.86734 -1.50332 H -4.11447 -1.32184 2.23332 H -6.12930 -1.66759 0.84535 C -0.72727 -1.61495 0.16594 C -0.75518 -1.16482 -1.15426 C 0.64168 -1.39133 0.67146 O 1.14198 -1.67736 1.72183 C 0.59588 -0.66047 -1.46920

	O 1.05157 -0.23742 -2.49330 H -1.32425 -2.41494 0.57880 H -1.37761 -1.55339 -1.94697 O 1.35663 -0.71992 -0.31007		O 1.05210 -0.23805 -2.49332 H -1.32429 -2.41515 0.57879 H -1.37765 -1.55358 -1.94707 O 1.35666 -0.72029 -0.31020
TSac $ClCH_2CH_2Cl$	C -4.20600 -0.05861 -1.44287 C -3.06336 0.18099 -0.65253 C -1.86235 0.77399 -1.16040 C -3.03256 -0.27420 0.68344 C -1.80296 -0.09816 1.39715 C -0.96455 1.01387 1.07570 C -0.99552 1.47002 -0.26215 C -5.29475 -0.69994 -0.90014 C -4.14483 -0.96244 1.20954 H -1.72496 -0.52209 2.39622 C -0.04908 1.58700 1.98523 C -0.11054 2.49214 -0.66953 C 0.74437 3.06239 0.24220 C 0.77532 2.60726 1.57691 H -0.01857 1.22276 3.00807 H -0.12768 2.82877 -1.70209 H 1.40713 3.86564 -0.06503 H 1.46154 3.06504 2.28287 C -5.26398 -1.15446 0.43369 H -4.22060 0.28219 -2.47453 H -1.83198 1.04879 -2.21278 H -6.18389 -0.86272 -1.50169 H -4.11205 -1.32240 2.23425 H -6.12971 -1.66305 0.84693 C -0.72706 -1.61854 0.16526 C -0.75496 -1.16755 -1.15619 C 0.63941 -1.39693 0.66909 O 1.14778 -1.68207 1.71770 C 0.59394 -0.66630 -1.47065 O 1.05858 -0.24459 -2.49319 H -1.32560 -2.41802 0.57838 H -1.37870 -1.55556 -1.94896 O 1.35662 -0.72542 -0.31188	**TSba** $CHCl_3$	N 0.82449 0.31828 0.58157 C 0.07472 1.42425 0.22596 C 0.08256 -0.43083 1.50680 N -1.12367 0.27308 1.74401 N -1.14818 1.33844 0.99251 O 0.36847 2.33154 -0.51373 O 0.42220 -1.45568 2.04769 C 2.13139 0.00860 0.11041 C 2.47758 -1.31599 -0.14509 C 3.05306 1.03349 -0.08930 C 3.75696 -1.61100 -0.59911 C 4.32482 0.72517 -0.55565 C 4.68241 -0.59454 -0.80910 H 1.75619 -2.10551 0.02416 H 2.77131 2.06011 0.10852 H 4.02752 -2.64436 -0.79330 H 5.04139 1.52516 -0.71461 H 5.67945 -0.83025 -1.16819 C -2.54416 -1.08299 0.62163 C -3.46468 0.08124 0.23984 C -2.64104 -0.76318 -1.68298 C -1.99098 -1.52277 -0.54030 H -2.51243 -1.58325 1.57734 H -1.19974 -2.25375 -0.65890 C -4.03357 -0.47885 -1.09095 H -4.60073 0.26091 -1.66503 H -4.62904 -1.38588 -0.94874 C -2.52112 1.16365 -0.33402 H -2.73905 2.22254 -0.29096 C -1.96769 0.55980 -1.46585 H -1.18450 0.97437 -2.08906 H -4.16579 0.41811 1.00081 H -2.55486 -1.20080 -2.67529
TSba **THF**	N 0.82359 0.32553 0.57792 C 0.07388 1.42991 0.21924 C 0.08532 -0.41715 1.51020 N -1.11996 0.28710 1.74649 N -1.14722 1.34838 0.98872 O 0.36738 2.33372 -0.52523 O 0.42916 -1.43749 2.05812	**TSba** **1,4-dioxane**	N 0.83232 0.30068 0.58639 C 0.07803 1.40343 0.22836 C 0.08495 -0.45883 1.50222 N -1.12518 0.24014 1.73719 N -1.14899 1.30720 0.99097 O 0.36685 2.31575 -0.50596 O 0.41993 -1.48844 2.03434

	C	2.12988	0.01320	0.10700	C	2.14199	-0.00273	0.11781
	C	2.46431	-1.30953	-0.17146	C	2.52090	-1.33072	-0.06639
	C	3.06196	1.03299	-0.06791	C	3.03532	1.03166	-0.15279
	C	3.74357	-1.60865	-0.62332	C	3.80163	-1.61795	-0.52099
	C	4.33350	0.72145	-0.53305	C	4.30856	0.72877	-0.61805
	C	4.67968	-0.59699	-0.80882	C	4.69800	-0.59311	-0.80173
	H	1.73313	-2.09472	-0.02351	H	1.82545	-2.12738	0.16271
	H	2.78880	2.05832	0.14913	H	2.72942	2.06032	-0.01371
	H	4.00554	-2.64067	-0.83586	H	4.09631	-2.65374	-0.65821
	H	5.05884	1.51712	-0.67313	H	5.00132	1.53666	-0.83226
	H	5.67656	-0.83556	-1.16666	H	5.69622	-0.82362	-1.16054
	C	-2.54339	-1.08051	0.62762	C	-2.55302	-1.10483	0.59524
	C	-3.46476	0.08066	0.23909	C	-3.46978	0.07213	0.24636
	C	-2.63872	-0.77395	-1.67847	C	-2.65297	-0.72364	-1.69874
	C	-1.98809	-1.52593	-0.53078	C	-2.00690	-1.51887	-0.57735
	H	-2.51010	-1.57369	1.58704	H	-2.50662	-1.61667	1.54396
	H	-1.19627	-2.25709	-0.64530	H	-1.21759	-2.24831	-0.71465
	C	-4.03202	-0.48816	-1.08884	C	-4.04412	-0.45088	-1.09700
	H	-4.60004	0.24742	-1.66738	H	-4.61034	0.30474	-1.65109
	H	-4.62614	-1.39526	-0.94151	H	-4.64196	-1.35955	-0.97659
	C	-2.52295	1.16074	-0.34092	C	-2.52647	1.17051	-0.30236
	H	-2.74139	2.21979	-0.30318	H	-2.75580	2.22577	-0.23652
	C	-1.96772	0.55147	-1.46870	C	-1.98064	0.59589	-1.45446
	H	-1.18494	0.96304	-2.09462	H	-1.20346	1.03016	-2.07095
	H	-4.16733	0.42085	0.99730	H	-4.16745	0.39078	1.01817
	H	-2.55076	-1.21722	-2.66812	H	-2.57264	-1.13621	-2.70230
TSba $PhCH_3$	N	0.83137	0.30217	0.58517	**TSba** $ClCH_2CH_2Cl$	N	0.82267	0.32947	0.57689
	C	0.07801	1.40579	0.22798		C	0.07341	1.43324	0.21643
	C	0.08424	-0.45641	1.50152		C	0.08597	-0.40961	1.51280
	N	-1.12503	0.24378	1.73736		N	-1.11890	0.29504	1.74811
	N	-1.14845	1.31106	0.99109		N	-1.14714	1.35400	0.98693
	O	0.36769	2.31749	-0.50692		O	0.36753	2.33547	-0.52991
	O	0.41907	-1.48621	2.03364		O	0.43166	-1.42729	2.06504
	C	2.14095	-0.00162	0.11676		C	2.12849	0.01539	0.10583
	C	2.51622	-1.32927	-0.07657		C	2.45663	-1.30620	-0.18489
	C	3.03768	1.03219	-0.14431		C	3.06580	1.03226	-0.05677
	C	3.79696	-1.61692	-0.53096		C	3.73556	-1.60750	-0.63635
	C	4.31093	0.72917	-0.60953		C	4.33701	0.71897	-0.52183
	C	4.69675	-0.59251	-0.80239		C	4.67712	-0.59860	-0.80944
	H	1.81770	-2.12557	0.14471		H	1.72046	-2.08888	-0.04775
	H	2.73454	2.06069	0.00236		H	2.79710	2.05676	0.17023
	H	4.08892	-2.65249	-0.67560		H	3.99294	-2.63863	-0.85871
	H	5.00651	1.53657	-0.81636		H	5.06678	1.51222	-0.65250
	H	5.69494	-0.82323	-1.16119		H	5.67371	-0.83867	-1.16718

	C	-2.55237	-1.10132	0.59921		C	-2.54215	-1.07874	0.63081
	C	-3.46936	0.07415	0.24563		C	-3.46432	0.08039	0.23824
	C	-2.65231	-0.72916	-1.69645		C	-2.63624	-0.77971	-1.67609
	C	-2.00577	-1.51946	-0.57206		C	-1.98542	-1.52725	-0.52555
	H	-2.50827	-1.61167	1.54886		H	-2.50867	-1.56845	1.59203
	H	-1.21629	-2.24927	-0.70665		H	-1.19318	-2.25843	-0.63766
	C	-4.04343	-0.45410	-1.09581		C	-4.03021	-0.49341	-1.08818
	H	-4.60958	0.29946	-1.65275		H	-4.59872	0.23967	-1.66941
	H	-4.64128	-1.36232	-0.97211		H	-4.62340	-1.40068	-0.93814
	C	-2.52567	1.16981	-0.30705		C	-2.52349	1.15943	-0.34492
	H	-2.75264	2.22576	-0.24424		H	-2.74225	2.21859	-0.31033
	C	-1.97916	0.59058	-1.45622		C	-1.96668	0.54704	-1.47005
	H	-1.20088	1.02158	-2.07370		H	-1.18398	0.95705	-2.09717
	H	-4.16713	0.39582	1.01611		H	-4.16791	0.42223	0.99480
	H	-2.57161	-1.14541	-2.69845		H	-2.54689	-1.22608	-2.66422
TSbb $CHCl_3$	C	0.88773	-0.21730	-1.87520	**TSbb** **THF**	C	0.88391	-0.21546	-1.87969
	C	0.92374	1.04364	-1.21228		C	0.92190	1.04427	-1.21616
	C	2.20206	1.03326	0.32467		C	2.20330	1.03239	0.32921
	C	2.06822	-0.33306	1.03987		C	2.07052	-0.33490	1.04233
	C	4.25713	-0.10777	0.52496		C	4.25874	-0.10690	0.52584
	C	3.54999	1.07065	-0.05860		C	3.55031	1.07309	-0.05373
	H	1.77021	1.95012	0.72335		H	1.76762	1.94853	0.72575
	H	4.01456	1.82786	-0.68337		H	4.01514	1.83396	-0.67417
	C	3.42265	-0.34758	1.79980		C	3.42548	-0.34803	1.80164
	H	3.64006	-1.31218	2.26681		H	3.64454	-1.31256	2.26804
	H	3.51297	0.45845	2.53458		H	3.51521	0.45801	2.53649
	C	2.38906	-1.36768	-0.03898		C	2.39247	-1.36977	-0.03611
	H	1.74665	-2.17896	-0.35234		H	1.74920	-2.17986	-0.35131
	C	3.67245	-1.16472	-0.40595		C	3.67510	-1.16676	-0.40323
	H	4.20564	-1.59765	-1.24370		H	4.21022	-1.60217	-1.23855
	H	1.15696	-0.48423	1.61627		H	1.15980	-0.48719	1.61943
	H	5.34180	-0.05076	0.58180		H	5.34344	-0.04837	0.58198
	C	-0.28348	1.39653	-0.48562		C	-0.28432	1.39790	-0.48886
	N	-1.22250	1.68196	0.12217		N	-1.22535	1.68166	0.11658
	C	1.48728	2.16486	-1.94113		C	1.48871	2.16439	-1.94337
	N	1.96605	3.05794	-2.49500		N	1.96759	3.05542	-2.50042
	C	1.80851	-0.49623	-2.91706		C	1.80248	-0.49586	-2.92295
	N	2.58589	-0.71439	-3.74933		N	2.57536	-0.71469	-3.75924
	C	-0.16163	-1.14373	-1.63914		C	-0.16468	-1.14182	-1.64122
	N	-1.00311	-1.91636	-1.44096		N	-1.00781	-1.91263	-1.44265
TSbb **1,4-dioxane**	C	0.89942	-0.22283	-1.86189	**TSbb** $PhCH_3$	C	0.89798	-0.22214	-1.86350
	C	0.92764	1.04209	-1.20247		C	0.92726	1.04224	-1.20351
	C	2.20080	1.03698	0.31462		C	2.20087	1.03644	0.31563
	C	2.06271	-0.32671	1.03466		C	2.06335	-0.32751	1.03523

	C 4.25327 -0.11085 0.52256		C 4.25372 -0.11047 0.52285
	C 3.55023 1.06461 -0.07084		C 3.55017 1.06526 -0.06951
	H 1.77684 1.95563 0.71632		H 1.77611 1.95490 0.71709
	H 4.01391 1.81091 -0.70843		H 4.01394 1.81277 -0.70571
	C 3.41616 -0.34667 1.79538		C 3.41689 -0.34670 1.79590
	H 3.62851 -1.31176 2.26362		H 3.62987 -1.31168 2.26408
	H 3.50961 0.45912 2.53004		H 3.50991 0.45917 2.53052
	C 2.37852 -1.36039 -0.04629		C 2.37986 -1.36138 -0.04535
	H 1.73768 -2.17483 -0.35295		H 1.73882 -2.17542 -0.35287
	C 3.66434 -1.15905 -0.41293		C 3.66534 -1.15976 -0.41209
	H 4.19164 -1.58609 -1.25713		H 4.19335 -1.58749 -1.25552
	H 1.15004 -0.47385 1.60953		H 1.15083 -0.47513 1.61026
	H 5.33791 -0.05863 0.58117		H 5.33837 -0.05764 0.58126
	C -0.28172 1.39120 -0.47626		C -0.28190 1.39183 -0.47728
	N -1.21631 1.67764 0.13789		N -1.21700 1.67830 0.13608
	C 1.48291 2.16590 -1.93528		C 1.48338 2.16581 -1.93589
	N 1.96083 3.06291 -2.48360		N 1.96137 3.06245 -2.48470
	C 1.82533 -0.49652 -2.90130		C 1.82337 -0.49648 -2.90311
	N 2.61419 -0.71179 -3.72335		N 2.61095 -0.71211 -3.72631
	C -0.15347 -1.14892 -1.63582		C -0.15449 -1.14827 -1.63627
	N -0.99207 -1.92543 -1.44162		N -0.99345 -1.92431 -1.44165
TSbb $ClCH_2CH_2Cl$	C 0.88147 -0.21444 -1.88219	**TSbc** $CHCl_3$	O 0.68724 0.25137 0.48827
	C 0.92112 1.04453 -1.21816		C 0.04933 1.48634 0.48976
	C 2.20342 1.03157 0.33165		C 0.05426 -0.58875 1.39824
	C 2.07187 -0.33640 1.04366		C -1.17388 0.08084 1.84325
	C 4.25954 -0.10610 0.52591		C -1.17810 1.35351 1.28515
	C 3.55003 1.07487 -0.05076		O 0.50289 2.41711 -0.11752
	H 1.76549 1.94710 0.72741		O 0.51341 -1.66444 1.66811
	H 4.01475 1.83846 -0.66808		C -2.51600 -1.02557 0.60378
	C 3.42723 -0.34829 1.80240		C -3.47060 0.11470 0.19757
	H 3.64767 -1.31274 2.26837		C -2.63233 -0.72090 -1.72133
	H 3.51637 0.45774 2.53732		C -1.94907 -1.43695 -0.58963
	C 2.39476 -1.37152 -0.03432		H -2.65938 -1.69380 1.44402
	H 1.75111 -2.18089 -0.35091		H -1.13180 -2.13908 -0.70902
	C 3.67662 -1.16768 -0.40214		C -4.02650 -0.46478 -1.13005
	H 4.21269 -1.60404 -1.23641		H -4.60701 0.26320 -1.70532
	H 1.16157 -0.48947 1.62127		H -4.60493 -1.38294 -0.98768
	H 5.34426 -0.04658 0.58145		C -2.51870 1.19072 -0.36211
	C -0.28479 1.39919 -0.49107		H -2.66766 2.26081 -0.28433
	N -1.22717 1.68282 0.11231		C -1.95173 0.59675 -1.47664
	C 1.49007 2.16376 -1.94473		H -1.13603 0.98904 -2.07326
	N 1.96981 3.05395 -2.50237		H -4.18530 0.44242 0.95145
	C 1.79909 -0.49620 -2.92579		H -2.53407 -1.15390 -2.71428
	N 2.56957 -0.71613 -3.76402		H -1.64507 2.22937 1.71338

	C -0.16682 -1.14054 -1.64206 N -1.01084 -1.91031 -1.44311		H -1.64007 -0.20205 2.77656
TSbc **THF**	O 0.68702 0.25126 0.48956 C 0.04870 1.48653 0.49113 C 0.05312 -0.58871 1.39906 C -1.17411 0.08082 1.84398 C -1.17731 1.35419 1.28658 O 0.50464 2.41655 -0.11665 O 0.51395 -1.66448 1.66840 C -2.51514 -1.02516 0.60323 C -3.47000 0.11500 0.19736 C -2.63294 -0.72116 -1.72194 C -1.94819 -1.43614 -0.59049 H -2.65901 -1.69356 1.44340 H -1.13156 -2.13894 -0.71101 C -4.02672 -0.46512 -1.12964 H -4.60783 0.26258 -1.70469 H -4.60493 -1.38330 -0.98646 C -2.51899 1.19082 -0.36354 H -2.66786 2.26092 -0.28451 C -1.95171 0.59630 -1.47757 H -1.13694 0.98831 -2.07574 H -4.18378 0.44296 0.95195 H -2.53493 -1.15444 -2.71481 H -1.64546 2.23000 1.71382 H -1.64109 -0.20222 2.77698	**TSbc** **1,4-dioxane**	O 0.68680 0.25040 0.48596 C 0.05027 1.48562 0.48615 C 0.05509 -0.59077 1.39496 C -1.17481 0.08028 1.84107 C -1.17917 1.35240 1.28287 O 0.49771 2.41715 -0.12173 O 0.50777 -1.66773 1.66465 C -2.51668 -1.02471 0.60580 C -3.47198 0.11461 0.19749 C -2.63013 -0.72004 -1.71952 C -1.94954 -1.43729 -0.58694 H -2.65939 -1.69351 1.44539 H -1.13000 -2.13701 -0.70295 C -4.02563 -0.46514 -1.13088 H -4.60559 0.26244 -1.70722 H -4.60362 -1.38378 -0.98967 C -2.51904 1.19148 -0.35961 H -2.66824 2.26142 -0.28295 C -1.95188 0.59879 -1.47467 H -1.13377 0.99181 -2.06710 H -4.18894 0.44156 0.94965 H -2.53111 -1.15293 -2.71238 H -1.64227 2.22901 1.71334 H -1.63695 -0.20104 2.77668
TSbc **$PhCH_3$**	O 0.68686 0.25046 0.48627 C 0.05018 1.48569 0.48661 C 0.05496 -0.59057 1.39533 C -1.17475 0.08034 1.84130 C -1.17900 1.35254 1.28317 O 0.49836 2.41711 -0.12121 O 0.50833 -1.66741 1.66506 C -2.51656 -1.02475 0.60557 C -3.47183 0.11464 0.19748 C -2.63040 -0.72014 -1.71974 C -1.94945 -1.43719 -0.58726 H -2.65934 -1.69355 1.44519 H -1.13015 -2.13717 -0.70366 C -4.02574 -0.46514 -1.13077 H -4.60580 0.26245 -1.70700 H -4.60375 -1.38374 -0.98940 C -2.51905 1.19142 -0.35996 H -2.66819 2.26138 -0.28312	**TSbc** **$ClCH_2CH_2Cl$**	O 0.68695 0.25133 0.49009 C 0.04837 1.48663 0.49173 C 0.05269 -0.58859 1.39951 C -1.17413 0.08078 1.84430 C -1.17705 1.35445 1.28711 O 0.50544 2.41637 -0.11622 O 0.51455 -1.66430 1.66863 C -2.51483 -1.02507 0.60295 C -3.46970 0.11514 0.19730 C -2.63323 -0.72127 -1.72222 C -1.94786 -1.43587 -0.59090 H -2.65899 -1.69343 1.44315 H -1.13160 -2.13906 -0.71200 C -4.02682 -0.46519 -1.12944 H -4.60817 0.26243 -1.70433 H -4.60497 -1.38336 -0.98590 C -2.51902 1.19082 -0.36410 H -2.66790 2.26094 -0.28465

	C	-1.95190	0.59858	-1.47494		C	-1.95163	0.59603	-1.47793
	H	-1.13409	0.99151	-2.06787		H	-1.13726	0.98791	-2.07680
	H	-4.18854	0.44167	0.94984		H	-4.18302	0.44323	0.95224
	H	-2.53146	-1.15306	-2.71260		H	-2.53536	-1.15466	-2.71507
	H	-1.64252	2.22909	1.71337		H	-1.64582	2.23019	1.71393
	H	-1.63727	-0.20113	2.77670		H	-1.64173	-0.20245	2.77700
TSca $CHCl_3$	C	-0.77643	1.16954	1.56583	**TSca** **THF**	C	-0.77380	1.18216	1.57327
	C	-1.41622	0.97904	0.34651		C	-1.42097	0.98457	0.35921
	C	-0.36004	2.51069	1.65320		C	-0.35190	2.52233	1.64810
	C	-0.73746	3.17235	0.49265		C	-0.73283	3.17660	0.48460
	C	-1.75389	2.32797	-0.21694		C	-1.75363	2.32978	-0.21511
	H	-0.56680	4.22095	0.28371		H	-0.56024	4.22316	0.26733
	H	-1.86859	0.05299	0.01536		H	-1.87921	0.05791	0.03751
	N	0.35871	1.00949	-0.86896		N	0.35511	0.99812	-0.86645
	N	0.75395	2.24710	-0.80884		N	0.75442	2.23493	-0.81675
	C	1.27038	0.17893	-0.11885		C	1.26563	0.17123	-0.11200
	O	1.20626	-1.02036	-0.02970		O	1.20002	-1.02773	-0.01443
	C	1.95500	2.32470	-0.01643		C	1.95721	2.31453	-0.02804
	O	2.59646	3.32406	0.18295		O	2.60505	3.31254	0.15968
	N	2.25513	1.02420	0.38038		N	2.25309	1.01712	0.37930
	H	0.24901	2.93076	2.44520		H	0.26108	2.94671	2.43495
	H	-0.53923	0.38775	2.27796		H	-0.53759	0.40564	2.29162
	H	-2.75342	2.61208	0.14422		H	-2.75134	2.62166	0.14515
	H	-1.74426	2.39784	-1.30305		H	-1.74708	2.38998	-1.30195
	C	3.38990	0.62790	1.14367		C	3.38842	0.62356	1.14317
	C	3.82773	1.43070	2.19385		C	3.80931	1.41578	2.20794
	C	4.05278	-0.55598	0.83071		C	4.06803	-0.54658	0.81548
	C	4.94081	1.04403	2.92954		C	4.92322	1.03235	2.94424
	C	5.15669	-0.93713	1.58313		C	5.17242	-0.92552	1.56850
	C	5.60590	-0.13999	2.63033		C	5.60503	-0.13852	2.63046
	H	3.30918	2.35371	2.42228		H	3.27540	2.32714	2.44898
	H	3.69972	-1.17430	0.01496		H	3.72818	-1.15566	-0.01307
	H	5.28497	1.67286	3.74490		H	5.25446	1.65237	3.77166
	H	5.67114	-1.86219	1.34176		H	5.70043	-1.84003	1.31624
	H	6.47246	-0.44027	3.21128		H	6.47195	-0.43673	3.21204
TSca **1,4-dioxane**	C	-0.78624	1.13988	1.54830	**TSca** $PhCH_3$	C	-0.78511	1.14334	1.55030
	C	-1.40900	0.96655	0.31742		C	-1.40972	0.96798	0.32066
	C	-0.38045	2.48204	1.66382		C	-0.37819	2.48543	1.66263
	C	-0.74801	3.16095	0.50990		C	-0.74690	3.16237	0.50796
	C	-1.75515	2.32365	-0.22217		C	-1.75499	2.32416	-0.22161
	H	-0.58068	4.21330	0.32069		H	-0.57919	4.21429	0.31649
	H	-1.84835	0.04301	-0.03642		H	-1.85056	0.04411	-0.03059
	N	0.36765	1.03631	-0.87443		N	0.36661	1.03324	-0.87375
	N	0.75160	2.27535	-0.78791		N	0.75198	2.27211	-0.79037

	C 1.28204 0.19807 -0.13426		C 1.28059 0.19584 -0.13235
	O 1.22099 -1.00172 -0.06411		O 1.21908 -1.00389 -0.05989
	C 1.94835 2.34876 0.01377		C 1.94920 2.34598 0.01028
	O 2.57228 3.35184 0.24214		O 2.57524 3.34862 0.23537
	N 2.26126 1.04154 0.38286		N 2.26053 1.03948 0.38263
	H 0.22079 2.89123 2.46701		H 0.22385 2.89594 2.46459
	H -0.54722 0.34618 2.24606		H -0.54630 0.35098 2.24971
	H -2.75881 2.59363 0.13785		H -2.75821 2.59568 0.13854
	H -1.73693 2.41344 -1.30662		H -1.73774 2.41167 -1.30628
	C 3.39503 0.63886 1.14500		C 3.39440 0.63750 1.14488
	C 3.87391 1.46453 2.15966		C 3.86850 1.46065 2.16372
	C 4.01802 -0.57586 0.86763		C 4.02206 -0.57376 0.86330
	C 4.98482 1.06940 2.89383		C 4.97973 1.06659 2.89800
	C 5.12080 -0.96280 1.61831		C 5.12502 -0.95998 1.61414
	C 5.60980 -0.14400 2.62986		C 5.60943 -0.14352 2.62985
	H 3.39218 2.41323 2.35788		H 3.38251 2.40653 2.36547
	H 3.63334 -1.21402 0.08293		H 3.64104 -1.20977 0.07498
	H 5.35995 1.71724 3.67998		H 5.35130 1.71237 3.68754
	H 5.60255 -1.91153 1.40331		H 5.61060 -1.90605 1.39602
	H 6.47529 -0.44967 3.20932		H 6.47510 -0.44850 3.20941
TSca $ClCH_2CH_2Cl$	C -0.77163 1.18977 1.57737	**TScb** $CHCl_3$	C 2.50322 0.21453 -0.51345
	C -1.42283 0.98754 0.36641		C 1.59575 -0.07172 -1.53883
	C -0.34694 2.52954 1.64455		C 2.36360 -0.73989 0.49314
	C -0.72996 3.17895 0.47904		C 1.36497 -1.64716 0.12303
	C -1.75346 2.33038 -0.21438		C 1.13218 -1.48355 -1.34806
	H -0.55656 4.22437 0.25661		H 1.10496 -2.54019 0.68119
	H -1.88399 0.06024 0.05055		H 1.54186 0.46075 -2.48235
	N 0.35341 0.99190 -0.86550		C -0.41607 -0.31772 0.53703
	N 0.75488 2.22817 -0.82146		C -0.27430 0.66318 -0.49290
	C 1.26310 0.16684 -0.10833		H 2.86846 -0.72218 1.45200
	O 1.19680 -1.03188 -0.00631		H 3.13426 1.09426 -0.46372
	C 1.95833 2.30902 -0.03398		H 1.84274 -2.14063 -1.87248
	O 2.60928 3.30630 0.14787		H 0.13757 -1.73053 -1.72053
	N 2.25137 1.01332 0.37949		C -0.13729 0.05453 1.89705
	H 0.26824 2.95680 2.42821		N 0.09426 0.34520 2.99176
	H -0.53574 0.41663 2.29955		C 0.14716 1.99044 -0.13772
	H -2.74963 2.62587 0.14733		N 0.49526 3.05708 0.14100
	H -1.74992 2.38514 -1.30153		C -1.12235 0.58930 -1.65020
	C 3.38710 0.62107 1.14342		N -1.78663 0.52342 -2.59449
	C 3.79857 1.40690 2.21641		C -1.40303 -1.35093 0.38600
	C 4.07603 -0.54099 0.80709		N -2.17913 -2.19905 0.26122
	C 4.91318 1.02525 2.95265		
	C 5.18090 -0.91875 1.56008		
	C 5.60439 -0.13785 2.63031		

	H 3.25601 2.31143 2.46467 H 3.74335 -1.14454 -0.02861 H 5.23733 1.63999 3.78682 H 5.71655 -1.82703 1.30140 H 6.47171 -0.43496 3.21192		
TScb **THF**	C 2.50345 0.21438 -0.51367 C 1.59759 -0.07258 -1.53970 C 2.36406 -0.74066 0.49311 C 1.36747 -1.64908 0.12225 C 1.13269 -1.48375 -1.34816 H 1.10617 -2.54185 0.68049 H 1.54278 0.46022 -2.48314 C -0.41825 -0.31606 0.53764 C -0.27608 0.66400 -0.49190 H 2.86873 -0.72294 1.45223 H 3.13417 1.09449 -0.46382 H 1.84279 -2.14105 -1.87310 H 0.13780 -1.73026 -1.72023 C -0.13806 0.05529 1.89729 N 0.09404 0.34712 2.99162 C 0.14634 1.99091 -0.13736 N 0.49416 3.05745 0.14216 C -1.12258 0.58958 -1.64998 N -1.78689 0.52307 -2.59422 C -1.40334 -1.35060 0.38635 N -2.17959 -2.19852 0.26083	**TScb** **1,4-dioxane**	C 2.49939 0.21531 -0.51147 C 1.58737 -0.06793 -1.53448 C 2.36102 -0.74000 0.49368 C 1.35927 -1.64462 0.12431 C 1.12904 -1.48280 -1.34795 H 1.09805 -2.53769 0.68112 H 1.53329 0.46393 -2.47790 C -0.41320 -0.31925 0.53606 C -0.26983 0.66102 -0.49514 H 2.86156 -0.71934 1.45437 H 3.12498 1.09832 -0.45825 H 1.84307 -2.13665 -1.87100 H 0.13476 -1.73044 -1.72021 C -0.13171 0.05251 1.89607 N 0.10615 0.33847 2.99064 C 0.15197 1.98908 -0.14059 N 0.50449 3.05548 0.13311 C -1.11908 0.58771 -1.65252 N -1.77849 0.52265 -2.60020 C -1.40087 -1.35267 0.38594 N -2.17380 -2.20394 0.26311
TScb **$PhCH_3$**	C 2.49960 0.21526 -0.51152 C 1.58806 -0.06827 -1.53482 C 2.36123 -0.74009 0.49366 C 1.35994 -1.64508 0.12408 C 1.12934 -1.48289 -1.34800 H 1.09883 -2.53818 0.68098 H 1.53411 0.46367 -2.47826 C -0.41352 -0.31903 0.53619 C -0.27015 0.66120 -0.49496 H 2.86215 -0.71974 1.45421 H 3.12558 1.09805 -0.45853 H 1.84295 -2.13701 -1.87137 H 0.13501 -1.73049 -1.72022 C -0.13212 0.05279 1.89614 N 0.10520 0.33931 2.99069 C 0.15153 1.98923 -0.14038 N 0.50342 3.05572 0.13379 C -1.11927 0.58784 -1.65235	**TScb** **$ClCH_2CH_2Cl$**	C 2.50322 0.21440 -0.51327 C 1.59859 -0.07326 -1.54015 C 2.36415 -0.74099 0.49320 C 1.36900 -1.65050 0.12148 C 1.13328 -1.48407 -1.34845 H 1.10795 -2.54326 0.68004 H 1.54438 0.45998 -2.48348 C -0.41902 -0.31537 0.53814 C -0.27654 0.66448 -0.49163 H 2.86925 -0.72372 1.45215 H 3.13408 1.09446 -0.46342 H 1.84200 -2.14201 -1.87474 H 0.13820 -1.73045 -1.72021 C -0.13813 0.05625 1.89741 N 0.09367 0.34995 2.99131 C 0.14580 1.99124 -0.13689 N 0.49226 3.05786 0.14408 C -1.12275 0.58946 -1.64976

	N	-1.77907	0.52273	-2.59977	N	-1.78764	0.52201	-2.59354
	C	-1.40105	-1.35247	0.38603	C	-1.40367	-1.35010	0.38646
	N	-2.17432	-2.20342	0.26309	N	-2.18064	-2.19723	0.25998
TScc $CHCl_3$	C	1.80240	1.48980	0.82789	**TScc** THF	C	1.80323	1.49134	0.82876
	C	1.78073	1.35389	-0.55963		C	1.78169	1.35450	-0.55898
	C	2.14541	0.25991	1.39973		C	2.14614	0.26196	1.40139
	C	2.34537	-0.67258	0.38242		C	2.34678	-0.67125	0.38461
	C	2.54460	0.10158	-0.89156		C	2.54369	0.10124	-0.89042
	H	2.71365	-1.68024	0.53871		H	2.71628	-1.67844	0.54157
	H	1.63858	2.17463	-1.25359		H	1.64139	2.17526	-1.25343
	C	-0.10190	0.18949	-0.81190		C	-0.10037	0.19076	-0.81168
	C	0.23876	-1.02982	-0.24210		C	0.23991	-1.02982	-0.24267
	C	-0.97086	0.89379	0.14475		C	-0.97101	0.89238	0.14435
	O	-1.56894	1.92919	0.05674		O	-1.57235	1.92663	0.05759
	C	-0.41458	-1.09613	1.07536		C	-0.41569	-1.09806	1.07256
	O	-0.47580	-1.97882	1.88445		O	-0.48149	-1.98218	1.88055
	H	-0.15515	0.42210	-1.86657		H	-0.15499	0.42405	-1.86622
	H	0.50273	-1.93985	-0.76308		H	0.50375	-1.93966	-0.76425
	O	-1.02297	0.13239	1.30721		O	-1.02389	0.13039	1.30642
	H	2.13931	0.03738	2.46073		H	2.14251	0.04071	2.46280
	H	1.48851	2.37105	1.37574		H	1.49183	2.37400	1.37602
	H	3.61065	0.36646	-0.96051		H	3.61005	0.36229	-0.96803
	H	2.26530	-0.40549	-1.81533		H	2.25829	-0.40733	-1.81146
TScc 1,4-dioxane	C	1.80251	1.49052	0.82759	**TScc** $PhCH_3$	C	1.80264	1.49061	0.82771
	C	1.78030	1.35350	-0.55967		C	1.78044	1.35359	-0.55960
	C	2.14557	0.26108	1.40020		C	2.14569	0.26118	1.40031
	C	2.34559	-0.67184	0.38367		C	2.34573	-0.67178	0.38376
	C	2.54621	0.10188	-0.89061		C	2.54603	0.10184	-0.89059
	H	2.71507	-1.67853	0.54187		H	2.71521	-1.67850	0.54187
	H	1.63987	2.17493	-1.25284		H	1.64003	2.17498	-1.25286
	C	-0.09966	0.19040	-0.81155		C	-0.09968	0.19046	-0.81154
	C	0.24019	-1.02926	-0.24296		C	0.24020	-1.02929	-0.24291
	C	-0.97097	0.89455	0.14701		C	-0.97101	0.89435	0.14678
	O	-1.56449	1.93077	0.05552		O	-1.56525	1.93037	0.05564
	C	-0.41532	-1.09711	1.07593		C	-0.41540	-1.09719	1.07564
	O	-0.47243	-1.98217	1.88080		O	-0.47328	-1.98221	1.88074
	H	-0.15858	0.42338	-1.86560		H	-0.15836	0.42340	-1.86564
	H	0.50004	-1.94048	-0.76347		H	0.50025	-1.94042	-0.76353
	O	-1.02382	0.13087	1.30705		O	-1.02392	0.13080	1.30696
	H	2.13583	0.03807	2.46079		H	2.13646	0.03830	2.46097
	H	1.48507	2.37084	1.37436		H	1.48571	2.37113	1.37452
	H	3.61231	0.36391	-0.96628		H	3.61215	0.36375	-0.96650
	H	2.26247	-0.40656	-1.81233		H	2.26213	-0.40661	-1.81224
TScc	C	1.80425	1.49184	0.82931					

$ClCH_2CH_2Cl$	C 1.78211 1.35489 -0.55857 C 2.14702 0.26246 1.40187 C 2.34686 -0.67105 0.38494 C 2.54358 0.10143 -0.89003 H 2.71637 -1.67829 0.54176 H 1.64177 2.17560 -1.25312 C -0.10062 0.19076 -0.81181 C 0.23996 -1.03000 -0.24255 C -0.97166 0.89180 0.14365 O -1.57416 1.92572 0.05748 C -0.41627 -1.09846 1.07195 O -0.48333 -1.98246 1.88034 H -0.15573 0.42292 -1.86665 H 0.50287 -1.93971 -0.76498 O -1.02481 0.12989 1.30590 H 2.14479 0.04151 2.46339 H 1.49426 2.37502 1.37664 H 3.61004 0.36187 -0.96878 H 2.25849 -0.40699 -1.81125		

BMK+IDSCRF/6-31G(d)

Species	Cartesian coordinates	Species	Cartesian coordinates
TSaa $CHCl_3$	C -4.21006 -0.01840 -1.46806 C -3.07168 0.21273 -0.66139 C -1.86108 0.81606 -1.15950 C -3.05013 -0.25577 0.67951 C -1.81794 -0.08678 1.40840 C -0.93757 0.99579 1.08806 C -0.96502 1.47418 -0.25677 C -5.31555 -0.66102 -0.92970 C -4.16836 -0.94850 1.19832 H -1.71363 -0.57294 2.37870 C 0.03617 1.50406 1.99322 C -0.02997 2.46395 -0.67003 C 0.87245 2.97751 0.24192 C 0.90988 2.49073 1.57866 H 0.07260 1.11353 3.00911 H -0.04745 2.81515 -1.70084 H 1.56881 3.75659 -0.06384 H 1.63972 2.89779 2.27608 C -5.29444 -1.12667 0.40749 H -4.21260 0.32320 -2.50250 H -1.79376 1.04695 -2.22304 H -6.20290 -0.81869 -1.54022	**TSaa** THF	C -4.20931 -0.01831 -1.47086 C -3.07184 0.21383 -0.66281 C -1.86311 0.82122 -1.15957 C -3.05074 -0.25585 0.67786 C-1.81899 -0.08672 1.40805 C -0.93909 0.99708 1.08867 C -0.96496 1.47512 -0.25657 C -5.31415 -0.66321 -0.93376 C -4.16839 -0.95033 1.19546 H -1.71727 -0.57055 2.37993 C 0.03122 1.50793 1.99579 C -0.02966 2.46512 -0.66898 C 0.87067 2.98005 0.24445 C 0.90489 2.49532 1.58203 H 0.06420 1.11993 3.01290 H -0.04629 2.81654 -1.69986 H 1.56725 3.75931 -0.06061 H 1.63173 2.90496 2.28125 C -5.29359 -1.12960 0.40326 H -4.21172 0.32473 -2.50493 H -1.79554 1.05280 -2.22314 H -6.20088 -0.82179 -1.54510

	H -4.13952 -1.32554 2.21997		H -4.14024 -1.32739 2.21725
	H -6.16613 -1.63751 0.81290		H -6.16518 -1.64161 0.80765
	N 1.36321 -0.85443 -0.31067		N 1.36388 -0.85287 -0.30408
	C 0.56387 -0.60747 -1.42589		C 0.56363 -0.61644 -1.42079
	C 0.55464 -1.38510 0.69157		C 0.55773 -1.37886 0.70143
	N -0.76838 -1.52133 0.14312		N -0.76555 -1.51985 0.15487
	N -0.76267 -1.06573 -1.10668		N -0.76086 -1.07367 -1.09859
	O 0.90344 -0.15364 -2.48852		O 0.90434 -0.17139 -2.48735
	O 0.88383 -1.72440 1.79978		O 0.88845 -1.71189 1.81143
	C 2.75998 -0.61133 -0.21091		C 2.76138 -0.61131 -0.20939
	C 3.57349 -1.52789 0.47151		C 3.57728 -1.53347 0.46254
	C 3.31488 0.53052 -0.80655		C 3.31384 0.53423 -0.79987
	C 4.94861 -1.29080 0.56116		C 4.95302 -1.29783 0.54770
	C 4.69416 0.74642 -0.72077		C 4.69366 0.74909 -0.71874
	C 5.51465 -0.15801 -0.03642		C 5.51660 -0.16067 -0.04421
	H 3.13222 -2.40729 0.93090		H 3.13767 -2.41672 0.91656
	H 2.67307 1.23044 -1.33187		H 2.66975 1.23794 -1.31771
	H 5.57751 -2.00172 1.09438		H 5.58421 -2.01295 1.07267
	H 5.12440 1.63019 -1.18896		H 5.12234 1.63621 -1.18212
	H 6.58718 0.01681 0.02809		H 6.58951 0.01352 0.01707
TSaa **1,4-dioxane**	C -4.18916 0.06787 -1.50655	**TSaa** **$PhCH_3$**	C -4.21097 -0.01228 -1.46608
	C -3.05518 0.25046 -0.67903		C -3.07113 0.21335 -0.66035
	C -1.84748 0.88198 -1.13630		C -1.85757 0.81201 -1.15774
	C -3.05710 -0.27043 0.64250		C -3.05013 -0.25759 0.67931
	C -1.81763 -0.16206 1.38392		C -1.81560 -0.09443 1.40598
	C -0.94279 0.95433 1.12427		C -0.93627 0.99049 1.08976
	C -0.93450 1.46215 -0.21069		C -0.96378 1.47171 -0.25374
	C -5.30878 -0.58030 -1.00777		C -5.31830 -0.65203 -0.92862
	C -4.18889 -0.96551 1.11944		C -4.17004 -0.94803 1.19698
	H -1.75655 -0.64378 2.35937		H -1.70904 -0.58520 2.37339
	C 0.00687 1.43877 2.06375		C 0.04034 1.49348 1.99469
	C 0.03794 2.43463 -0.58564		C -0.02634 2.45995 -0.66527
	C 0.92921 2.91214 0.35402		C 0.87866 2.96859 0.24646
	C 0.91089 2.41415 1.68701		C 0.91652 2.47816 1.58174
	H 0.01258 1.03170 3.07296		H 0.07988 1.09733 3.00796
	H 0.05164 2.80245 -1.61079		H -0.04234 2.81168 -1.69568
	H 1.65749 3.67177 0.07632		H 1.57734 3.74565 -0.05845
	H 1.62628 2.79833 2.41155		H 1.64980 2.87951 2.27853
	C -5.30947 -1.09701 0.30995		C -5.29737 -1.12093 0.40722
	H -4.17495 0.45055 -2.52617		H -4.21286 0.33051 -2.49990
	H -1.75400 1.13004 -2.19407		H -1.78732 1.04106 -2.22115
	H -6.19014 -0.70261 -1.63449		H -6.20635 -0.80547 -1.53886
	H -4.17683 -1.38559 2.12426		H -4.14088 -1.32869 2.21702
	H -6.19201 -1.61144 0.68569		H -6.16977 -1.63053 0.81213

	N 1.35806 -0.90263 -0.26205 C 0.52464 -0.78304 -1.38314 C 0.58435 -1.32037 0.80989 N -0.75938 -1.50815 0.30419 N -0.78552 -1.20193 -0.99022 O 0.84888 -0.44260 -2.49178 O 0.92945 -1.54267 1.94129 C 2.74894 -0.61713 -0.22242 C 3.60126 -1.42177 0.54820 C 3.25957 0.46004 -0.96118 C 4.96972 -1.13608 0.58100 C 4.63237 0.72346 -0.92991 C 5.49144 -0.06858 -0.15909 H 3.19573 -2.25061 1.12022 H 2.58792 1.07268 -1.55350 H 5.62849 -1.75988 1.18251 H 5.02761 1.55502 -1.51081 H 6.55890 0.14325 -0.13700		N 1.36255 -0.85992 -0.31534 C 0.56043 -0.60488 -1.42772 C 0.55410 -1.38659 0.69005 N -0.77151 -1.52049 0.14275 N -0.76715 -1.06386 -1.10602 O 0.89504 -0.14115 -2.48657 O 0.88283 -1.72269 1.79839 C 2.75789 -0.61145 -0.21440 C 3.57170 -1.51460 0.48528 C 3.31212 0.52276 -0.82529 C 4.94572 -1.27244 0.57527 C 4.69034 0.74337 -0.73839 C 5.51114 -0.14807 -0.03806 H 3.13104 -2.38654 0.95854 H 2.67004 1.21220 -1.36317 H 5.57444 -1.97311 1.12177 H 5.11976 1.62051 -1.21936 H 6.58294 0.03023 0.02668
TSaa $ClCH_2CH_2Cl$	C -4.19587 -0.04158 -1.47701 C -3.06644 0.20385 -0.66259 C -1.85171 0.80357 -1.15769 C -3.05563 -0.24881 0.68412 C -1.83402 -0.06211 1.42545 C -0.95189 1.01620 1.09837 C -0.96707 1.47704 -0.25285 C -5.30352 -0.68286 -0.94084 C -4.17622 -0.93944 1.20161 H -1.73710 -0.53862 2.40167 C 0.00805 1.54102 2.00899 C -0.03294 2.46661 -0.66752 C 0.85649 2.99640 0.24878 C 0.88080 2.52780 1.59228 H 0.03054 1.16765 3.03192 H -0.04076 2.80533 -1.70271 H 1.55213 3.77570 -0.05863 H 1.59877 2.94947 2.29359 C -5.29384 -1.13233 0.40212 H -4.19046 0.28708 -2.51573 H -1.77929 1.02957 -2.22208 H -6.18446 -0.85168 -1.55789 H -4.15629 -1.30109 2.22917 H -6.16774 -1.64165 0.80505 N 1.36797 -0.84547 -0.30095 C 0.56836 -0.60438 -1.41471	**TSab** $CHCl_3$	C -4.28952 0.06253 -1.47991 C -3.13873 0.31794 -0.68525 C -2.07313 1.13023 -1.15404 C -3.02659 -0.26543 0.61399 C -1.73602 -0.13630 1.29343 C -0.93743 1.05800 1.01108 C -1.06425 1.63238 -0.29082 C -5.32269 -0.70271 -0.96493 C -4.07912 -1.05429 1.10879 H -1.70293 -0.49804 2.32527 C 0.03918 1.55414 1.89145 C -0.17857 2.66703 -0.69831 C 0.76432 3.15313 0.19215 C 0.86404 2.60353 1.49045 H 0.14730 1.11494 2.88170 H -0.26651 3.07851 -1.70282 H 1.43485 3.95646 -0.10617 H 1.60558 2.99632 2.18419 C -5.22083 -1.25058 0.33395 H -4.35196 0.48990 -2.47968 H -2.11039 1.49749 -2.18244 H -6.21429 -0.88891 -1.56017 H -3.99635 -1.50931 2.09433 H -6.04088 -1.84667 0.73098 C -0.69258 -1.51831 0.40919 C -0.55704 -1.29627 -1.03307

	C 0.56132 -1.37390 0.70487 N -0.75985 -1.51654 0.16007 N -0.75686 -1.06222 -1.09137 O 0.90696 -0.15559 -2.48064 O 0.89618 -1.70886 1.81344 C 2.76778 -0.61536 -0.21240 C 3.58287 -1.55985 0.42834 C 3.32263 0.54024 -0.78014 C 4.96101 -1.33606 0.50657 C 4.70455 0.74419 -0.70606 C 5.52682 -0.18773 -0.06142 H 3.14085 -2.45218 0.86219 H 2.67844 1.25960 -1.27612 H 5.59226 -2.06880 1.00664 H 5.13558 1.63971 -1.15083 H 6.60145 -0.02230 -0.00536		C 0.56043 -1.45592 1.16442 N 1.52953 -1.38770 1.79138 C -1.43925 -2.72171 0.78142 N -2.04550 -3.65099 1.10666 C -1.46655 -1.90506 -1.93954 N -2.23848 -2.38893 -2.66283 C 0.57629 -0.61101 -1.54830 N 1.49691 -0.02273 -1.94774
TSab **THF**	C -4.29057 0.06475 -1.48020 C -3.13916 0.31961 -0.68568 C -2.07747 1.13711 -1.15301 C -3.02592 -0.26554 0.61310 C -1.73925 -0.13210 1.29632 C -0.93729 1.05750 1.01026 C -1.06519 1.63359 -0.29120 C -5.32268 -0.70221 -0.96599 C -4.07823 -1.05570 1.10740 H -1.70559 -0.49486 2.32790 C 0.04032 1.55299 1.89050 C -0.17974 2.66904 -0.69834 C 0.76427 3.15361 0.19157 C 0.86507 2.60229 1.48950 H 0.14670 1.11490 2.88156 H -0.27056 3.08314 -1.70169 H 1.43392 3.95819 -0.10579 H 1.60643 2.99541 2.18347 C -5.21973 -1.25191 0.33247 H -4.35444 0.49575 -2.47849 H -2.11956 1.51145 -2.17888 H -6.21523 -0.88721 -1.56041 H -3.99605 -1.50894 2.09394 H -6.04007 -1.84784 0.72954 C -0.68830 -1.52486 0.40873 C -0.55339 -1.30321 -1.03188 C 0.56259 -1.45758 1.16528 N 1.53350 -1.38470 1.78901	**TSab** **1,4-dixoane**	C -4.20563 -0.07240 -1.43947 C -3.08187 0.20459 -0.62986 C -1.86237 0.79332 -1.13666 C -3.06066 -0.23463 0.72391 C -1.83998 -0.02104 1.45547 C -0.98030 1.08315 1.11996 C -1.00053 1.52296 -0.23363 C -5.29820 -0.73230 -0.89259 C -4.16294 -0.95060 1.24839 H -1.75424 -0.45638 2.45342 C -0.05691 1.65041 2.03007 C -0.10225 2.52683 -0.65833 C 0.76200 3.10653 0.26106 C 0.78586 2.66734 1.60515 H -0.02531 1.29172 3.05744 H -0.10163 2.84350 -1.69990 H 1.43887 3.89626 -0.05906 H 1.48141 3.12244 2.30743 C -5.27643 -1.17287 0.45109 H -4.20913 0.24171 -2.48181 H -1.82648 1.05528 -2.19662 H -6.17429 -0.92629 -1.50833 H -4.13126 -1.30929 2.27576 H -6.13568 -1.70270 0.85738 C -0.63035 -1.55549 0.20786 C -0.68902 -1.05148 -1.16265 C 0.59857 -1.41865 0.94574 N 1.56477 -1.27264 1.56908

	C -1.43829 -2.72450 0.78284 N -2.04818 -3.65278 1.10429 C -1.46379 -1.91017 -1.93835 N -2.23394 -2.39613 -2.66222 C 0.57844 -0.61660 -1.54805 N 1.50021 -0.03084 -1.94869		C -1.42704 -2.70193 0.56052 N -2.09880 -3.59353 0.87232 C -1.49475 -1.78281 -2.11722 N -2.16828 -2.32466 -2.88769 C 0.52338 -0.50420 -1.73344 N 1.46830 -0.02045 -2.19602
TSab **$PhCH_3$**	C -4.20506 -0.07316 -1.43925 C -3.08155 0.20391 -0.62948 C -1.86159 0.79203 -1.13640 C -3.06084 -0.23454 0.72456 C -1.84118 -0.01967 1.45708 C -0.98051 1.08324 1.12065 C -1.00011 1.52229 -0.23321 C -5.29799 -0.73250 -0.89226 C -4.16345 -0.95006 1.24918 H -1.75561 -0.45481 2.45517 C -0.05748 1.65097 2.03095 C -0.10177 2.52590 -0.65809 C 0.76206 3.10615 0.26145 C 0.78543 2.66769 1.60580 H -0.02677 1.29318 3.05870 H -0.10083 2.84213 -1.69983 H 1.43887 3.89593 -0.05877 H 1.48052 3.12347 2.30814 C -5.27674 -1.17246 0.45164 H -4.20824 0.24058 -2.48174 H -1.82607 1.05461 -2.19628 H -6.17408 -0.92636 -1.50810 H -4.13232 -1.30770 2.27697 H -6.13642 -1.70163 0.85795 C -0.62953 -1.55627 0.20642 C -0.68970 -1.05029 -1.16341 C 0.59920 -1.41876 0.94398 N 1.56578 -1.27238 1.56672 C -1.42652 -2.70223 0.55888 N -2.09846 -3.59394 0.87013 C -1.49473 -1.78249 -2.11812 N -2.16728 -2.32549 -2.88859 C 0.52317 -0.50401 -1.73457 N 1.46863 -0.02167 -2.19744	**TSab** **$ClCH_2CH_2Cl$**	C -4.28930 0.06241 -1.47954 C -3.13808 0.31781 -0.68470 C -2.07545 1.13379 -1.15272 C -3.02668 -0.26451 0.61563 C -1.74271 -0.12802 1.30087 C -0.93859 1.05819 1.01268 C -1.06434 1.63168 -0.29026 C -5.32261 -0.70224 -0.96423 C -4.07994 -1.05359 1.11064 H -1.70661 -0.49427 2.33114 C 0.03830 1.55484 1.89364 C -0.17841 2.66677 -0.69768 C 0.76379 3.15319 0.19317 C 0.86312 2.60370 1.49230 H 0.14306 1.11782 2.88545 H -0.26807 3.07955 -1.70176 H 1.43303 3.95827 -0.10405 H 1.60289 2.99874 2.18698 C -5.22101 -1.25000 0.33547 H -4.35227 0.49191 -2.47862 H -2.11537 1.50508 -2.17990 H -6.21548 -0.88666 -1.55849 H -3.99828 -1.50504 2.09816 H -6.04263 -1.84374 0.73335 C -0.68584 -1.52728 0.40391 C -0.55320 -1.30243 -1.03525 C 0.56390 -1.45727 1.16067 N 1.53594 -1.38230 1.78248 C -1.43794 -2.72469 0.77804 N -2.04968 -3.65263 1.09716 C -1.46264 -1.90993 -1.94269 N -2.23101 -2.39761 -2.66717 C 0.57904 -0.61671 -1.55235 N 1.50189 -0.03315 -1.95350
TSac **$CHCl_3$**	C -4.22861 -0.06441 -1.45573 C -3.08267 0.18690 -0.65744 C -1.87984 0.79476 -1.16752 C -3.04999 -0.27469 0.68805	**TSac** **THF**	C -4.22834 -0.06308 -1.45607 C -3.08199 0.18731 -0.65794 C -1.88002 0.79638 -1.16839 C -3.04878 -0.27502 0.68731

	C -1.81413 -0.09303 1.40806 C -0.96799 1.02328 1.08312 C -0.99935 1.48409 -0.26498 C -5.31882 -0.72284 -0.91205 C -4.16224 -0.98086 1.21396 H -1.73137 -0.52462 2.40761 C -0.02969 1.58158 1.99209 C -0.09283 2.49587 -0.68159 C 0.78338 3.05383 0.23142 C 0.81489 2.59439 1.57472 H 0.00413 1.21271 3.01636 H -0.10821 2.83028 -1.71806 H 1.46239 3.84496 -0.08192 H 1.51761 3.03838 2.27769 C -5.28552 -1.18366 0.42973 H -4.24519 0.27952 -2.48959 H -1.84713 1.06746 -2.22419 H -6.20765 -0.89273 -1.51746 H -4.12783 -1.34269 2.24126 H -6.14879 -1.70321 0.84237 C -0.73285 -1.61842 0.17075 C -0.75541 -1.17078 -1.15914 C 0.64146 -1.36548 0.68175 O 1.14507 -1.63908 1.73385 C 0.60052 -0.63917 -1.45455 O 1.06633 -0.20798 -2.47088 H -1.32763 -2.42022 0.59304 H -1.37738 -1.55092 -1.96114 O 1.34377 -0.68542 -0.29158		C -1.81224 -0.09462 1.40683 C -0.96615 1.02210 1.08202 C -0.99814 1.48390 -0.26576 C -5.31863 -0.72102 -0.91175 C -4.16100 -0.98076 1.21383 H -1.73060 -0.52549 2.40688 C -0.02949 1.58186 1.99185 C -0.09331 2.49779 -0.68151 C 0.78151 3.05707 0.23229 C 0.81324 2.59692 1.57549 H 0.00334 1.21357 3.01650 H -0.11020 2.83388 -1.71755 H 1.45830 3.85068 -0.07994 H 1.51379 3.04300 2.27949 C -5.28489 -1.18231 0.42997 H -4.24486 0.28082 -2.49001 H -1.84812 1.06930 -2.22513 H -6.20788 -0.89052 -1.51680 H -4.12597 -1.34342 2.24090 H -6.14831 -1.70161 0.84287 C -0.73321 -1.61968 0.17206 C -0.75516 -1.17375 -1.15889 C 0.64164 -1.36912 0.68122 O 1.14811 -1.64389 1.73209 C 0.60027 -0.64437 -1.45502 O 1.06899 -0.21515 -2.47138 H -1.32875 -2.42081 0.59487 H -1.37900 -1.55258 -1.96021 O 1.34429 -0.68963 -0.29213
TSac **1,4-dioxane**	C -4.23216 -0.06408 -1.45536 C -3.08617 0.18900 -0.65771 C -1.88467 0.79873 -1.16738 C -3.05173 -0.27486 0.68707 C -1.81457 -0.09405 1.40510 C -0.96998 1.02360 1.08184 C -1.00336 1.48649 -0.26552 C -5.32079 -0.72561 -0.91289 C -4.16282 -0.98351 1.21174 H -1.72861 -0.52805 2.40302 C -0.02811 1.57804 1.98917 C -0.09214 2.49348 -0.68337 C 0.78805 3.04710 0.22794 C 0.81933 2.58769 1.57104 H 0.00912 1.20586 3.01182	**TSac** **$PhCH_3$**	C -4.22942 -0.06633 -1.45510 C -3.08332 0.18559 -0.65754 C -1.87993 0.79282 -1.16732 C -3.05060 -0.27555 0.68820 C -1.81468 -0.09335 1.40756 C -0.96871 1.02265 1.08289 C -1.00073 1.48379 -0.26498 C -5.31975 -0.72454 -0.91163 C -4.16358 -0.98028 1.21418 H -1.72969 -0.52585 2.40629 C -0.02922 1.57991 1.99099 C -0.09265 2.49346 -0.68250 C 0.78468 3.05033 0.22966 C 0.81614 2.59137 1.57289 H 0.00754 1.20871 3.01403

	H -0.10442 2.82466 -1.72062		H -0.10528 2.82458 -1.71978
	H 1.47222 3.83266 -0.08729		H 1.46630 3.83836 -0.08500
	H 1.52628 3.02701 2.27229		H 1.52108 3.03308 2.27471
	C -5.28617 -1.18768 0.42818		C -5.28678 -1.18405 0.43032
	H -4.24998 0.28082 -2.48874		H -4.24636 0.27708 -2.48899
	H -1.85063 1.07029 -2.22402		H -1.84497 1.06438 -2.22397
	H -6.20930 -0.89627 -1.51818		H -6.20834 -0.89454 -1.51702
	H -4.12811 -1.34589 2.23871		H -4.13004 -1.34036 2.24200
	H -6.14824 -1.70883 0.84080		H -6.15017 -1.70253 0.84359
	C -0.73380 -1.61397 0.17373		C -0.73309 -1.61784 0.16887
	C -0.75301 -1.17046 -1.15645		C -0.75433 -1.16809 -1.15952
	C 0.64101 -1.35619 0.68840		C 0.64063 -1.36126 0.68435
	O 1.13573 -1.62486 1.74469		O 1.13751 -1.63439 1.73863
	C 0.60139 -0.62934 -1.44869		C 0.60175 -0.62940 -1.45107
	O 1.06041 -0.18907 -2.46287		O 1.06227 -0.19111 -2.46554
	H -1.32547 -2.41783 0.59587		H -1.32719 -2.42080 0.58908
	H -1.37364 -1.54949 -1.95948		H -1.37285 -1.54959 -1.96319
	O 1.34280 -0.67760 -0.28483		O 1.34226 -0.67849 -0.28707
TSac $ClCH_2CH_2Cl$	C -4.22815 -0.06259 -1.45626	**TSba** $CHCl_3$	N 0.80625 0.33237 0.60334
	C -3.08155 0.18742 -0.65826		C 0.06189 1.45565 0.28357
	C -1.88020 0.79745 -1.16886		C 0.07692 -0.42130 1.53880
	C -3.04806 -0.27526 0.68694		N -1.12732 0.28434 1.81047
	C -1.81118 -0.09549 1.40613		N -1.16395 1.36577 1.05921
	C -0.96525 1.02153 1.08144		O 0.35302 2.37592 -0.43690
	C -0.99757 1.48389 -0.26617		O 0.42147 -1.44973 2.06528
	C -5.31845 -0.72027 -0.91158		C 2.10223 0.01533 0.11200
	C -4.16033 -0.98064 1.21385		C 2.44433 -1.32498 -0.12183
	H -1.72996 -0.52596 2.40645		C 3.02777 1.04130 -0.13022
	C -0.02933 1.58195 1.99172		C 3.72224 -1.63428 -0.59768
	C -0.09344 2.49873 -0.68152		C 4.29774 0.71629 -0.61784
	C 0.78071 3.05859 0.23268		C 4.65136 -0.61791 -0.85092
	C 0.81252 2.59806 1.57588		H 1.72464 -2.11063 0.08657
	H 0.00297 1.21389 3.01655		H 2.75297 2.07518 0.05348
	H -0.11113 2.83572 -1.71732		H 3.98768 -2.67533 -0.77355
	H 1.45644 3.85342 -0.07897		H 5.01267 1.51476 -0.80917
	H 1.51194 3.04518 2.28042		H 5.64405 -0.86475 -1.22320
	C -5.28450 -1.18166 0.43018		C -2.54842 -1.10407 0.62010
	H -4.24462 0.28121 -2.49027		C -3.47298 0.06341 0.22300
	H -1.84837 1.07017 -2.22570		C -2.58233 -0.75867 -1.69665
	H -6.20791 -0.88965 -1.51642		C -1.95113 -1.52812 -0.53203
	H -4.12497 -1.34363 2.24083		H -2.51096 -1.58918 1.58755
	H -6.14801 -1.70076 0.84326		H -1.13533 -2.23964 -0.63319
	C -0.73353 -1.62030 0.17260		C -4.00504 -0.49410 -1.13743
	C -0.75509 -1.17512 -1.15880		H -4.56330 0.24946 -1.72051

	C	0.64134	-1.37086	0.68118	H	-4.59261	-1.41272	-1.01610
	O	1.14906	-1.64600	1.73157	C	-2.52063	1.16998	-0.31860
	C	0.59990	-0.64672	-1.45530	H	-2.74296	2.23079	-0.25828
	O	1.07008	-0.21809	-2.47152	C	-1.92920	0.58362	-1.44942
	H	-1.32958	-2.42118	0.59537	H	-1.12768	1.01075	-2.04704
	H	-1.37975	-1.55350	-1.95980	H	-4.19905	0.38769	0.97034
	O	1.34441	-0.69173	-0.29230	H	-2.46106	-1.18809	-2.69207
TSba **THF**	N	0.81036	0.32883	0.56573	**TSba** **1,4-dioxane**	N	0.81993	0.31488	0.58323
	C	0.06863	1.45162	0.23867		C	0.07279	1.43249	0.24854
	C	0.08912	-0.40817	1.51856		C	0.08515	-0.43887	1.51625
	N	-1.10977	0.30849	1.79214		N	-1.11905	0.27189	1.78449
	N	-1.14774	1.38062	1.02917		N	-1.15321	1.34778	1.02832
	O	0.35862	2.35782	-0.49998		O	0.35984	2.34499	-0.48193
	O	0.43602	-1.42844	2.05919		O	0.42249	-1.47005	2.03887
	C	2.11349	0.01729	0.09113		C	2.12414	0.00757	0.10893
	C	2.44276	-1.31210	-0.20903		C	2.48717	-1.33073	-0.10493
	C	3.05998	1.04107	-0.06176		C	3.03960	1.04196	-0.13534
	C	3.73273	-1.61504	-0.65631		C	3.77398	-1.62828	-0.56430
	C	4.34169	0.72498	-0.52362		C	4.31868	0.72812	-0.60513
	C	4.68428	-0.60044	-0.81772		C	4.69252	-0.60340	-0.81989
	H	1.70283	-2.09722	-0.08288		H	1.77724	-2.12315	0.10957
	H	2.79090	2.06703	0.17286		H	2.75118	2.07454	0.03186
	H	3.98973	-2.64823	-0.88376		H	4.05466	-2.66780	-0.72356
	H	5.07450	1.52098	-0.64523		H	5.02508	1.53396	-0.79634
	H	5.68606	-0.84200	-1.16875		H	5.69245	-0.84031	-1.17847
	C	-2.55652	-1.08544	0.64336		C	-2.56084	-1.11084	0.61151
	C	-3.47646	0.08308	0.23384		C	-3.47993	0.07090	0.23697
	C	-2.62871	-0.79778	-1.68027		C	-2.63417	-0.75047	-1.70089
	C	-1.98233	-1.54178	-0.50904		C	-1.99256	-1.53605	-0.55386
	H	-2.51542	-1.55417	1.61892		H	-2.50555	-1.59679	1.57732
	H	-1.17614	-2.26469	-0.60784		H	-1.18838	-2.25726	-0.67411
	C	-4.03787	-0.50309	-1.10363		C	-4.04377	-0.47265	-1.11583
	H	-4.59694	0.23251	-1.69589		H	-4.60294	0.28034	-1.68568
	H	-4.63428	-1.41102	-0.94970		H	-4.63986	-1.38508	-0.98952
	C	-2.52269	1.16228	-0.35392		C	-2.52627	1.17169	-0.31653
	H	-2.72024	2.22877	-0.31205		H	-2.74262	2.23285	-0.24837
	C	-1.95363	0.54055	-1.47443		C	-1.96232	0.58462	-1.46115
	H	-1.15505	0.94103	-2.09454		H	-1.16778	1.00946	-2.06912
	H	-4.18624	0.43316	0.98520		H	-4.18669	0.39850	1.00103
	H	-2.52839	-1.25138	-2.66732		H	-2.53766	-1.17567	-2.70088
TSba **$PhCH_3$**	N	0.82010	0.31561	0.58360	**TSba** **$ClCH_2CH_2Cl$**	N	0.80830	0.33084	0.58693
	C	0.07250	1.43359	0.25086		C	0.06430	1.45687	0.27639
	C	0.08568	-0.43972	1.51526		C	0.08475	-0.42321	1.52414
	N	-1.11847	0.27011	1.78478		N	-1.11518	0.28645	1.80793

	N	-1.15314	1.34768	1.03072	N	-1.15366	1.37088	1.06134
	O	0.35949	2.34710	-0.47852	O	0.35276	2.37576	-0.44751
	O	0.42344	-1.47154	2.03672	O	0.43199	-1.45357	2.04638
	C	2.12401	0.00843	0.10835	C	2.10731	0.01993	0.10036
	C	2.48620	-1.32978	-0.10743	C	2.44428	-1.31578	-0.16305
	C	3.04010	1.04270	-0.13403	C	3.04099	1.04722	-0.10088
	C	3.77312	-1.62751	-0.56634	C	3.72758	-1.62022	-0.62775
	C	4.31925	0.72874	-0.60364	C	4.31659	0.72795	-0.57774
	C	4.69243	-0.60277	-0.81984	C	4.66581	-0.60234	-0.83988
	H	1.77548	-2.12207	0.10497	H	1.71474	-2.10085	0.01403
	H	2.75212	2.07520	0.03472	H	2.76787	2.07734	0.10773
	H	4.05330	-2.66699	-0.72693	H	3.99055	-2.65762	-0.82781
	H	5.02626	1.53440	-0.79348	H	5.03927	1.52666	-0.73692
	H	5.69251	-0.83986	-1.17796	H	5.66279	-0.84524	-1.20358
	C	-2.56175	-1.10954	0.61241	C	-2.55892	-1.09146	0.63480
	C	-3.48015	0.07215	0.23640	C	-3.47519	0.07995	0.22527
	C	-2.63461	-0.75232	-1.70054	C	-2.60743	-0.78637	-1.68753
	C	-1.99279	-1.53603	-0.55242	C	-1.97161	-1.53778	-0.51545
	H	-2.50944	-1.59604	1.57816	H	-2.53002	-1.57169	1.60515
	H	-1.18867	-2.25751	-0.67160	H	-1.16350	-2.25898	-0.61199
	C	-4.04409	-0.47280	-1.11594	C	-4.02220	-0.49645	-1.12265
	H	-4.60282	0.27981	-1.68672	H	-4.57575	0.24358	-1.71463
	H	-4.64064	-1.38480	-0.98856	H	-4.61968	-1.40587	-0.98196
	C	-2.52522	1.17088	-0.31837	C	-2.51422	1.16211	-0.34412
	H	-2.73928	2.23263	-0.25160	H	-2.70911	2.22888	-0.29494
	C	-1.96108	0.58196	-1.46173	C	-1.93317	0.54839	-1.46350
	H	-1.16591	1.00489	-2.07029	H	-1.12762	0.95208	-2.07247
	H	-4.18663	0.40151	0.99996	H	-4.19284	0.42430	0.97174
	H	-2.53801	-1.17899	-2.69989	H	-2.49649	-1.23264	-2.67677
TSbb $CHCl_3$	C	0.88176	-0.18981	-1.94295	**TSbb** **THF**	C	0.87937	-0.18884	-1.94694
	C	0.89223	1.04847	-1.23021		C	0.88999	1.04879	-1.23460
	C	2.21953	1.04710	0.31826		C	2.22098	1.04741	0.32449
	C	2.07497	-0.29892	1.09102		C	2.07743	-0.29972	1.09504
	C	4.26191	-0.14786	0.48639		C	4.26325	-0.14729	0.48662
	C	3.55899	1.05168	-0.10439		C	3.55910	1.05423	-0.09940
	H	1.78541	1.98469	0.67421		H	1.78229	1.98420	0.67728
	H	4.02329	1.79318	-0.75464		H	4.02367	1.79871	-0.74630
	C	3.46484	-0.31144	1.81273		C	3.46860	-0.31242	1.81449
	H	3.67621	-1.26405	2.31297		H	3.68128	-1.26553	2.31328
	H	3.59736	0.52980	2.50455		H	3.60173	0.52831	2.50684
	C	2.33906	-1.39848	0.04713		C	2.34066	-1.39928	0.05074
	H	1.63979	-2.17563	-0.24392		H	1.64052	-2.17571	-0.24070
	C	3.61918	-1.25403	-0.36709		C	3.61977	-1.25454	-0.36561
	H	4.11737	-1.74343	-1.19997		H	4.11821	-1.74572	-1.19741

	H 1.17738 -0.40229 1.70446 H 5.35204 -0.11221 0.50343 C -0.31410 1.34063 -0.46242 N -1.24846 1.56998 0.17861 C 1.44073 2.21619 -1.91152 N 1.90923 3.14264 -2.42107 C 1.87429 -0.43477 -2.93589 N 2.71024 -0.61501 -3.72144 C -0.14419 -1.16107 -1.74783 N -0.97021 -1.96270 -1.59479		H 1.18101 -0.40384 1.71016 H 5.35346 -0.11093 0.50182 C -0.31583 1.34103 -0.46694 N -1.25275 1.56850 0.17104 C 1.44246 2.21537 -1.91346 N 1.91202 3.14015 -2.42508 C 1.87012 -0.43512 -2.94131 N 2.70209 -0.61551 -3.73100 C -0.14626 -1.16001 -1.75027 N -0.97427 -1.95959 -1.59716
TSbb **1,4-dioxane**	C 0.88357 -0.19278 -1.93291 C 0.89860 1.04807 -1.22080 C 2.21269 1.04405 0.30509 C 2.06904 -0.30242 1.07837 C 4.25886 -0.14492 0.48859 C 3.55647 1.04915 -0.11144 H 1.78594 1.98080 0.67106 H 4.01861 1.78575 -0.76804 C 3.45392 -0.31170 1.80868 H 3.66448 -1.26395 2.30972 H 3.58066 0.52918 2.50202 C 2.34148 -1.39800 0.03257 H 1.64666 -2.17708 -0.26261 C 3.62419 -1.24794 -0.37367 H 4.12431 -1.72719 -1.21093 H 1.16773 -0.40870 1.68553 H 5.34861 -0.10738 0.51281 C -0.30931 1.34687 -0.45577 N -1.23732 1.58699 0.19049 C 1.44405 2.21471 -1.90921 N 1.91614 3.14160 -2.41459 C 1.87714 -0.44021 -2.92416 N 2.72073 -0.62324 -3.70096 C -0.14358 -1.16210 -1.73304 N -0.96479 -1.96687 -1.57117	**TSbb** **$PhCH_3$**	C 0.88612 -0.19094 -1.93622 C 0.89758 1.04781 -1.22074 C 2.21541 1.04594 0.30439 C 2.06938 -0.29736 1.08260 C 4.25813 -0.14950 0.48571 C 3.55790 1.04557 -0.11567 H 1.79104 1.98518 0.66683 H 4.02110 1.77952 -0.77458 C 3.45642 -0.30897 1.80890 H 3.66513 -1.26020 2.31271 H 3.58783 0.53389 2.49896 C 2.33516 -1.39765 0.04011 H 1.63575 -2.17388 -0.25186 C 3.61721 -1.25393 -0.37004 H 4.11370 -1.73845 -1.20648 H 1.16943 -0.39858 1.69265 H 5.34808 -0.11524 0.50675 C -0.30997 1.33975 -0.45278 N -1.23823 1.57276 0.19573 C 1.43888 2.21793 -1.90640 N 1.90780 3.14714 -2.41047 C 1.88338 -0.43338 -2.92490 N 2.73025 -0.61095 -3.69939 C -0.13915 -1.16340 -1.74272 N -0.95945 -1.97041 -1.58748
TSbb **$ClCH_2CH_2Cl$**	C 0.87903 -0.18867 -1.94825 C 0.88918 1.04900 -1.23675 C 2.22171 1.04788 0.32761 C 2.07833 -0.29979 1.09698 C 4.26374 -0.14705 0.48644 C 3.55915 1.05570 -0.09678 H 1.78084 1.98438 0.67867 H 4.02405 1.80222 -0.74117 C 3.47029 -0.31319 1.81516	**TSbc** **$CHCl_3$**	O 0.66413 0.24551 0.46063 C 0.04683 1.47300 0.44900 C 0.05708 -0.57424 1.40797 C -1.13665 0.12421 1.90358 C -1.19062 1.36780 1.27256 O 0.48867 2.39308 -0.18027 O 0.51967 -1.65109 1.66780 C -2.55332 -1.08720 0.58991 C -3.48557 0.08586 0.20618

	H 3.68344 -1.26673 2.31295 H 3.60401 0.52707 2.50798 C 2.34071 -1.39924 0.05239 H 1.64073 -2.17626 -0.23819 C 3.61942 -1.25458 -0.36508 H 4.11786 -1.74686 -1.19629 H 1.18251 -0.40410 1.71298 H 5.35400 -0.11068 0.50056 C -0.31636 1.34118 -0.46914 N -1.25459 1.56757 0.16732 C 1.44317 2.21490 -1.91487 N 1.91314 3.13889 -2.42757 C 1.86898 -0.43538 -2.94331 N 2.69885 -0.61639 -3.73505 C -0.14695 -1.15946 -1.75168 N -0.97635 -1.95775 -1.59929		C -2.62135 -0.71235 -1.73231 C -1.96713 -1.48294 -0.59331 H -2.62618 -1.70243 1.48091 H -1.14484 -2.18408 -0.71510 C -4.03458 -0.45024 -1.15703 H -4.59295 0.30718 -1.72135 H -4.62695 -1.36705 -1.04596 C -2.50509 1.18086 -0.31107 H -2.68994 2.25170 -0.25038 C -1.93416 0.60474 -1.44971 H -1.10725 1.00743 -2.03096 H -4.20852 0.40382 0.96085 H -2.50846 -1.12508 -2.73558 H -1.63518 2.26495 1.68983 H -1.62875 -0.17043 2.82220
TSbc **THF**	O 0.66389 0.24496 0.46205 C 0.04664 1.47209 0.44848 C 0.05658 -0.57246 1.41260 C -1.13498 0.12685 1.90693 C -1.19119 1.36835 1.27120 O 0.49079 2.39094 -0.18186 O 0.52263 -1.64814 1.67426 C -2.55366 -1.09094 0.58703 C -3.48458 0.08385 0.20689 C -2.62226 -0.71146 -1.73387 C -1.96802 -1.48501 -0.59630 H -2.62228 -1.70337 1.48036 H -1.14705 -2.18732 -0.72075 C -4.03492 -0.44888 -1.15701 H -4.59298 0.31019 -1.71944 H -4.62811 -1.36533 -1.04741 C -2.50376 1.17947 -0.30911 H -2.69191 2.25005 -0.24989 C -1.93393 0.60434 -1.44946 H -1.10827 1.00780 -2.03216 H -4.20638 0.40121 0.96292 H -2.51010 -1.12266 -2.73792 H -1.63576 2.26617 1.68747 H -1.63147 -0.16768 2.82335	**TSbc** **1,4-dioxane**	O 0.66289 0.24798 0.45530 C 0.04557 1.47721 0.45282 C 0.05816 -0.57982 1.39295 C -1.14240 0.11430 1.89329 C -1.18837 1.36609 1.28073 O 0.48098 2.40136 -0.17265 O 0.51269 -1.65970 1.64633 C -2.55080 -1.07393 0.59875 C -3.48703 0.09375 0.20335 C -2.61841 -0.71602 -1.72774 C -1.96470 -1.47763 -0.58410 H -2.63825 -1.69659 1.48320 H -1.13943 -2.17638 -0.69787 C -4.03308 -0.45465 -1.15657 H -4.59289 0.29692 -1.72717 H -4.62272 -1.37246 -1.03935 C -2.50835 1.18575 -0.32047 H -2.68041 2.25765 -0.25311 C -1.93501 0.60612 -1.45319 H -1.10501 1.00592 -2.03144 H -4.21228 0.41482 0.95453 H -2.50407 -1.13441 -2.72837 H -1.63679 2.25929 1.70118 H -1.62139 -0.18254 2.81798
TSbc **$PhCH_3$**	O 0.66309 0.25000 0.45514 C 0.04471 1.47839 0.45308 C 0.05901 -0.57833 1.39359 C -1.14101 0.11483 1.89448	**TSbc** **$ClCH_2CH_2Cl$**	O 0.66431 0.24603 0.46237 C 0.04663 1.47310 0.44923 C 0.05651 -0.57169 1.41254 C -1.13465 0.12710 1.90692

	C	-1.18971	1.36585	1.28012		C	-1.19120	1.36877	1.27114
	O	0.47982	2.40320	-0.17190		O	0.49235	2.39217	-0.18010
	O	0.51565	-1.65765	1.64636		O	0.52360	-1.64750	1.67332
	C	-2.55203	-1.07595	0.59791		C	-2.55393	-1.09160	0.58681
	C	-3.48669	0.09318	0.20353		C	-3.48430	0.08368	0.20706
	C	-2.61898	-0.71632	-1.72807		C	-2.62253	-0.71179	-1.73409
	C	-1.96629	-1.47967	-0.58476		C	-1.96838	-1.48560	-0.59659
	H	-2.63770	-1.69710	1.48357		H	-2.62311	-1.70367	1.48045
	H	-1.14189	-2.17938	-0.69918		H	-1.14852	-2.18914	-0.72176
	C	-4.03335	-0.45320	-1.15680		C	-4.03498	-0.44867	-1.15688
	H	-4.59198	0.29972	-1.72683		H	-4.59285	0.31070	-1.71908
	H	-4.62444	-1.37019	-1.04043		H	-4.62852	-1.36490	-1.04729
	C	-2.50644	1.18456	-0.31910		C	-2.50347	1.17897	-0.30915
	H	-2.67936	2.25661	-0.25443		H	-2.69177	2.24958	-0.24964
	C	-1.93367	0.60442	-1.45240		C	-1.93341	0.60351	-1.44932
	H	-1.10351	1.00367	-2.03087		H	-1.10804	1.00679	-2.03264
	H	-4.21159	0.41449	0.95494		H	-4.20573	0.40121	0.96337
	H	-2.50503	-1.13410	-2.72901		H	-2.51046	-1.12288	-2.73822
	H	-1.63891	2.25857	1.70088		H	-1.63690	2.26636	1.68686
	H	-1.62082	-0.18258	2.81855		H	-1.63174	-0.16750	2.82305
TSca $CHCl_3$	C	-0.76622	1.13696	1.54538	**TSca** THF	C	-0.76216	1.13791	1.54730
	C	-1.40458	0.98294	0.30783		C	-1.40899	0.98449	0.31532
	C	-0.36605	2.49205	1.68828		C	-0.35943	2.49335	1.68798
	C	-0.77447	3.20209	0.56484		C	-0.77405	3.20384	0.56788
	C	-1.76003	2.35959	-0.20884		C	-1.76006	2.36075	-0.20409
	H	-0.60109	4.25895	0.38328		H	-0.60193	4.26101	0.38593
	H	-1.86125	0.06500	-0.05003		H	-1.86863	0.06714	-0.04063
	N	0.34514	0.99525	-0.87751		N	0.34671	0.99249	-0.88331
	N	0.77183	2.23628	-0.86563		N	0.77410	2.23226	-0.87276
	C	1.25577	0.16737	-0.09914		C	1.25678	0.16525	-0.10363
	O	1.16995	-1.02553	0.02080		O	1.17193	-1.02808	0.01565
	C	1.97554	2.30902	-0.07525		C	1.97799	2.30508	-0.08281
	O	2.64407	3.29527	0.08590		O	2.64971	3.29050	0.07302
	N	2.25084	1.01371	0.37278		N	2.25133	1.01136	0.36872
	H	0.24087	2.88755	2.49848		H	0.25036	2.88850	2.49640
	H	-0.51895	0.32863	2.22847		H	-0.51430	0.33028	2.23122
	H	-2.77789	2.60320	0.14276		H	-2.77791	2.60741	0.14587
	H	-1.72346	2.47533	-1.29369		H	-1.72427	2.47451	-1.28928
	C	3.38440	0.62608	1.13834		C	3.38358	0.62478	1.13693
	C	3.82923	1.45107	2.18114		C	3.82221	1.44854	2.18319
	C	4.04831	-0.57254	0.84058		C	4.05187	-0.57084	0.83737
	C	4.94926	1.07032	2.92687		C	4.94143	1.06933	2.93107
	C	5.15852	-0.94718	1.60417		C	5.16109	-0.94427	1.60318
	C	5.61405	-0.12943	2.64533		C	5.61086	-0.12762	2.64790

	H	3.31164	2.38191	2.39492		H	3.29979	2.37663	2.39845
	H	3.69674	-1.20280	0.02929		H	3.70406	-1.19928	0.02275
	H	5.29651	1.71413	3.73311		H	5.28418	1.71177	3.74043
	H	5.67004	-1.88065	1.37591		H	5.67640	-1.87551	1.37393
	H	6.48114	-0.42513	3.23328		H	6.47721	-0.42217	3.23767
TSca	C	-0.77267	1.13247	1.54208	**TSca**	C	-0.76780	1.10739	1.52755
1,4-dioxane	C	-1.39731	0.97964	0.29600	**$PhCH_3$**	C	-1.38686	0.96399	0.27765
	C	-0.37720	2.48755	1.69072		C	-0.38957	2.46469	1.69540
	C	-0.77635	3.19853	0.56402		C	-0.79304	3.18516	0.57521
	C	-1.76000	2.35740	-0.21465		C	-1.76586	2.34331	-0.21568
	H	-0.60129	4.25504	0.38457		H	-0.63194	4.24647	0.41149
	H	-1.84800	0.06119	-0.06704		H	-1.82207	0.04406	-0.10047
	N	0.34186	1.00226	-0.86836		N	0.36037	1.03418	-0.88557
	N	0.76630	2.24495	-0.85330		N	0.76899	2.28123	-0.83517
	C	1.25582	0.17194	-0.09495		C	1.27501	0.19743	-0.12344
	O	1.16912	-1.02014	0.02334		O	1.19799	-0.99809	-0.03273
	C	1.97220	2.31748	-0.06412		C	1.96638	2.34831	-0.03221
	O	2.63456	3.30508	0.10536		O	2.61173	3.34137	0.17066
	N	2.25152	1.01895	0.37667		N	2.26011	1.04217	0.37579
	H	0.22639	2.88196	2.50347		H	0.20652	2.85603	2.51513
	H	-0.52405	0.32176	2.22128		H	-0.51163	0.29111	2.19729
	H	-2.77919	2.59646	0.13521		H	-2.78793	2.56670	0.13614
	H	-1.71820	2.47717	-1.29876		H	-1.72449	2.47785	-1.29814
	C	3.38627	0.62933	1.13905		C	3.39101	0.64296	1.14013
	C	3.84306	1.45791	2.17406		C	3.88877	1.49120	2.14050
	C	4.04044	-0.57643	0.84798		C	4.00063	-0.59484	0.88468
	C	4.96295	1.07373	2.91790		C	5.00366	1.09345	2.88518
	C	5.15070	-0.95382	1.60972		C	5.10731	-0.98226	1.64645
	C	5.61719	-0.13294	2.64306		C	5.61414	-0.14305	2.64557
	H	3.33639	2.39530	2.38271		H	3.42006	2.45366	2.31868
	H	3.68254	-1.21081	0.04339		H	3.60451	-1.24610	0.11227
	H	5.31885	1.72133	3.71706		H	5.39048	1.75623	3.65713
	H	5.65366	-1.89277	1.38580		H	5.57555	-1.94500	1.44981
	H	6.48432	-0.43114	3.22933		H	6.47781	-0.45020	3.23234
TSca	C	-0.75908	1.13887	1.54905	**TScb**	C	2.50942	0.22195	-0.51524
$ClCH_2CH_2Cl$	C	-1.41166	0.98524	0.32119	**$CHCl_3$**	C	1.61236	-0.07580	-1.55268
	C	-0.35477	2.49477	1.68751		C	2.36864	-0.74312	0.50173
	C	-0.77352	3.20490	0.56933		C	1.38033	-1.66442	0.12170
	C	-1.75984	2.36086	-0.20104		C	1.12976	-1.49128	-1.35585
	H	-0.60128	4.26184	0.38581		H	1.10992	-2.55560	0.68494
	H	-1.87266	0.06785	-0.03312		H	1.54950	0.46332	-2.49605
	N	0.34799	0.99125	-0.88840		C	-0.43648	-0.30579	0.54808
	N	0.77558	2.23007	-0.87787		C	-0.29403	0.67744	-0.48481
	C	1.25770	0.16407	-0.10806		H	2.86701	-0.71923	1.46743

	O	1.17396	-1.02965	0.00934	H	3.13388	1.10994	-0.46018
	C	1.97874	2.30312	-0.08635	H	1.82395	-2.16137	-1.89483
	O	2.65128	3.28842	0.06793	H	0.12158	-1.72043	-1.71356
	N	2.25064	1.01024	0.36715	C	-0.13964	0.05813	1.91400
	H	0.25742	2.89011	2.49415	N	0.10372	0.34292	3.00954
	H	-0.51045	0.33201	2.23372	C	0.14540	2.00823	-0.13555
	H	-2.77770	2.61022	0.14722	N	0.50387	3.07454	0.13841
	H	-1.72359	2.47239	-1.28647	C	-1.12609	0.59455	-1.66160
	C	3.38236	0.62401	1.13647	N	-1.77474	0.51916	-2.61815
	C	3.81749	1.44675	2.18496	C	-1.40928	-1.36104	0.39151
	C	4.05330	-0.56974	0.83555	N	-2.17162	-2.22295	0.25987
	C	4.93641	1.06841	2.93380				
	C	5.16207	-0.94251	1.60245				
	C	5.60862	-0.12676	2.64934				
	H	3.29224	2.37305	2.40156				
	H	3.70782	-1.19715	0.01903				
	H	5.27659	1.70993	3.74501				
	H	5.67954	-1.87240	1.37238				
	H	6.47463	-0.42074	3.23998				
TScb **THF**	C	2.50913	0.22183	-0.51535	**TScb** **1,4-dioxane**	C	2.50724	0.22224	-0.51410
	C	1.61532	-0.07753	-1.55431		C	1.60343	-0.07165	-1.54832
	C	2.36884	-0.74424	0.50176		C	2.36688	-0.74211	0.50182
	C	1.38448	-1.66790	0.12004		C	1.37219	-1.65918	0.12430
	C	1.13104	-1.49212	-1.35639		C	1.12708	-1.49086	-1.35563
	H	1.11411	-2.55938	0.68316		H	1.10168	-2.54975	0.68773
	H	1.55272	0.46178	-2.49779		H	1.54026	0.46804	-2.49090
	C	-0.43998	-0.30270	0.54958		C	-0.43165	-0.30967	0.54614
	C	-0.29687	0.67938	-0.48290		C	-0.28893	0.67467	-0.48799
	H	2.86824	-0.72106	1.46710		H	2.86247	-0.71628	1.46846
	H	3.13417	1.10958	-0.46036		H	3.12850	1.11190	-0.45739
	H	1.82482	-2.16190	-1.89668		H	1.82677	-2.15717	-1.89111
	H	0.12252	-1.72141	-1.71344		H	0.12032	-1.72272	-1.71507
	C	-0.14116	0.06001	1.91500		C	-0.13531	0.05515	1.91256
	N	0.10174	0.34634	3.01028		N	0.11270	0.33508	3.00822
	C	0.14389	2.00973	-0.13477		C	0.14974	2.00620	-0.13811
	N	0.50119	3.07615	0.14038		N	0.51336	3.07179	0.13149
	C	-1.12676	0.59491	-1.66080		C	-1.12415	0.59334	-1.66355
	N	-1.77635	0.51783	-2.61659		N	-1.76967	0.52038	-2.62234
	C	-1.41042	-1.35945	0.39200		C	-1.40780	-1.36292	0.39074
	N	-2.17324	-2.22073	0.25876		N	-2.16765	-2.22736	0.26175
TScb **$PhCH_3$**	C	2.50750	0.22220	-0.51423	**TScb** **$ClCH_2CH_2Cl$**	C	2.50991	0.22170	-0.51548
	C	1.60439	-0.07212	-1.54882		C	1.61784	-0.07846	-1.55522
	C	2.36706	-0.74217	0.50180		C	2.36958	-0.74473	0.50182
	C	1.37300	-1.65969	0.12404		C	1.38685	-1.66930	0.11943

	C	1.12742	-1.49093	-1.35567	C	1.13166	-1.49207	-1.35630
	H	1.10262	-2.55035	0.68748	H	1.11616	-2.56088	0.68235
	H	1.54135	0.46753	-2.49149	H	1.55487	0.46093	-2.49869
	C	-0.43207	-0.30934	0.54631	C	-0.44124	-0.30184	0.54992
	C	-0.28944	0.67494	-0.48769	C	-0.29826	0.67999	-0.48222
	H	2.86304	-0.71660	1.46832	H	2.86933	-0.72176	1.46706
	H	3.12921	1.11162	-0.45777	H	3.13519	1.10938	-0.46046
	H	1.82657	-2.15766	-1.89144	H	1.82269	-2.16321	-1.89863
	H	0.12057	-1.72264	-1.71508	H	0.12222	-1.71985	-1.71184
	C	-0.13580	0.05545	1.91269	C	-0.14214	0.06089	1.91513
	N	0.11158	0.33598	3.00835	N	0.10006	0.34860	3.01022
	C	0.14923	2.00640	-0.13781	C	0.14261	2.01018	-0.13416
	N	0.51220	3.07208	0.13234	N	0.49883	3.07670	0.14208
	C	-1.12440	0.59351	-1.66332	C	-1.12696	0.59496	-1.66071
	N	-1.77038	0.52044	-2.62180	N	-1.77701	0.51715	-2.61614
	C	-1.40797	-1.36271	0.39083	C	-1.41078	-1.35917	0.39220
	N	-2.16821	-2.22678	0.26166	N	-2.17396	-2.22005	0.25832
TScc **$CHCl_3$**	C	1.80021	1.49815	0.83337	**TScc** **THF**	C	1.80096	1.50095	0.83349
	C	1.79099	1.36502	-0.56055		C	1.79274	1.36650	-0.56049
	C	2.14875	0.25625	1.41036		C	2.14766	0.25926	1.41203
	C	2.36371	-0.67584	0.38753		C	2.36292	-0.67406	0.39038
	C	2.55445	0.10121	-0.89895		C	2.55281	0.10050	-0.89725
	H	2.72602	-1.68972	0.54120		H	2.72436	-1.68810	0.54557
	H	1.63937	2.18566	-1.25800		H	1.64270	2.18618	-1.25950
	C	-0.11495	0.18149	-0.82714		C	-0.11518	0.18175	-0.82746
	C	0.22451	-1.04226	-0.25527		C	0.22556	-1.04274	-0.25701
	C	-0.97584	0.89306	0.15108		C	-0.97529	0.89111	0.15176
	O	-1.56881	1.93098	0.06861		O	-1.57126	1.92818	0.07239
	C	-0.42196	-1.09057	1.08057		C	-0.42185	-1.09403	1.07708
	O	-0.47790	-1.96628	1.89653		O	-0.48343	-1.97213	1.89084
	H	-0.15772	0.43219	-1.88136		H	-0.15859	0.43321	-1.88160
	H	0.50643	-1.95770	-0.76368		H	0.50722	-1.95721	-0.76761
	O	-1.02124	0.13427	1.30535		O	-1.01915	0.13146	1.30581
	H	2.13094	0.02966	2.47345		H	2.13505	0.03588	2.47603
	H	1.47393	2.37734	1.38332		H	1.47993	2.38277	1.38257
	H	3.62415	0.36523	-0.97729		H	3.62325	0.36010	-0.98118
	H	2.26074	-0.40940	-1.81968		H	2.25536	-0.41083	-1.81636
TScc **1,4-dioxane**	C	1.80074	1.50023	0.83209	**TScc** **$PhCH_3$**	C	1.80085	1.50032	0.83222
	C	1.79160	1.36560	-0.56137		C	1.79173	1.36568	-0.56129
	C	2.14721	0.25839	1.41052		C	2.14734	0.25848	1.41065
	C	2.36095	-0.67482	0.38903		C	2.36114	-0.67474	0.38914
	C	2.55556	0.10121	-0.89764		C	2.55537	0.10117	-0.89761
	H	2.72245	-1.68822	0.54573		H	2.72264	-1.68820	0.54574
	H	1.64143	2.18610	-1.25883		H	1.64157	2.18614	-1.25885

	C -0.11483 0.18109 -0.82747 C 0.22616 -1.04218 -0.25717 C -0.97533 0.89324 0.15452 O -1.56308 1.93238 0.07028 C -0.42132 -1.09302 1.08078 O -0.47372 -1.97213 1.89122 H -0.16308 0.43297 -1.88085 H 0.50338 -1.95859 -0.76583 O -1.01893 0.13195 1.30664 H 2.12738 0.03290 2.47351 H 1.47281 2.37931 1.38060 H 3.62574 0.36195 -0.97840 H 2.26065 -0.40962 -1.81788		C -0.11487 0.18114 -0.82747 C 0.22611 -1.04222 -0.25716 C -0.97536 0.89304 0.15429 O -1.56388 1.93196 0.07039 C -0.42139 -1.09310 1.08047 O -0.47463 -1.97217 1.89114 H -0.16285 0.43299 -1.88091 H 0.50357 -1.95853 -0.76593 O -1.01898 0.13191 1.30657 H 2.12807 0.03316 2.47372 H 1.47347 2.37961 1.38078 H 3.62557 0.36179 -0.97865 H 2.26029 -0.40969 -1.81776
TScc $ClCH_2CH_2Cl$	C 1.80097 1.50107 0.83374 C 1.79282 1.36662 -0.56033 C 2.14768 0.25939 1.41228 C 2.36305 -0.67396 0.39058 C 2.55238 0.10043 -0.89714 H 2.72448 -1.68811 0.54554 H 1.64279 2.18618 -1.25957 C -0.11533 0.18175 -0.82761 C 0.22542 -1.04291 -0.25710 C -0.97517 0.89084 0.15133 O -1.57218 1.92769 0.07272 C -0.42177 -1.09416 1.07655 O -0.48451 -1.97204 1.89087 H -0.15811 0.43316 -1.88186 H 0.50764 -1.95715 -0.76796 O -1.01897 0.13145 1.30569 H 2.13605 0.03627 2.47641 H 1.48090 2.38327 1.38288 H 3.62287 0.35988 -0.98141 H 2.25472 -0.41093 -1.81615		

M06-2x+IDSCRF/6-31G(d)

Species	Cartesian coordinates	Species	Cartesian coordinates
TSaa $CHCl_3$	C -4.20915 0.00796 -1.43884 C -3.06317 0.21395 -0.64934 C -1.85008 0.79157 -1.15654 C -3.03073 -0.26143 0.67884 C -1.78693 -0.12383 1.38377 C -0.90540 0.95008 1.06866 C -0.94686 1.43915 -0.26164 C -5.31161 -0.61683 -0.89260	**TSaa** THF	C -4.20513 0.00752 -1.44445 C -3.06139 0.21444 -0.65169 C -1.84751 0.79299 -1.15564 C -3.03309 -0.25974 0.67716 C -1.79176 -0.12125 1.38618 C -0.90842 0.95168 1.07203 C -0.94499 1.43881 -0.25918 C -5.30892 -0.61739 -0.90070

	C -4.14661 -0.93728 1.20585		C -4.15028 -0.93525 1.20188
	H -1.67279 -0.62530 2.34308		H -1.68265 -0.61952 2.34788
	C 0.10005 1.41422 1.95310		C 0.09292 1.41768 1.95985
	C 0.00307 2.40111 -0.68341		C 0.00698 2.39974 -0.67918
	C 0.93886 2.87041 0.20695		C 0.93921 2.87071 0.21429
	C 0.99295 2.36891 1.53020		C 0.98752 2.37178 1.53876
	H 0.14861 1.00850 2.95980		H 0.13599 1.01530 2.96822
	H -0.02258 2.75721 -1.70966		H -0.01542 2.75514 -1.70588
	H 1.65803 3.62070 -0.10840		H 1.65958 3.62063 -0.09944
	H 1.75365 2.73911 2.21049		H 1.74455 2.74431 2.22200
	C -5.27981 -1.09046 0.43378		C -5.28116 -1.08960 0.42641
	H -4.21802 0.35490 -2.46856		H -4.21148 0.35438 -2.47430
	H -1.79332 1.03520 -2.21590		H -1.78771 1.03570 -2.21522
	H -6.20745 -0.75621 -1.49018		H -6.20311 -0.75752 -1.50068
	H -4.10819 -1.32112 2.22168		H -4.11524 -1.31688 2.21877
	H -6.15179 -1.58946 0.84542		H -6.15445 -1.58817 0.83601
	N 1.33069 -0.83255 -0.33487		N 1.33063 -0.83089 -0.32717
	C 0.53571 -0.57844 -1.44919		C 0.53552 -0.58869 -1.44374
	C 0.52513 -1.39733 0.64978		C 0.52705 -1.39165 0.66052
	N -0.79120 -1.53430 0.08755		N -0.78903 -1.53433 0.10000
	N -0.78701 -1.05789 -1.13624		N -0.78609 -1.06595 -1.12731
	O 0.87048 -0.09746 -2.50119		O 0.87124 -0.11836 -2.50067
	O 0.84886 -1.74731 1.75645		O 0.85258 -1.73605 1.76882
	C 2.72331 -0.56864 -0.21353		C 2.72411 -0.56809 -0.21151
	C 3.52152 -1.44548 0.52198		C 3.52597 -1.44891 0.51513
	C 3.27872 0.54924 -0.83650		C 3.27606 0.55225 -0.83288
	C 4.88231 -1.18669 0.64601		C 4.88785 -1.19168 0.63172
	C 4.64389 0.78762 -0.71175		C 4.64232 0.78901 -0.71627
	C 5.44856 -0.07274 0.03108		C 5.45089 -0.07552 0.01755
	H 3.07765 -2.31334 0.99493		H 3.08426 -2.31921 0.98608
	H 2.64825 1.21466 -1.41335		H 2.64204 1.22149 -1.40155
	H 5.50213 -1.86782 1.22121		H 5.51104 -1.87575 1.19985
	H 5.07784 1.65671 -1.19712		H 5.07389 1.66016 -1.20021
	H 6.51231 0.12234 0.12791		H 6.51548 0.11831 0.10826
TSaa **1,4-dioxane**	C -4.21632 0.01399 -1.42963	**TSaa** **PhCH$_3$**	C -4.21753 0.01199 -1.42912
	C -3.06666 0.21564 -0.64520		C -3.06847 0.21631 -0.64439
	C -1.85299 0.78977 -1.15638		C -1.85605 0.79287 -1.15562
	C -3.02794 -0.26435 0.68080		C -3.02905 -0.26338 0.68175
	C -1.78045 -0.13013 1.37990		C -1.78203 -0.12666 1.38119
	C -0.90067 0.94468 1.06562		C -0.90334 0.94871 1.06617
	C -0.94921 1.43911 -0.26248		C -0.95215 1.44238 -0.26223
	C -5.31690 -0.61163 -0.88113		C -5.31684 -0.61603 -0.88078
	C -4.14173 -0.94218 1.20941		C -4.14150 -0.94353 1.21024
	H -1.65835 -0.64025 2.33342		H -1.65943 -0.63582 2.33515

	C 0.11406 1.40068 1.94414		C 0.11227 1.40442 1.94396
	C 0.00054 2.40010 -0.68611		C -0.00114 2.40178 -0.68718
	C 0.94470 2.86150 0.19885		C 0.94390 2.86281 0.19701
	C 1.00754 2.35334 1.51914		C 1.00660 2.35574 1.51784
	H 0.17143 0.98679 2.94685		H 0.16917 0.99177 2.94723
	H -0.02920 2.75816 -1.71128		H -0.03122 2.75951 -1.71248
	H 1.66496 3.60962 -0.11870		H 1.66504 3.60970 -0.12151
	H 1.77709 2.71460 2.19400		H 1.77664 2.71695 2.19218
	C -5.27870 -1.09132 0.44258		C -5.27790 -1.09537 0.44307
	H -4.22925 0.36391 -2.45812		H -4.23106 0.36195 -2.45761
	H -1.79938 1.03562 -2.21490		H -1.80320 1.03849 -2.21428
	H -6.21549 -0.74742 -1.47507		H -6.21500 -0.75396 -1.47490
	H -4.09786 -1.33240 2.22239		H -4.09715 -1.33333 2.22338
	H -6.14852 -1.59217 0.85608		H -6.14678 -1.59796 0.85651
	N 1.33059 -0.83876 -0.35264		N 1.33098 -0.83513 -0.34981
	C 0.53462 -0.55563 -1.45975		C 0.53524 -0.55442 -1.45764
	C 0.52015 -1.41047 0.62659		C 0.52080 -1.40643 0.62952
	N -0.79737 -1.53353 0.06182		N -0.79650 -1.53036 0.06491
	N -0.79070 -1.03890 -1.15340		N -0.78979 -1.03684 -1.15091
	O 0.86512 -0.04713 -2.49907		O 0.86639 -0.04826 -2.49804
	O 0.84024 -1.77238 1.72943		O 0.84096 -1.76718 1.73286
	C 2.72094 -0.56991 -0.21938		C 2.72207 -0.56928 -0.21838
	C 3.51295 -1.43475 0.53715		C 3.51384 -1.43745 0.53449
	C 3.28200 0.54216 -0.84851		C 3.28395 0.54302 -0.84630
	C 4.87079 -1.16941 0.67611		C 4.87251 -1.17506 0.67128
	C 4.64423 0.78702 -0.70724		C 4.64700 0.78488 -0.70749
	C 5.44198 -0.06086 0.05658		C 5.44456 -0.06623 0.05297
	H 3.06584 -2.29660 1.01699		H 3.06606 -2.29970 1.01311
	H 2.65819 1.19613 -1.44475		H 2.66008 1.19950 -1.43978
	H 5.48459 -1.84142 1.26797		H 5.48625 -1.84952 1.26042
	H 5.08155 1.65119 -1.19805		H 5.08505 1.64922 -1.19736
	H 6.50345 0.13922 0.16565		H 6.50666 0.13152 0.16034
TSaa $ClCH_2CH_2Cl$	C -4.20340 0.00755 -1.44674	**TSab** $CHCl_3$	C -4.19923 -0.06502 -1.44073
	C -3.06038 0.21468 -0.65280		C -3.08370 0.21865 -0.63177
	C -1.84638 0.79375 -1.15559		C -1.88065 0.82175 -1.13431
	C -3.03369 -0.25911 0.67632		C -3.05291 -0.23312 0.70794
	C -1.79310 -0.12076 1.38663		C -1.82206 -0.03994 1.42301
	C -0.90909 0.95193 1.07291		C -0.98084 1.07965 1.10284
	C -0.94370 1.43833 -0.25863		C -1.01146 1.53096 -0.23703
	C -5.30772 -0.61730 -0.90385		C -5.27329 -0.74644 -0.90334
	C -4.15145 -0.93427 1.20030		C -4.13817 -0.96372 1.22538
	H -1.68593 -0.61772 2.34929		H -1.73756 -0.47348 2.42054
	C 0.09023 1.41892 1.96231		C -0.04972 1.62660 2.00459
	C 0.00907 2.39891 -0.67786		C -0.11024 2.52425 -0.66188

	C 0.93966 2.87071 0.21703 C 0.98542 2.37295 1.54203 H 0.13088 1.01801 2.97140 H -0.01199 2.75412 -1.70471 H 1.66050 3.62054 -0.09595 H 1.74068 2.74674 2.22661 C -5.28151 -1.08891 0.42359 H -4.20890 0.35457 -2.47658 H -1.78541 1.03588 -2.21534 H -6.20135 -0.75766 -1.50467 H -4.11770 -1.31493 2.21764 H -6.15537 -1.58713 0.83252 N 1.33048 -0.83145 -0.32369 C 0.53509 -0.59449 -1.44109 C 0.52777 -1.38938 0.66589 N -0.78826 -1.53483 0.10621 N -0.78572 -1.07107 -1.12304 O 0.87115 -0.12844 -2.50005 O 0.85394 -1.73039 1.77523 C 2.72416 -0.56814 -0.21041 C 3.52802 -1.45002 0.51271 C 3.27394 0.55337 -0.83139 C 4.89025 -1.19281 0.62582 C 4.64057 0.79009 -0.71854 C 5.45130 -0.07567 0.01150 H 3.08764 -2.32138 0.98315 H 2.63801 1.22377 -1.39662 H 5.51531 -1.87763 1.19108 H 5.07065 1.66219 -1.20219 H 6.51619 0.11809 0.09927		C 0.76794 3.07965 0.24754 C 0.79811 2.63084 1.58100 H -0.01225 1.25717 3.02563 H -0.11949 2.84762 -1.69906 H 1.45206 3.86060 -0.06954 H 1.50505 3.07076 2.27753 C -5.24277 -1.19581 0.42992 H -4.20582 0.26052 -2.47726 H -1.84389 1.08225 -2.19306 H -6.14528 -0.95079 -1.51680 H -4.09776 -1.33175 2.24681 H -6.09162 -1.74160 0.82993 C -0.66671 -1.50733 0.24176 C -0.69955 -1.04445 -1.13298 C 0.56883 -1.38164 0.96688 N 1.54512 -1.23616 1.57146 C -1.45150 -2.66280 0.58402 N -2.12069 -3.56069 0.87695 C -1.51675 -1.76716 -2.06988 N -2.21308 -2.31200 -2.81695 C 0.50447 -0.48683 -1.68733 N 1.45424 0.01114 -2.12301
TSab **THF**	C -4.19911 -0.06466 -1.44062 C -3.08295 0.21760 -0.63200 C -1.88049 0.82167 -1.13487 C -3.05235 -0.23387 0.70791 C -1.82279 -0.03921 1.42446 C -0.98038 1.07883 1.10280 C -1.01074 1.52987 -0.23726 C -5.27396 -0.74456 -0.90250 C -4.13824 -0.96324 1.22602 H -1.73910 -0.47168 2.42273 C -0.05031 1.62678 2.00516 C -0.11059 2.52428 -0.66186 C 0.76633 3.08094 0.24824 C 0.79650 2.63213 1.58182	**TSab** **1,4-dixoane**	C -4.19946 -0.06595 -1.44063 C -3.08506 0.22062 -0.63128 C -1.88028 0.82077 -1.13328 C -3.05393 -0.23145 0.70808 C -1.82058 -0.04128 1.42002 C -0.98184 1.08127 1.10289 C -1.01288 1.53300 -0.23660 C -5.27192 -0.75032 -0.90461 C -4.13767 -0.96503 1.22411 H -1.73422 -0.47721 2.41590 C -0.04819 1.62580 2.00327 C -0.10958 2.52415 -0.66173 C 0.77103 3.07708 0.24636 C 0.80163 2.62783 1.57939

	H -0.01428 1.25828 3.02672 H -0.12110 2.84865 -1.69884 H 1.44875 3.86383 -0.06811 H 1.50181 3.07393 2.27899 C -5.24347 -1.19398 0.43087 H -4.20614 0.26240 -2.47678 H -1.84415 1.08285 -2.19367 H -6.14717 -0.94669 -1.51514 H -4.09823 -1.32969 2.24816 H -6.09350 -1.73764 0.83159 C -0.66518 -1.50941 0.24066 C -0.69874 -1.04554 -1.13375 C 0.57055 -1.38330 0.96465 N 1.54892 -1.23708 1.56576 C -1.45011 -2.66468 0.58176 N -2.11983 -3.56349 0.87078 C -1.51503 -1.76963 -2.07017 N -2.21029 -2.31818 -2.81553 C 0.50602 -0.48945 -1.68771 N 1.45818 0.00561 -2.12146		H -0.00733 1.25371 3.02290 H -0.11609 2.84530 -1.69932 H 1.45844 3.85416 -0.07219 H 1.51222 3.06343 2.27450 C -5.24104 -1.19993 0.42828 H -4.20508 0.25609 -2.47796 H -1.84234 1.07937 -2.19201 H -6.14139 -0.95915 -1.51964 H -4.09584 -1.33683 2.24381 H -6.08713 -1.75053 0.82682 C -0.66939 -1.50375 0.24306 C -0.70134 -1.04179 -1.13176 C 0.56498 -1.37722 0.97125 N 1.53612 -1.22978 1.58351 C -1.45564 -2.65823 0.58794 N -2.12687 -3.55193 0.88875 C -1.52022 -1.76207 -2.06973 N -2.21890 -2.29981 -2.81971 C 0.50165 -0.48125 -1.68654 N 1.44698 0.02262 -2.12501
TSab **$PhCH_3$**	C -4.19949 -0.06576 -1.44066 C -3.08498 0.22050 -0.63135 C -1.88043 0.82105 -1.13339 C -3.05384 -0.23160 0.70803 C -1.82069 -0.04119 1.42025 C -0.98174 1.08113 1.10285 C -1.01279 1.53288 -0.23665 C -5.27209 -0.74988 -0.90452 C -4.13772 -0.96490 1.22418 H -1.73451 -0.47691 2.41629 C -0.04834 1.62588 2.00337 C -0.10969 2.52425 -0.66175 C 0.77071 3.07738 0.24646 C 0.80128 2.62815 1.57952 H -0.00781 1.25407 3.02315 H -0.11650 2.84566 -1.69930 H 1.45780 3.85485 -0.07194 H 1.51151 3.06417 2.27478 C -5.24123 -1.19951 0.42840 H -4.20524 0.25668 -2.47790 H -1.84265 1.07990 -2.19212 H -6.14182 -0.95826 -1.51939 H -4.09604 -1.33634 2.24406 H -6.08759 -1.74964 0.82708	**TSab** **$ClCH_2CH_2Cl$**	C -4.19911 -0.06433 -1.44066 C -3.08263 0.21724 -0.63217 C -1.88069 0.82210 -1.13521 C -3.05202 -0.23426 0.70778 C -1.82296 -0.03910 1.42497 C -0.98014 1.07839 1.10266 C -1.01049 1.52945 -0.23745 C -5.27433 -0.74349 -0.90219 C -4.13822 -0.96302 1.22620 H -1.73955 -0.47122 2.42352 C -0.05057 1.62683 2.00531 C -0.11085 2.52442 -0.66193 C 0.76546 3.08169 0.24848 C 0.79562 2.63285 1.58213 H -0.01522 1.25876 3.02711 H -0.12203 2.84928 -1.69881 H 1.44701 3.86558 -0.06749 H 1.50005 3.07565 2.27965 C -5.24383 -1.19295 0.43124 H -4.20632 0.26354 -2.47663 H -1.84461 1.08369 -2.19402 H -6.14818 -0.94446 -1.51441 H -4.09838 -1.32874 2.24868 H -6.09450 -1.73546 0.83235

	C -0.66918 -1.50402 0.24303 C -0.70112 -1.04214 -1.13185 C 0.56537 -1.37774 0.97086 N 1.53710 -1.23075 1.58230 C -1.45513 -2.65874 0.58764 N -2.12591 -3.55304 0.88765 C -1.51986 -1.76267 -2.06966 N -2.21830 -2.30122 -2.81928 C 0.50196 -0.48189 -1.68657 N 1.44779 0.02132 -2.12472		C -0.66452 -1.51036 0.24037 C -0.69810 -1.04648 -1.13409 C 0.57151 -1.38427 0.96360 N 1.55124 -1.23784 1.56244 C -1.44932 -2.66577 0.58072 N -2.11913 -3.56532 0.86725 C -1.51427 -1.77115 -2.06995 N -2.20960 -2.32180 -2.81371 C 0.50696 -0.49085 -1.68750 N 1.46056 0.00306 -2.11942
TSac **$CHCl_3$**	C -4.21759 -0.07331 -1.45067 C -3.08226 0.18482 -0.65211 C -1.88274 0.78471 -1.15895 C -3.05143 -0.27166 0.68563 C -1.82278 -0.08995 1.40243 C -0.97927 1.01896 1.07872 C -1.00969 1.47577 -0.26138 C -5.30011 -0.73326 -0.91317 C -4.15571 -0.98078 1.20589 H -1.73735 -0.52222 2.39926 C -0.02857 1.55610 1.97766 C -0.08848 2.46265 -0.68308 C 0.80255 2.99720 0.21792 C 0.83264 2.54171 1.55527 H 0.00656 1.18180 2.99729 H -0.09991 2.78956 -1.71941 H 1.49848 3.76765 -0.10010 H 1.55183 2.96672 2.24895 C -5.26897 -1.18981 0.42273 H -4.23031 0.26824 -2.48265 H -1.84502 1.05124 -2.21507 H -6.18346 -0.91054 -1.51930 H -4.12018 -1.34244 2.23047 H -6.12866 -1.71363 0.82969 C -0.73932 -1.59286 0.17492 C -0.76798 -1.14483 -1.14618 C 0.61109 -1.29900 0.70114 O 1.10768 -1.55106 1.76172 C 0.56375 -0.57258 -1.43752 O 1.01449 -0.12002 -2.45083 H -1.31916 -2.40405 0.59410 H -1.37561 -1.53901 -1.94942 O 1.30391 -0.58832 -0.26594	**TSac** **THF**	C -4.21700 -0.07294 -1.45082 C -3.08158 0.18467 -0.65216 C -1.88210 0.78448 -1.15933 C -3.05078 -0.27176 0.68563 C -1.82229 -0.09019 1.40280 C -0.97814 1.01822 1.07855 C -1.00856 1.47499 -0.26160 C -5.29976 -0.73228 -0.91289 C -4.15522 -0.98041 1.20631 H -1.73762 -0.52222 2.39990 C -0.02839 1.55652 1.97795 C -0.08836 2.46305 -0.68300 C 0.80175 2.99879 0.21842 C 0.83188 2.54328 1.55588 H 0.00545 1.18339 2.99818 H -0.10113 2.79119 -1.71905 H 1.49601 3.77116 -0.09894 H 1.54939 2.97030 2.25023 C -5.26867 -1.18876 0.42313 H -4.22932 0.26819 -2.48301 H -1.84507 1.05144 -2.21547 H -6.18328 -0.90944 -1.51893 H -4.11942 -1.34233 2.23085 H -6.12858 -1.71235 0.83014 C -0.73949 -1.59420 0.17452 C -0.76820 -1.14592 -1.14683 C 0.61052 -1.30154 0.70013 O 1.10969 -1.55447 1.75975 C 0.56318 -0.57494 -1.43830 O 1.01651 -0.12332 -2.45136 H -1.32011 -2.40491 0.59389 H -1.37658 -1.53965 -1.94991 O 1.30373 -0.59030 -0.26664
TSac	C -4.21827 -0.07570 -1.45051	**TSac**	C -4.21799 -0.07509 -1.45047

1,4-dioxane				**$PhCH_3$**			
	C	-3.08402	0.18512 -0.65159		C	-3.08323	0.18464 -0.65186
	C	-1.88366	0.78439 -1.15738		C	-1.88299	0.78380 -1.15787
	C	-3.05356	-0.27077 0.68630		C	-3.05275	-0.27132 0.68606
	C	-1.82524	-0.08802 1.40307		C	-1.82454	-0.08882 1.40298
	C	-0.98301	1.02184 1.08062		C	-0.98174	1.02051 1.08014
	C	-1.01326	1.47816 -0.25958		C	-1.01200	1.47687 -0.26008
	C	-5.30025	-0.73736 -0.91435		C	-5.30040	-0.73575 -0.91390
	C	-4.15751	-0.98118 1.20530		C	-4.15719	-0.98074 1.20548
	H	-1.73844	-0.52108 2.39918		H	-1.73768	-0.52206 2.39902
	C	-0.02868	1.55517 1.97771		C	-0.02876	1.55529 1.97779
	C	-0.08853	2.46085 -0.68285		C	-0.08867	2.46107 -0.68282
	C	0.80560	2.99200 0.21659		C	0.80418	2.99362 0.21716
	C	0.83563	2.53691 1.55374		C	0.83426	2.53846 1.55432
	H	0.00935	1.17845 2.99605		H	0.00923	1.17862 2.99618
	H	-0.09669	2.78390 -1.72013		H	-0.09696	2.78429 -1.72008
	H	1.50663	3.75646 -0.10384		H	1.50373	3.75973 -0.10267
	H	1.55938	2.95693 2.24532		H	1.55659	2.96001 2.24650
	C	-5.26967	-1.19291 0.42157		C	-5.26979	-1.19139 0.42206
	H	-4.23113	0.26564 -2.48241		H	-4.23081	0.26624 -2.48240
	H	-1.84402	1.05035 -2.21332		H	-1.84318	1.04963 -2.21386
	H	-6.18261	-0.91615 -1.52112		H	-6.18313	-0.91371 -1.52041
	H	-4.12324	-1.34124 2.23033		H	-4.12283	-1.34092 2.23048
	H	-6.12879	-1.71744 0.82836		H	-6.12927	-1.71515 0.82913
	C	-0.73893	-1.58914 0.17471		C	-0.73866	-1.59077 0.17431
	C	-0.76844	-1.13987 -1.14517		C	-0.76819	-1.14180 -1.14565
	C	0.61223	-1.29263 0.70261		C	0.61227	-1.29385 0.70209
	O	1.10295	-1.54358 1.76493		O	1.10336	-1.54424 1.76452
	C	0.56441	-0.56472 -1.43642		C	0.56428	-0.56621 -1.43682
	O	1.00885	-0.10954 -2.45012		O	1.00890	-0.11054 -2.45037
	H	-1.31750	-2.40066 0.59417		H	-1.31689	-2.40263 0.59369
	H	-1.37470	-1.53453 -1.94886		H	-1.37432	-1.53687 -1.94927
	O	1.30357	-0.58184 -0.26488		O	1.30364	-0.58313 -0.26539
TSac	C	-4.21647	-0.07295 -1.45090	**TSba**	N	0.76582	0.34232 0.63549
$ClCH_2CH_2Cl$	C	-3.08104	0.18441 -0.65216	**$CHCl_3$**	C	0.04717	1.50814 0.38798
	C	-1.88145	0.78397 -1.15950		C	0.01592	-0.45567 1.49588
	C	-3.05037	-0.27183 0.68572		N	-1.19077	0.27394 1.78318
	C	-1.82220	-0.09016 1.40332		N	-1.17388	1.40502 1.14224
	C	-0.97751	1.01778 1.07866		O	0.37378	2.44823 -0.29078
	C	-1.00786	1.47435 -0.26156		O	0.31247	-1.52907 1.95470
	C	-5.29949	-0.73172 -0.91270		C	2.04880	0.02968 0.10843
	C	-4.15503	-0.98002 1.20666		C	2.32720	-1.27414 -0.29965
	H	-1.73792	-0.52220 2.40051		C	3.01095	1.03366 0.00427
	C	-0.02836	1.55684 1.97829		C	3.58594	-1.57151 -0.81200
	C	-0.08830	2.46313 -0.68285		C	4.26058	0.72414 -0.52276

	C 0.80116 2.99972 0.21881 C 0.83129 2.54431 1.55636 H 0.00485 1.18435 2.99884 H -0.10162 2.79159 -1.71885 H 1.49451 3.77311 -0.09825 H 1.54776 2.97263 2.25107 C -5.26857 -1.18796 0.42345 H -4.22845 0.26774 -2.48326 H -1.84467 1.05120 -2.21562 H -6.18311 -0.90881 -1.51871 H -4.11921 -1.34188 2.23125 H -6.12870 -1.71123 0.83053 C -0.73948 -1.59515 0.17391 C -0.76843 -1.14638 -1.14741 C 0.61027 -1.30306 0.69922 O 1.11078 -1.55650 1.75831 C 0.56281 -0.57602 -1.43897 O 1.01735 -0.12471 -2.45188 H -1.32052 -2.40556 0.59342 H -1.37717 -1.53993 -1.95040 O 1.30362 -0.59131 -0.26732		C 4.55298 -0.57578 -0.92883 H 1.56973 -2.04440 -0.20703 H 2.77600 2.04188 0.32611 H 3.80696 -2.58688 -1.12677 H 5.01076 1.50446 -0.60728 H 5.53194 -0.81301 -1.33393 C -2.51016 -0.94196 0.73509 C -3.42557 0.15638 0.16351 C -2.49345 -0.89278 -1.61063 C -1.87720 -1.48313 -0.36743 H -2.64638 -1.45461 1.67760 H -1.06730 -2.20505 -0.35895 C -3.91528 -0.56737 -1.12084 H -4.45656 0.09634 -1.80215 H -4.50459 -1.46409 -0.90589 C -2.44827 1.15918 -0.47472 H -2.54021 2.23667 -0.45050 C -1.81549 0.44755 -1.47695 H -0.96479 0.77476 -2.06592 H -4.16934 0.56936 0.84195 H -2.34447 -1.43313 -2.54233
TSba **THF**	N 0.76404 0.35040 0.62869 C 0.04667 1.51624 0.37937 C 0.01776 -0.44231 1.49518 N -1.18755 0.28931 1.78341 N -1.17159 1.41797 1.13742 O 0.37482 2.45362 -0.30304 O 0.31673 -1.51352 1.95875 C 2.04710 0.03539 0.10289 C 2.31087 -1.26031 -0.33837 C 3.02312 1.02873 0.03512 C 3.57002 -1.56111 -0.84811 C 4.27341 0.71692 -0.48933 C 4.55130 -0.57555 -0.92866 H 1.54070 -2.02150 -0.27555 H 2.79904 2.03047 0.38474 H 3.78015 -2.57019 -1.18963 H 5.03513 1.48864 -0.54539 H 5.53050 -0.81504 -1.33201 C -2.50939 -0.93306 0.74538 C -3.42446 0.15899 0.16175 C -2.49338 -0.91052 -1.60065 C -1.87747 -1.48729 -0.35161 H -2.64955 -1.43737 1.69202	**TSba** **1,4-dioxane**	N 0.77158 0.32278 0.64739 C 0.04820 1.48951 0.40914 C 0.01290 -0.49222 1.48692 N -1.19613 0.23345 1.77964 N -1.17639 1.37307 1.15654 O 0.36960 2.43844 -0.25840 O 0.29976 -1.57626 1.92373 C 2.05572 0.01797 0.11800 C 2.37116 -1.30038 -0.21147 C 2.98517 1.04183 -0.06737 C 3.63005 -1.59040 -0.72665 C 4.23505 0.73659 -0.59566 C 4.56339 -0.57610 -0.92433 H 1.64384 -2.08692 -0.04957 H 2.72409 2.06124 0.19009 H 3.87772 -2.61703 -0.97833 H 4.95796 1.53292 -0.74341 H 5.54288 -0.80760 -1.33113 C -2.51305 -0.95866 0.71239 C -3.42910 0.15425 0.16796 C -2.50345 -0.85379 -1.63144 C -1.88254 -1.47211 -0.40442 H -2.64532 -1.48901 1.64525

	H	-1.07052	-2.21265	-0.33658	H	-1.06761	-2.18790	-0.41474
	C	-3.91491	-0.57834	-1.11454	C	-3.92308	-0.53922	-1.13058
	H	-4.45547	0.07866	-1.80279	H	-4.46666	0.13950	-1.79518
	H	-4.50498	-1.47227	-0.88992	H	-4.51203	-1.44034	-0.93345
	C	-2.44714	1.15392	-0.48894	C	-2.45006	1.17212	-0.44767
	H	-2.53434	2.23201	-0.47273	H	-2.54395	2.24832	-0.40172
	C	-1.81312	0.43060	-1.48088	C	-1.82399	0.48267	-1.47033
	H	-0.96183	0.74942	-2.07396	H	-0.97483	0.82292	-2.05369
	H	-4.16821	0.58004	0.83529	H	-4.16887	0.55202	0.85955
	H	-2.34418	-1.46118	-2.52623	H	-2.35873	-1.37253	-2.57598
TSba $PhCH_3$	N	0.77147	0.32502	0.64834	**TSba** $ClCH_2CH_2Cl$	N	0.76382	0.35386	0.62550
	C	0.04828	1.49126	0.40831		C	0.04631	1.51876	0.37431
	C	0.01313	-0.48863	1.48925		C	0.01922	-0.43640	1.49520
	N	-1.19609	0.23723	1.78051		N	-1.18541	0.29566	1.78374
	N	-1.17628	1.37599	1.15584		N	-1.17076	1.42239	1.13432
	O	0.37025	2.43918	-0.26051		O	0.37393	2.45468	-0.31065
	O	0.30086	-1.57151	1.92858		O	0.32006	-1.50614	1.96153
	C	2.05501	0.01923	0.11817		C	2.04700	0.03781	0.10033
	C	2.36667	-1.29812	-0.21849		C	2.30549	-1.25469	-0.35296
	C	2.98732	1.04151	-0.06087		C	3.02821	1.02675	0.04657
	C	3.62507	-1.58888	-0.73453		C	3.56505	-1.55703	-0.86091
	C	4.23667	0.73584	-0.59023		C	4.27901	0.71385	-0.47621
	C	4.56135	-0.57602	-0.92597		C	4.55170	-0.57568	-0.92754
	H	1.63668	-2.08343	-0.06215		H	1.53058	-2.01217	-0.30165
	H	2.72887	2.06015	0.20254		H	2.80801	2.02586	0.40644
	H	3.87004	-2.61474	-0.99199		H	3.77131	-2.56363	-1.21207
	H	4.96196	1.53092	-0.73309		H	5.04505	1.48203	-0.52142
	H	5.54041	-0.80814	-1.33348		H	5.53119	-0.81620	-1.32963
	C	-2.51283	-0.95729	0.71420		C	-2.50986	-0.93142	0.74847
	C	-3.42866	0.15439	0.16692		C	-3.42472	0.15895	0.16168
	C	-2.50161	-0.85759	-1.62980		C	-2.49418	-0.91653	-1.59729
	C	-1.88129	-1.47295	-0.40104		C	-1.87803	-1.48917	-0.34652
	H	-2.64579	-1.48611	1.64788		H	-2.64951	-1.43131	1.69758
	H	-1.06673	-2.18924	-0.40920		H	-1.07171	-2.21534	-0.33005
	C	-3.92168	-0.54223	-1.13044		C	-3.91556	-0.58233	-1.11220
	H	-4.46505	0.13488	-1.79685		H	-4.45604	0.07270	-1.80238
	H	-4.51050	-1.44303	-0.93167		H	-4.50582	-1.47537	-0.88445
	C	-2.44974	1.17089	-0.45060		C	-2.44746	1.15174	-0.49272
	H	-2.54333	2.24723	-0.40643		H	-2.53454	2.22995	-0.48032
	C	-1.82269	0.47950	-1.47118		C	-1.81338	0.42479	-1.48195
	H	-0.97341	0.81872	-2.05497		H	-0.96210	0.74105	-2.07657
	H	-4.16907	0.55351	0.85707		H	-4.16857	0.58207	0.83385
	H	-2.35600	-1.37843	-2.57306		H	-2.34497	-1.47041	-2.52093
TSbb	C	0.96636	-0.31313	-1.70825	**TSbb**	C	0.94473	-0.29223	-1.74611

$CHCl_3$				**THF**			
	C	0.87696	1.04329	-1.31998	C	0.89287	1.04267	-1.28340
	C	2.22870	1.11191	0.50116	C	2.22288	1.09525	0.44835
	C	2.04583	-0.33033	1.00342	C	2.04748	-0.33145	1.00513
	C	4.25204	-0.06248	0.56099	C	4.25370	-0.07352	0.55759
	C	3.54826	1.19241	0.11198	C	3.55131	1.15787	0.05976
	H	1.63138	1.96936	0.79177	H	1.67130	1.97293	0.77216
	H	4.02189	2.00065	-0.43583	H	4.02645	1.94846	-0.51313
	C	3.39393	-0.49366	1.76409	C	3.39391	-0.45662	1.77592
	H	3.58397	-1.52601	2.07238	H	3.58733	-1.47454	2.12675
	H	3.48474	0.18756	2.61523	H	3.47973	0.25963	2.59852
	C	2.36017	-1.19783	-0.22955	C	2.37244	-1.24269	-0.18906
	H	1.89724	-2.14909	-0.47151	H	1.85849	-2.16022	-0.45335
	C	3.67142	-0.89648	-0.54823	C	3.67599	-0.96039	-0.51939
	H	4.21010	-1.19126	-1.44328	H	4.21748	-1.28767	-1.40099
	H	1.12336	-0.55251	1.53877	H	1.12451	-0.53678	1.54639
	H	5.33581	-0.02231	0.63501	H	5.33740	-0.02931	0.63200
	C	-0.29677	1.48358	-0.61830	C	-0.29089	1.46035	-0.57442
	N	-1.22265	1.83611	-0.02002	N	-1.22214	1.79042	0.02679
	C	1.60241	2.04334	-2.04910	C	1.57342	2.07390	-2.02184
	N	2.21710	2.84370	-2.61607	N	2.14841	2.89928	-2.59321
	C	1.74593	-0.67356	-2.86093	C	1.76625	-0.62759	-2.87040
	N	2.40231	-0.97134	-3.76616	N	2.45783	-0.89851	-3.75866
	C	-0.13766	-1.18279	-1.39606	C	-0.14512	-1.17570	-1.44892
	N	-1.00400	-1.89644	-1.11591	N	-1.00686	-1.90086	-1.18086
TSbb	C	0.96473	-0.30946	-1.71359	**TSbb**	C	0.96473	-0.30983	-1.71302
1,4-dioxane	C	0.88527	1.04160	-1.30254	**$PhCH_3$**	C	0.88439	1.04165	-1.30378
	C	2.22380	1.10764	0.47782		C	2.22434	1.10798	0.47996
	C	2.04330	-0.32862	1.00045		C	2.04363	-0.32893	1.00053
	C	4.25013	-0.06588	0.55788		C	4.25046	-0.06573	0.55793
	C	3.54722	1.17932	0.08800		C	3.54741	1.18030	0.08996
	H	1.64326	1.97171	0.78206		H	1.64248	1.97159	0.78307
	H	4.01856	1.97848	-0.47459		H	4.01918	1.98038	-0.47099
	C	3.39027	-0.48107	1.76497		C	3.39075	-0.48249	1.76460
	H	3.58046	-1.50900	2.08740		H	3.58077	-1.51090	2.08558
	H	3.47984	0.21112	2.60734		H	3.48049	0.20854	2.60790
	C	2.35904	-1.20808	-0.22236		C	2.35927	-1.20719	-0.22324
	H	1.88285	-2.15138	-0.46637		H	1.88419	-2.15129	-0.46670
	C	3.66925	-0.91115	-0.54378		C	3.66950	-0.90959	-0.54462
	H	4.20498	-1.21093	-1.43843		H	4.20549	-1.20891	-1.43931
	H	1.11989	-0.54447	1.53645		H	1.12037	-0.54558	1.53653
	H	5.33360	-0.02545	0.63343		H	5.33396	-0.02525	0.63319
	C	-0.29239	1.47484	-0.59856		C	-0.29281	1.47550	-0.59976
	N	-1.21515	1.82449	0.00566		N	-1.21567	1.82567	0.00405
	C	1.59545	2.05286	-2.03525		C	1.59572	2.05229	-2.03590

	N 2.20039 2.86445 -2.59617 C 1.75704 -0.66103 -2.85915 N 2.42812 -0.95471 -3.75508 C -0.13579 -1.18450 -1.40842 N -0.99522 -1.90809 -1.13159		N 2.20093 2.86348 -2.59716 C 1.75558 -0.66175 -2.85955 N 2.42515 -0.95501 -3.75674 C -0.13585 -1.18458 -1.40707 N -0.99557 -1.90768 -1.12985
TSbb **$ClCH_2CH_2Cl$**	C 0.90730 -0.23775 -1.83536 C 0.91368 1.04355 -1.22832 C 2.21103 1.05829 0.35832 C 2.05632 -0.32568 1.02909 C 4.25300 -0.10166 0.52671 C 3.55005 1.09295 -0.03915 H 1.74330 1.97037 0.72767 H 4.01793 1.85235 -0.66091 C 3.41256 -0.37728 1.78955 H 3.61849 -1.36009 2.22268 H 3.50656 0.40753 2.54642 C 2.37164 -1.33101 -0.08432 H 1.75568 -2.17064 -0.38245 C 3.66017 -1.10896 -0.44958 H 4.19160 -1.51119 -1.30531 H 1.14108 -0.48546 1.59818 H 5.33796 -0.05394 0.58352 C -0.28846 1.40128 -0.49879 N -1.22847 1.67592 0.11442 C 1.51184 2.14299 -1.95864 N 2.02409 3.01441 -2.51930 C 1.82520 -0.52844 -2.88383 N 2.60277 -0.74918 -3.71519 C -0.15308 -1.15520 -1.58255 N -1.00336 -1.91050 -1.35723	**TSbc** **$CHCl_3$**	O 0.63087 0.22685 0.43396 C 0.01961 1.47324 0.46327 C 0.02378 -0.60016 1.36991 C -1.17726 0.09114 1.86409 C -1.18041 1.36233 1.30759 O 0.46092 2.39477 -0.16479 O 0.46922 -1.68556 1.61888 C -2.51513 -1.02214 0.61210 C -3.47094 0.11648 0.20136 C -2.61686 -0.71884 -1.71594 C -1.92970 -1.42274 -0.57710 H -2.64795 -1.68774 1.45742 H -1.09959 -2.11229 -0.69122 C -4.01579 -0.46584 -1.13148 H -4.59136 0.26263 -1.71091 H -4.58895 -1.38745 -0.99098 C -2.51904 1.19498 -0.35544 H -2.65649 2.26693 -0.27001 C -1.93346 0.59692 -1.45876 H -1.10565 0.98476 -2.04347 H -4.19121 0.44238 0.95081 H -2.50661 -1.15143 -2.70748 H -1.64211 2.24481 1.72848 H -1.63700 -0.20103 2.79806
TSbc **THF**	O 0.63028 0.22706 0.43424 C 0.01889 1.47362 0.46440 C 0.02311 -0.59952 1.37088 C -1.17695 0.09151 1.86514 C -1.18019 1.36284 1.30853 O 0.46267 2.39472 -0.16353 O 0.47105 -1.68453 1.61951 C -2.51476 -1.02259 0.61138 C -3.47017 0.11650 0.20145 C -2.61739 -0.71913 -1.71656 C -1.92953 -1.42294 -0.57802 H -2.64768 -1.68767 1.45725 H -1.10041 -2.11362 -0.69335 C -4.01586 -0.46563 -1.13119	**TSbc** **1,4-dioxane**	O 0.63185 0.22567 0.43339 C 0.02103 1.47181 0.46028 C 0.02469 -0.60250 1.36727 C -1.17851 0.09000 1.86161 C -1.18035 1.36120 1.30638 O 0.45534 2.39385 -0.16948 O 0.46265 -1.68948 1.61627 C -2.51509 -1.02010 0.61416 C -3.47237 0.11687 0.20107 C -2.61523 -0.71792 -1.71437 C -1.92931 -1.42134 -0.57470 H -2.64837 -1.68696 1.45806 H -1.09627 -2.10750 -0.68566 C -4.01525 -0.46690 -1.13180

	H	-4.59162	0.26304	-1.71019		H	-4.59082	0.26051	-1.71246
	H	-4.58924	-1.38705	-0.99029		H	-4.58733	-1.38930	-0.99177
	C	-2.51860	1.19468	-0.35619		C	-2.52031	1.19623	-0.35432
	H	-2.65620	2.26668	-0.27010		H	-2.65709	2.26800	-0.26938
	C	-1.93322	0.59627	-1.45946		C	-1.93412	0.59912	-1.45758
	H	-1.10632	0.98389	-2.04576		H	-1.10378	0.98749	-2.03794
	H	-4.18962	0.44270	0.95155		H	-4.19451	0.44197	0.94913
	H	-2.50743	-1.15174	-2.70818		H	-2.50446	-1.15079	-2.70562
	H	-1.64357	2.24497	1.72859		H	-1.63855	2.24456	1.72862
	H	-1.63835	-0.20104	2.79830		H	-1.63491	-0.20148	2.79721
TSbc $PhCH_3$	O	0.63182	0.22587	0.43358	**TSbc** $ClCH_2CH_2Cl$	O	0.62994	0.22713	0.43436
	C	0.02087	1.47198	0.46062		C	0.01850	1.47379	0.46494
	C	0.02460	-0.60220	1.36761		C	0.02273	-0.59923	1.37135
	C	-1.17834	0.09017	1.86193		C	-1.17682	0.09169	1.86567
	C	-1.18037	1.36133	1.30651		C	-1.18006	1.36311	1.30903
	O	0.45590	2.39398	-0.16898		O	0.46349	2.39464	-0.16298
	O	0.46336	-1.68903	1.61661		O	0.47189	-1.68407	1.61977
	C	-2.51509	-1.02041	0.61389		C	-2.51452	-1.02278	0.61104
	C	-3.47213	0.11681	0.20114		C	-3.46976	0.11653	0.20150
	C	-2.61544	-0.71802	-1.71457		C	-2.61763	-0.71927	-1.71687
	C	-1.92938	-1.42154	-0.57502		C	-1.92939	-1.42300	-0.57847
	H	-2.64832	-1.68705	1.45801		H	-2.64755	-1.68761	1.45717
	H	-1.09666	-2.10808	-0.68638		H	-1.10077	-2.11422	-0.69440
	C	-4.01532	-0.46676	-1.13174		C	-4.01587	-0.46555	-1.13103
	H	-4.59086	0.26080	-1.71223		H	-4.59174	0.26321	-1.70983
	H	-4.58755	-1.38906	-0.99165		H	-4.58935	-1.38687	-0.98992
	C	-2.52011	1.19608	-0.35447		C	-2.51838	1.19455	-0.35659
	H	-2.65701	2.26785	-0.26944		H	-2.65606	2.26657	-0.27012
	C	-1.93402	0.59887	-1.45775		C	-1.93309	0.59596	-1.45982
	H	-1.10398	0.98715	-2.03863		H	-1.10666	0.98348	-2.04692
	H	-4.19403	0.44200	0.94937		H	-4.18879	0.44287	0.95193
	H	-2.50478	-1.15084	-2.70586		H	-2.50782	-1.15190	-2.70852
	H	-1.63904	2.24458	1.72852		H	-1.64432	2.24505	1.72866
	H	-1.63521	-0.20146	2.79728		H	-1.63908	-0.20107	2.79841
TSca $CHCl_3$	C	-0.65180	1.14804	1.57463	**TSca** **THF**	C	-0.64254	1.15857	1.58150
	C	-1.36637	0.96096	0.39741		C	-1.36657	0.96452	0.41143
	C	-0.23888	2.49566	1.64448		C	-0.22690	2.50613	1.63894
	C	-0.68949	3.16101	0.51048		C	-0.68496	3.16433	0.50376
	C	-1.73954	2.31089	-0.14478		C	-1.73956	2.31081	-0.13905
	H	-0.53551	4.21179	0.29519		H	-0.53237	4.21384	0.28085
	H	-1.82254	0.03016	0.08150		H	-1.82733	0.03243	0.10575
	N	0.34757	1.02975	-0.93915		N	0.34508	1.02215	-0.94146
	N	0.73811	2.26126	-0.86866		N	0.73851	2.25289	-0.87796
	C	1.26939	0.18836	-0.20061		C	1.26648	0.18270	-0.20108

	O	1.21120	-1.00992	-0.12673		
	C	1.94976	2.33642	-0.07543		
	O	2.58911	3.33344	0.12781		
	N	2.24375	1.03444	0.31897		
	H	0.41889	2.91511	2.39822		
	H	-0.35778	0.36290	2.26270		
	H	-2.71831	2.59153	0.27278		
	H	-1.78499	2.37987	-1.23068		
	C	3.35520	0.63847	1.11337		
	C	3.75514	1.44376	2.17914		
	C	4.02569	-0.54768	0.81868		
	C	4.84397	1.05523	2.95249		
	C	5.10447	-0.92964	1.60976		
	C	5.51793	-0.13153	2.67381		
	H	3.22379	2.36585	2.38814		
	H	3.69751	-1.16173	-0.01212		
	H	5.16185	1.68249	3.77981		
	H	5.62777	-1.85441	1.38658		
	H	6.36396	-0.43305	3.28383		
TSca **1,4-dioxane**	C	-0.66618	1.13174	1.56521	**TSca** **$PhCH_3$**	C -0.66255 1.13309 1.56495
	C	-1.36779	0.95405	0.37900		C -1.36530 0.95463 0.37931
	C	-0.25640	2.47934	1.65097		C -0.25428 2.48115 1.65036
	C	-0.69486	3.15324	0.51699		C -0.69570 3.15487 0.51760
	C	-1.74144	2.30866	-0.15258		C -1.74160 2.30898 -0.15116
	H	-0.53951	4.20556	0.31220		H -0.54135 4.20726 0.31211
	H	-1.81488	0.02463	0.04750		H -1.81275 0.02491 0.04905
	N	0.35196	1.04505	-0.93715		N 0.35129 1.04399 -0.93740
	N	0.73466	2.27778	-0.84982		N 0.73559 2.27648 -0.85293
	C	1.27671	0.19936	-0.20549		C 1.27576 0.19846 -0.20508
	O	1.21990	-0.99859	-0.14075		O 1.21846 -0.99953 -0.13957
	C	1.94537	2.35150	-0.05265		C 1.94634 2.35003 -0.05636
	O	2.57140	3.35166	0.17006		O 2.57512 3.34936 0.16288
	N	2.24897	1.04482	0.32269		N 2.24830 1.04383 0.32195
	H	0.39734	2.89160	2.41164		H 0.39954 2.89418 2.41061
	H	-0.37335	0.33994	2.24564		H -0.36783 0.34175 2.24516
	H	-2.72311	2.58419	0.26092		H -2.72236 2.58175 0.26645
	H	-1.77748	2.38681	-1.23815		H -1.78067 2.38793 -1.23652
	C	3.36007	0.64484	1.11533		C 3.35925 0.64424 1.11503
	C	3.78675	1.46330	2.16098		C 3.78338 1.46174 2.16242
	C	4.00612	-0.55963	0.83952		C 4.00729 -0.55888 0.83803
	C	4.87540	1.06940	2.93150		C 4.87177 1.06830 2.93361
	C	5.08539	-0.94525	1.62768		C 5.08623 -0.94421 1.62685
	C	5.52473	-0.13469	2.67130		C 5.52316 -0.13447 2.67218
	H	3.27905	2.40130	2.35405		H 3.27361 2.39845 2.35669

	H	3.65778	-1.18558	0.02668		H	3.66082	-1.18389	0.02360
	H	5.21350	1.70795	3.74176		H	5.20795	1.70598	3.74537
	H	5.58857	-1.88403	1.41784		H	5.59107	-1.88194	1.41625
	H	6.37117	-0.43952	3.27877		H	6.36933	-0.43902	3.28020
TSca	C	-0.64127	1.16294	1.58399	**TScb**	C	2.48622	0.22451	-0.50842
$ClCH_2CH_2Cl$	C	-1.36814	0.96784	0.41579	**$CHCl_3$**	C	1.59175	-0.07081	-1.54140
	C	-0.22249	2.50977	1.63765		C	2.34695	-0.73553	0.50116
	C	-0.68203	3.16666	0.50252		C	1.36237	-1.65260	0.12197
	C	-1.73848	2.31363	-0.13745		C	1.12094	-1.48116	-1.34786
	H	-0.52754	4.21540	0.27696		H	1.09479	-2.54429	0.68115
	H	-1.83257	0.03631	0.11373		H	1.53165	0.46528	-2.48394
	N	0.34257	1.01560	-0.93985		C	-0.42445	-0.30726	0.54018
	N	0.73868	2.24575	-0.88297		C	-0.28241	0.66754	-0.48503
	C	1.26334	0.17783	-0.19678		H	2.83812	-0.70807	1.46753
	O	1.20282	-1.02020	-0.11273		H	3.10247	1.11480	-0.44930
	C	1.95308	2.32306	-0.09511		H	1.82549	-2.14110	-1.87869
	O	2.60050	3.31833	0.09400		H	0.12029	-1.72064	-1.71330
	N	2.24209	1.02456	0.31118		C	-0.11761	0.05767	1.89807
	H	0.44090	2.93492	2.38357		N	0.14621	0.35133	2.98538
	H	-0.34602	0.38352	2.27830		C	0.16388	1.99002	-0.13403
	H	-2.71273	2.60241	0.28563		N	0.53870	3.04664	0.15079
	H	-1.79367	2.37341	-1.22351		C	-1.11507	0.57784	-1.65495
	C	3.35245	0.63254	1.10927		N	-1.76719	0.48305	-2.60602
	C	3.72633	1.42457	2.19387		C	-1.39645	-1.35555	0.37783
	C	4.04638	-0.53567	0.79874		N	-2.15920	-2.21253	0.22758
	C	4.81411	1.04099	2.97138					
	C	5.12337	-0.91431	1.59417					
	C	5.51136	-0.12878	2.67728					
	H	3.17400	2.33167	2.41611					
	H	3.73925	-1.13799	-0.04902					
	H	5.11204	1.65735	3.81432					
	H	5.66539	-1.82554	1.35977					
	H	6.35613	-0.42715	3.29081					
TScb	C	2.48695	0.22401	-0.50876	**TScb**	C	2.48308	0.22438	-0.50729
THF	C	1.59437	-0.07202	-1.54257	**1,4-dioxane**	C	1.58194	-0.06678	-1.53709
	C	2.34813	-0.73700	0.50081		C	2.34427	-0.73543	0.50088
	C	1.36624	-1.65561	0.12056		C	1.35358	-1.64825	0.12376
	C	1.12175	-1.48151	-1.34824		C	1.11767	-1.48082	-1.34817
	H	1.09802	-2.54726	0.67984		H	1.08477	-2.53912	0.68292
	H	1.53415	0.46431	-2.48517		H	1.52099	0.47010	-2.47869
	C	-0.42759	-0.30500	0.54119		C	-0.41996	-0.30966	0.53919
	C	-0.28452	0.66847	-0.48391		C	-0.27729	0.66563	-0.48741
	H	2.84066	-0.71028	1.46666		H	2.83338	-0.70708	1.46787
	H	3.10428	1.11372	-0.44959		H	3.09693	1.11582	-0.44675

	H 1.82598 -2.14133 -1.88000		H 1.83309 -2.13375 -1.87247
	H 0.12041 -1.71984 -1.71241		H 0.12086 -1.72698 -1.71898
	C -0.11978 0.05945 1.89866		C -0.11296 0.05515 1.89764
	N 0.14328 0.35577 2.98546		N 0.15566 0.34399 2.98502
	C 0.16198 1.99085 -0.13349		C 0.16829 1.98919 -0.13701
	N 0.53503 3.04756 0.15336		N 0.54765 3.04534 0.14330
	C -1.11563 0.57820 -1.65474		C -1.11306 0.57675 -1.65601
	N -1.76827 0.48297 -2.60541		N -1.76180 0.48287 -2.60943
	C -1.39744 -1.35485 0.37851		C -1.39486 -1.35618 0.37776
	N -2.16055 -2.21148 0.22793		N -2.15476 -2.21603 0.22966
TScb $PhCH_3$	C 2.48330 0.22430 -0.50736	**TScb** $ClCH_2CH_2Cl$	C 2.48710 0.22393 -0.50912
	C 1.58291 -0.06722 -1.53753		C 1.59621 -0.07309 -1.54368
	C 2.34451 -0.73566 0.50088		C 2.34827 -0.73726 0.50074
	C 1.35457 -1.64896 0.12344		C 1.36797 -1.65690 0.11990
	C 1.11801 -1.48094 -1.34824		C 1.12250 -1.48198 -1.34852
	H 1.08588 -2.53996 0.68253		H 1.09974 -2.54864 0.67917
	H 1.52207 0.46965 -2.47919		H 1.53584 0.46316 -2.48641
	C -0.42062 -0.30918 0.53938		C -0.42913 -0.30393 0.54171
	C -0.27795 0.66596 -0.48708		C -0.28612 0.66930 -0.48304
	H 2.83397 -0.70754 1.46775		H 2.84098 -0.71061 1.46657
	H 3.09745 1.11559 -0.44694		H 3.10458 1.11363 -0.45011
	H 1.83301 -2.13406 -1.87296		H 1.82684 -2.14182 -1.88032
	H 0.12100 -1.72682 -1.71872		H 0.12107 -1.72020 -1.71247
	C -0.11345 0.05557 1.89774		C -0.12061 0.06039 1.89891
	N 0.15475 0.34492 2.98509		N 0.14281 0.35869 2.98509
	C 0.16771 1.98944 -0.13676		C 0.16115 1.99126 -0.13263
	N 0.54650 3.04569 0.14397		N 0.53433 3.04734 0.15642
	C -1.11329 0.57687 -1.65588		C -1.11638 0.57838 -1.65426
	N -1.76240 0.48293 -2.60905		N -1.76979 0.48204 -2.60429
	C -1.39514 -1.35593 0.37789		C -1.39817 -1.35427 0.37846
	N -2.15534 -2.21551 0.22972		N -2.16174 -2.21027 0.22656
TScc $CHCl_3$	C 1.77553 1.48436 0.82564	**TScc** THF	C 1.77623 1.48522 0.82677
	C 1.77508 1.35311 -0.56271		C 1.77540 1.35349 -0.56190
	C 2.11976 0.25056 1.39976		C 2.12032 0.25166 1.40102
	C 2.34130 -0.67632 0.38162		C 2.34128 -0.67571 0.38271
	C 2.54223 0.10048 -0.89211		C 2.54181 0.10073 -0.89085
	H 2.70593 -1.68624 0.53766		H 2.70618 -1.68561 0.53873
	H 1.62933 2.17303 -1.25819		H 1.62976 2.17335 -1.25761
	C -0.10615 0.18145 -0.82434		C -0.10598 0.18138 -0.82535
	C 0.23350 -1.03642 -0.25597		C 0.23389 -1.03705 -0.25688
	C -0.94625 0.90259 0.15168		C -0.94534 0.90185 0.15066
	O -1.52664 1.94729 0.07272		O -1.52693 1.94660 0.07362
	C -0.39075 -1.08635 1.08061		C -0.39022 -1.08696 1.07893
	O -0.43436 -1.96052 1.89822		O -0.43593 -1.96078 1.89749

	H -0.15331 0.42575 -1.87724 H 0.50773 -1.94853 -0.76917 O -0.98073 0.14802 1.31670 H 2.09593 0.02249 2.45990 H 1.44387 2.36070 1.37200 H 3.60823 0.37018 -0.95021 H 2.26553 -0.40689 -1.81709		H -0.15538 0.42546 -1.87837 H 0.50644 -1.94976 -0.77026 O -0.98072 0.14735 1.31604 H 2.09727 0.02377 2.46134 H 1.44517 2.36213 1.37283 H 3.60808 0.36854 -0.95403 H 2.26444 -0.40693 -1.81538
TScc **1,4-dioxane**	C 1.77670 1.48500 0.82589 C 1.77406 1.35267 -0.56225 C 2.12077 0.25141 1.40018 C 2.33978 -0.67607 0.38219 C 2.54364 0.10110 -0.89112 H 2.70463 -1.68532 0.54013 H 1.62830 2.17350 -1.25625 C -0.10428 0.18167 -0.82472 C 0.23539 -1.03600 -0.25665 C -0.94643 0.90318 0.15289 O -1.52192 1.94878 0.07020 C -0.39102 -1.08661 1.08153 O -0.42984 -1.96238 1.89569 H -0.15696 0.42633 -1.87700 H 0.50519 -1.94987 -0.76849 O -0.98058 0.14758 1.31656 H 2.09265 0.02238 2.45970 H 1.44088 2.35979 1.37158 H 3.60969 0.36836 -0.95523 H 2.26512 -0.40675 -1.81535	**TScc** **$PhCH_3$**	C 1.77667 1.48501 0.82593 C 1.77421 1.35275 -0.56224 C 2.12076 0.25142 1.40024 C 2.33997 -0.67604 0.38223 C 2.54354 0.10107 -0.89111 H 2.70481 -1.68534 0.54003 H 1.62844 2.17349 -1.25637 C -0.10444 0.18163 -0.82477 C 0.23523 -1.03609 -0.25668 C -0.94633 0.90307 0.15273 O -1.52231 1.94861 0.07049 C -0.39098 -1.08663 1.08132 O -0.43036 -1.96226 1.89583 H -0.15694 0.42626 -1.87710 H 0.50519 -1.94989 -0.76862 O -0.98061 0.14756 1.31652 H 2.09301 0.02247 2.45982 H 1.44118 2.35997 1.37164 H 3.60959 0.36845 -0.95505 H 2.26513 -0.40678 -1.81536
TScc **$ClCH_2CH_2Cl$**	C 1.77608 1.48519 0.82689 C 1.77558 1.35358 -0.56186 C 2.12022 0.25164 1.40111 C 2.34163 -0.67566 0.38276 C 2.54154 0.10067 -0.89084 H 2.70652 -1.68567 0.53841 H 1.62996 2.17326 -1.25785 C -0.10629 0.18132 -0.82543 C 0.23352 -1.03721 -0.25692 C -0.94517 0.90169 0.15034 O -1.52747 1.94643 0.07418 C -0.39008 -1.08694 1.07858 O -0.43652 -1.96035 1.89795 H -0.15499 0.42531 -1.87858 H 0.50665 -1.94969 -0.77055 O -0.98084 0.14736 1.31599 H 2.09771 0.02380 2.46152		

	H 1.44551 2.36234 1.37297			
	H 3.60785 0.36861 -0.95374			
	H 2.26434 -0.40694 -1.81544			

wB97xd+IDSCRF/6-31G(d)

Species	Cartesian coordinates			Species	Cartesian coordinates		
TSaa	C	-4.18732	0.00901 -1.45889	**TSaa**	C	-4.18679	-0.01307 -1.45799
$CHCl_3$	C	-3.04972	0.21555 -0.65893	THF	C	-3.05059	0.20625 -0.65955
	C	-1.83156	0.79067 -1.15438		C	-1.83468	0.78150 -1.16091
	C	-3.03498	-0.25186 0.67111		C	-3.03308	-0.24785 0.67519
	C	-1.79916	-0.11072 1.38926		C	-1.80053	-0.09042 1.39423
	C	-0.92210	0.97167 1.08081		C	-0.92548	0.98867 1.07330
	C	-0.94032	1.44516 -0.25471		C	-0.94804	1.45073 -0.26616
	C	-5.29649	-0.61161 -0.92193		C	-5.29334	-0.63356 -0.91514
	C	-4.15640	-0.92183 1.18950		C	-4.15178	-0.91839 1.19972
	H	-1.70589	-0.59175 2.35973		H	-1.70437	-0.56267 2.36890
	C	0.04574	1.46890 1.98482		C	0.03966	1.50092 1.97230
	C	0.00137	2.41888 -0.66354		C	-0.01725	2.43084 -0.68324
	C	0.90426	2.91744 0.24440		C	0.88029	2.94657 0.22071
	C	0.93053	2.43594 1.57332		C	0.91379	2.47436 1.55283
	H	0.07585	1.08053 2.99847		H	0.07320	1.12165 2.98943
	H	-0.00486	2.76442 -1.69330		H	-0.02893	2.77021 -1.71499
	H	1.61678	3.67757 -0.06185		H	1.58304	3.71350 -0.09141
	H	1.66329	2.83162 2.26972		H	1.64248	2.88348 2.24582
	C	-5.28121	-1.07835 0.40564		C	-5.27557	-1.08744 0.41690
	H	-4.18705	0.35027 -2.49041		H	-4.18812	0.32022 -2.49216
	H	-1.75995	1.02244 -2.21419		H	-1.76736	1.00891 -2.22210
	H	-6.18603	-0.75155 -1.52896		H	-6.18265	-0.78247 -1.52045
	H	-4.13181	-1.29918 2.20814		H	-4.12593	-1.28562 2.22206
	H	-6.15889	-1.57323 0.81058		H	-6.15117	-1.58211 0.82676
	N	1.34941	-0.89327 -0.32087		N	1.35366	-0.88451 -0.31739
	C	0.54155	-0.66243 -1.43141		C	0.55104	-0.64632 -1.42814
	C	0.54775	-1.39365 0.69960		C	0.54905	-1.39181 0.69737
	N	-0.77575	-1.52554 0.16329		N	-0.77126	-1.52283 0.15673
	N	-0.77935	-1.09726 -1.08562		N	-0.77084	-1.08515 -1.08928
	O	0.87617	-0.23444 -2.50934		O	0.88974	-0.21187 -2.50255
	O	0.88431	-1.71491 1.81356		O	0.88566	-1.71905 1.81002
	C	2.74102	-0.61704 -0.22333		C	2.74779	-0.62217 -0.21717
	C	3.57045	-1.50626 0.45847		C	3.57426	-1.54966 0.41505
	C	3.26392	0.53338 -0.81160		C	3.27418	0.55155 -0.75296
	C	4.92941	-1.22935 0.56199		C	4.93594	-1.28794 0.52276
	C	4.62688	0.79057 -0.71292		C	4.63972	0.79442 -0.65135
	C	5.46252	-0.08433 -0.02400		C	5.47291	-0.11913 -0.01095
	H	3.15299	-2.39780 0.91149		H	3.15194	-2.45974 0.82564

	H	2.61026	1.21387	-1.34230	H	2.62062	1.26227	-1.24335
	H	5.57440	-1.91938	1.09795	H	5.57986	-2.00725	1.02022
	H	5.03474	1.68464	-1.17534	H	5.05139	1.70754	-1.07126
	H	6.52514	0.12488	0.05571	H	6.53745	0.07905	0.07227
TSaa **1,4-dioxane**	C	-4.19274	0.01729	-1.45393	**TSaa** **$PhCH_3$**	C	-4.19211	0.01576	-1.45409
	C	-3.05248	0.21929	-0.65679		C	-3.05200	0.21844	-0.65691
	C	-1.83394	0.79380	-1.15235		C	-1.83346	0.79255	-1.15289
	C	-3.03465	-0.25464	0.67072		C	-3.03440	-0.25418	0.67111
	C	-1.79520	-0.12132	1.38419		C	-1.79540	-0.11967	1.38506
	C	-0.92007	0.96379	1.08140		C	-0.91995	0.96485	1.08091
	C	-0.94215	1.44544	-0.25108		C	-0.94162	1.44494	-0.25217
	C	-5.30117	-0.60414	-0.91718		C	-5.30062	-0.60523	-0.91689
	C	-4.15577	-0.92507	1.18887		C	-4.15555	-0.92422	1.18973
	H	-1.69667	-0.61297	2.34841		H	-1.69745	-0.60961	2.35025
	C	0.05498	1.45074	1.98353		C	0.05399	1.45368	1.98315
	C	0.00328	2.41665	-0.65793		C	0.00282	2.41683	-0.65944
	C	0.91341	2.90445	0.24812		C	0.91185	2.90658	0.24675
	C	0.94327	2.41488	1.57414		C	0.94151	2.41836	1.57324
	H	0.09036	1.05306	2.99313		H	0.08886	1.05748	2.99339
	H	-0.00357	2.76550	-1.68638		H	-0.00405	2.76499	-1.68815
	H	1.62995	3.66090	-0.05731		H	1.62749	3.66378	-0.05899
	H	1.68327	2.79965	2.26874		H	1.68051	2.80489	2.26795
	C	-5.28304	-1.07658	0.40820		C	-5.28268	-1.07648	0.40893
	H	-4.19431	0.36101	-2.48447		H	-4.19359	0.35873	-2.48490
	H	-1.76252	1.02772	-2.21129		H	-1.76204	1.02563	-2.21207
	H	-6.19193	-0.74111	-1.52277		H	-6.19135	-0.74264	-1.52246
	H	-4.12819	-1.30893	2.20482		H	-4.12819	-1.30694	2.20613
	H	-6.15979	-1.57285	0.81305		H	-6.15952	-1.57235	0.81412
	N	1.34810	-0.89319	-0.33135		N	1.34847	-0.89446	-0.33039
	C	0.53933	-0.64702	-1.43920		C	0.53938	-0.64962	-1.43814
	C	0.54448	-1.39904	0.68609		C	0.54532	-1.39902	0.68796
	N	-0.78066	-1.52341	0.14771		N	-0.77983	-1.52420	0.15034
	N	-0.78344	-1.08549	-1.09653		N	-0.78307	-1.08759	-1.09451
	O	0.87037	-0.20228	-2.51020		O	0.87043	-0.20670	-2.51005
	O	0.87716	-1.72702	1.79823		O	0.87887	-1.72580	1.80030
	C	2.73835	-0.61354	-0.22765		C	2.73872	-0.61444	-0.22741
	C	3.56195	-1.48294	0.48640		C	3.56330	-1.48609	0.48263
	C	3.26745	0.52128	-0.84075		C	3.26661	0.52258	-0.83736
	C	4.91932	-1.20187	0.59607		C	4.92073	-1.20500	0.59179
	C	4.62888	0.78229	-0.73418		C	4.62811	0.78369	-0.73156
	C	5.45824	-0.07263	-0.01392		C	5.45850	-0.07346	-0.01506
	H	3.14096	-2.36108	0.96065		H	3.14300	-2.36620	0.95402
	H	2.61980	1.18482	-1.39882		H	2.61792	1.18797	-1.39208
	H	5.55865	-1.87698	1.15697		H	5.56101	-1.88176	1.14963

	H 5.04083 1.66374 -1.21656		H 5.03927 1.66690 -1.21139
	H 6.51976 0.13943 0.07090		H 6.52006 0.13866 0.06928
TSaa	C -4.18464 -0.01923 -1.45944	**TSab**	C -4.19369 -0.07116 -1.43139
$ClCH_2CH_2Cl$	C -3.04981 0.20339 -0.65999	$CHCl_3$	C -3.07929 0.21167 -0.62387
	C -1.83379 0.77830 -1.16156		C -1.86607 0.79694 -1.12818
	C -3.03378 -0.24616 0.67647		C -3.05830 -0.22472 0.72047
	C -1.80363 -0.08374 1.39802		C -1.84316 -0.01377 1.44719
	C -0.92720 0.99266 1.07363		C -0.98919 1.08597 1.11473
	C -0.94896 1.45094 -0.26723		C -1.00900 1.52264 -0.22954
	C -5.29160 -0.63864 -0.91605		C -5.27338 -0.74171 -0.89199
	C -4.15299 -0.91566 1.20166		C -4.15010 -0.94392 1.24083
	H -1.70919 -0.55239 2.37470		H -1.75988 -0.44524 2.44416
	C 0.03627 1.50907 1.97226		C -0.06637 1.64336 2.01901
	C -0.02018 2.43210 -0.68590		C -0.10945 2.51513 -0.65353
	C 0.87496 2.95259 0.21782		C 0.76078 3.08010 0.25742
	C 0.90854 2.48351 1.55110		C 0.78333 2.64368 1.59392
	H 0.06882 1.13324 2.99075		H -0.03863 1.28768 3.04477
	H -0.03220 2.76982 -1.71823		H -0.10940 2.83225 -1.69222
	H 1.57568 3.72097 -0.09538		H 1.44486 3.86026 -0.06187
	H 1.63533 2.89638 2.24395		H 1.48534 3.08979 2.29141
	C -5.27543 -1.08810 0.41760		C -5.25154 -1.17933 0.44414
	H -4.18488 0.31167 -2.49443		H -4.19806 0.24361 -2.47079
	H -1.76643 1.00442 -2.22308		H -1.83662 1.06798 -2.18331
	H -6.18016 -0.78962 -1.52199		H -6.14405 -0.94615 -1.50737
	H -4.12854 -1.27930 2.22535		H -4.11918 -1.29805 2.26703
	H -6.15146 -1.58166 0.82794		H -6.10410 -1.71831 0.84536
	N 1.35541 -0.88469 -0.31615		C -0.64366 -1.53501 0.21197
	C 0.55329 -0.64642 -1.42655		C -0.70003 -1.03789 -1.15294
	C 0.55064 -1.39105 0.69897		C 0.58359 -1.40083 0.93878
	N -0.76893 -1.52268 0.15865		N 1.56005 -1.25192 1.54665
	N -0.76873 -1.08469 -1.08738		C -1.43332 -2.67969 0.55632
	O 0.89247 -0.21321 -2.50155		N -2.10685 -3.57669 0.85110
	O 0.88835 -1.71773 1.81169		C -1.50123 -1.77149 -2.09747
	C 2.75000 -0.62426 -0.21662		N -2.17734 -2.32655 -2.85739
	C 3.57726 -1.55997 0.40216		C 0.50928 -0.49763 -1.71676
	C 3.27548 0.55524 -0.74027		N 1.46348 -0.01935 -2.16781
	C 4.93942 -1.30039 0.50957		
	C 4.64150 0.79620 -0.63938		
	C 5.47555 -0.12544 -0.01168		
	H 3.15515 -2.47499 0.80225		
	H 2.62064 1.27186 -1.22053		
	H 5.58437 -2.02588 0.99668		
	H 5.05282 1.71397 -1.04945		
	H 6.54042 0.07120 0.07134		

TSab **THF**				**TSab** **1,4-dixoane**			
	C	-4.14872	-0.15865 -1.40754		C	-4.20045	-0.06039 -1.43412
	C	-3.05978	0.16532 -0.58962		C	-3.08357	0.21992 -0.62800
	C	-1.80959	0.69886 -1.10068		C	-1.87641	0.81411 -1.13076
	C	-3.08647	-0.19444 0.78031		C	-3.05548	-0.22726 0.71219
	C	-1.95291	0.12462 1.56803		C	-1.82827	-0.03159 1.42817
	C	-1.01980	1.11477 1.17293		C	-0.98588	1.08374 1.10659
	C	-0.98540	1.47991 -0.19540		C	-1.01342	1.53072 -0.23366
	C	-5.24262	-0.81189 -0.86670		C	-5.27673	-0.73630 -0.89635
	C	-4.19037	-0.90226 1.30286		C	-4.14384	-0.95157 1.23036
	H	-1.90266	-0.25986 2.58629		H	-1.74541	-0.46241 2.42510
	C	-0.10212	1.68777 2.07972		C	-0.05937	1.63618 2.00881
	C	-0.05790	2.43421 -0.62989		C	-0.11546	2.52627 -0.65605
	C	0.80287	3.01942 0.28249		C	0.75859	3.08607 0.25341
	C	0.78765	2.64199 1.63622		C	0.78709	2.64047 1.58650
	H	-0.11833	1.37955 3.12107		H	-0.02063	1.26969 3.03014
	H	-0.01870	2.70932 -1.67975		H	-0.11834	2.84717 -1.69329
	H	1.51064	3.77104 -0.05410		H	1.44279	3.86624 -0.06459
	H	1.48500	3.09933 2.33094		H	1.49341	3.08061 2.28310
	C	-5.26216	-1.19138 0.48638		C	-5.24826	-1.18273 0.43648
	H	-4.12879	0.10383 -2.46117		H	-4.20737	0.25845 -2.47198
	H	-1.81458	1.01918 -2.14334		H	-1.84286	1.07903 -2.18681
	H	-6.09287	-1.04792 -1.49956		H	-6.14779	-0.94100 -1.51057
	H	-4.18786	-1.19823 2.34789		H	-4.10654	-1.31951 2.25122
	H	-6.12182	-1.72057 0.88518		H	-6.09704	-1.72797 0.83667
	C	-0.57785	-1.60062 0.07250		C	-0.65464	-1.52339 0.23090
	C	-0.73642	-0.95671 -1.22503		C	-0.69507	-1.04910 -1.14253
	C	0.60286	-1.39031 0.82826		C	0.57691	-1.39872 0.95821
	N	1.56171	-1.17682 1.45072		N	1.54974	-1.26038 1.57346
	C	-1.42770	-2.67436 0.43894		C	-1.43740	-2.67630 0.57637
	N	-2.15763	-3.52896 0.73772		N	-2.10160	-3.57630 0.88117
	C	-1.50829	-1.70797 -2.20047		C	-1.50237	-1.77607 -2.08447
	N	-2.14620	-2.27834 -2.97963		N	-2.18413	-2.32198 -2.84637
	C	0.48776	-0.44443 -1.81711		C	0.50998	-0.50091 -1.70361
	N	1.44789	-0.00375 -2.28965		N	1.45864	-0.01314 -2.15686
TSab **$PhCH_3$**				**TSab** **$ClCH_2CH_2Cl$**			
	C	-4.19924	-0.06217 -1.43361		C	-4.14839	-0.15965 -1.40791
	C	-3.08278	0.21835 -0.62722		C	-3.06006	0.16561 -0.58957
	C	-1.87429	0.81052 -1.13011		C	-1.81078	0.70077 -1.10060
	C	-3.05582	-0.22704 0.71361		C	-3.08741	-0.19326 0.78070
	C	-1.83042	-0.02907 1.43113		C	-1.95566	0.12788 1.56969
	C	-0.98632	1.08391 1.10795		C	-1.02099	1.11581 1.17361
	C	-1.01261	1.52923 -0.23291		C	-0.98561	1.48009 -0.19505
	C	-5.27625	-0.73682 -0.89547		C	-5.24196	-0.81365 -0.86718
	C	-4.14495	-0.95010 1.23227		C	-4.19097	-0.90199 1.30313
	H	-1.74708	-0.46052 2.42777		H	-1.90757	-0.25391 2.58914

	C -0.06067 1.63748 2.01059 C -0.11460 2.52439 -0.65565 C 0.75856 3.08533 0.25410 C 0.78605 2.64133 1.58781 H -0.02375 1.27294 3.03271 H -0.11682 2.84442 -1.69319 H 1.44260 3.86561 -0.06410 H 1.49148 3.08266 2.28459 C -5.24897 -1.18165 0.43797 H -4.20559 0.25570 -2.47181 H -1.84131 1.07624 -2.18604 H -6.14730 -0.94133 -1.50984 H -4.10886 -1.31564 2.25407 H -6.09849 -1.72558 0.83841 C -0.65266 -1.52554 0.22745 C -0.69592 -1.04702 -1.14445 C 0.57805 -1.39952 0.95509 N 1.55094 -1.25970 1.57003 C -1.43656 -2.67708 0.57307 N -2.10217 -3.57634 0.87727 C -1.50195 -1.77504 -2.08722 N -2.18246 -2.32196 -2.84943 C 0.50988 -0.50027 -1.70624 N 1.45914 -0.01405 -2.15978		C -0.10271 1.68793 2.08055 C -0.05678 2.43314 -0.62966 C 0.80449 3.01755 0.28285 C 0.78849 2.64074 1.63685 H -0.12044 1.38073 3.12225 H -0.01787 2.70865 -1.67946 H 1.51295 3.76862 -0.05370 H 1.48591 3.09801 2.33162 C -5.26198 -1.19260 0.48615 H -4.12858 0.10350 -2.46141 H -1.81588 1.02158 -2.14320 H -6.09201 -1.05023 -1.50022 H -4.18898 -1.19647 2.34864 H -6.12175 -1.72185 0.88477 C -0.57615 -1.60134 0.07061 C -0.73621 -0.95693 -1.22625 C 0.60420 -1.38985 0.82607 N 1.56398 -1.17640 1.44722 C -1.42598 -2.67430 0.43825 N -2.15539 -3.52953 0.73679 C -1.50903 -1.70838 -2.20049 N -2.14794 -2.28069 -2.97741 C 0.48744 -0.44416 -1.81852 N 1.44849 -0.00377 -2.28945
TSac **$CHCl_3$**	C -4.21203 -0.06749 -1.44749 C -3.07761 0.19240 -0.64902 C -1.88079 0.79525 -1.15503 C -3.04685 -0.26338 0.68810 C -1.82103 -0.07895 1.40635 C -0.97835 1.02868 1.08178 C -1.00945 1.48562 -0.25737 C -5.29288 -0.73028 -0.91191 C -4.15099 -0.97268 1.20738 H -1.73902 -0.50727 2.40392 C -0.03816 1.57745 1.98335 C -0.10081 2.48499 -0.67424 C 0.78081 3.02950 0.22903 C 0.81245 2.57301 1.56493 H -0.00153 1.20632 3.00378 H -0.11332 2.81616 -1.70891 H 1.46706 3.80997 -0.08562 H 1.52286 3.00762 2.26171 C -5.26210 -1.18572 0.42345 H -4.22591 0.27267 -2.47988	**TSac** **THF**	C -4.21145 -0.06690 -1.44761 C -3.07682 0.19222 -0.64913 C -1.88001 0.79491 -1.15552 C -3.04605 -0.26358 0.68800 C -1.82024 -0.07950 1.40646 C -0.97702 1.02776 1.08143 C -1.00811 1.48471 -0.25774 C -5.29262 -0.72888 -0.91150 C -4.15036 -0.97234 1.20775 H -1.73892 -0.50763 2.40427 C -0.03808 1.57790 1.98362 C -0.10075 2.48557 -0.67416 C 0.77973 3.03139 0.22966 C 0.81138 2.57484 1.56567 H -0.00293 1.20804 3.00469 H -0.11475 2.81818 -1.70847 H 1.46413 3.81392 -0.08423 H 1.51996 3.01149 2.26320 C -5.26182 -1.18440 0.42393 H -4.22496 0.27283 -2.48019

	H -1.84564 1.06481 -2.20930 H -6.17506 -0.91074 -1.51899 H -4.11738 -1.33479 2.23181 H -6.12092 -1.71188 0.82957 C -0.73764 -1.60039 0.17202 C -0.76569 -1.15062 -1.14872 C 0.62566 -1.35526 0.68234 O 1.13020 -1.63244 1.73517 C 0.57965 -0.62665 -1.45477 O 1.03988 -0.19689 -2.47623 H -1.33419 -2.40001 0.58843 H -1.38802 -1.53694 -1.94377 O 1.33526 -0.67428 -0.29385		H -1.84561 1.06481 -2.20982 H -6.17508 -0.90900 -1.51841 H -4.11633 -1.33498 2.23203 H -6.12090 -1.71023 0.83012 C -0.73772 -1.60187 0.17176 C -0.76578 -1.15208 -1.14939 C 0.62511 -1.35786 0.68137 O 1.13216 -1.63561 1.73333 C 0.57910 -0.62950 -1.45565 O 1.04189 -0.20090 -2.47694 H -1.33495 -2.40105 0.58833 H -1.38889 -1.53798 -1.94419 O 1.33515 -0.67650 -0.29464
TSac **1,4-dioxane**	C -4.21329 -0.06794 -1.44713 C -3.07939 0.19401 -0.64868 C -1.88236 0.79649 -1.15410 C -3.04839 -0.26215 0.68835 C -1.82198 -0.07805 1.40550 C -0.98056 1.03061 1.08215 C -1.01187 1.48783 -0.25688 C -5.29310 -0.73320 -0.91291 C -4.15171 -0.97361 1.20624 H -1.73794 -0.50735 2.40224 C -0.03753 1.57621 1.98240 C -0.10084 2.48444 -0.67453 C 0.78315 3.02609 0.22765 C 0.81514 2.56923 1.56316 H 0.00227 1.20212 3.00133 H -0.11086 2.81328 -1.70969 H 1.47289 3.80258 -0.08839 H 1.52944 2.99941 2.25837 C -5.26202 -1.18906 0.42209 H -4.22815 0.27345 -2.47899 H -1.84536 1.06481 -2.20839 H -6.17452 -0.91478 -1.52047 H -4.11851 -1.33543 2.23067 H -6.11986 -1.71680 0.82780 C -0.73850 -1.59750 0.17310 C -0.76599 -1.14884 -1.14713 C 0.62581 -1.34965 0.68550 O 1.12355 -1.62411 1.74105 C 0.58022 -0.62138 -1.45285 O 1.03425 -0.18847 -2.47450 H -1.33339 -2.39807 0.58943	**TSac** **$PhCH_3$**	C -4.21318 -0.06781 -1.44719 C -3.07924 0.19396 -0.64871 C -1.88226 0.79649 -1.15421 C -3.04823 -0.26222 0.68831 C -1.82179 -0.07823 1.40550 C -0.98027 1.03038 1.08206 C -1.01161 1.48764 -0.25695 C -5.29307 -0.73286 -0.91283 C -4.15159 -0.97354 1.20633 H -1.73795 -0.50744 2.40231 C -0.03752 1.57629 1.98244 C -0.10087 2.48460 -0.67452 C 0.78288 3.02652 0.22778 C 0.81489 2.56963 1.56331 H 0.00195 1.20250 3.00153 H -0.11127 2.81380 -1.70959 H 1.47222 3.80347 -0.08810 H 1.52879 3.00025 2.25867 C -5.26200 -1.18873 0.42219 H -4.22796 0.27350 -2.47908 H -1.84540 1.06486 -2.20852 H -6.17457 -0.91434 -1.52033 H -4.11833 -1.33544 2.23074 H -6.11991 -1.71635 0.82793 C -0.73846 -1.59782 0.17309 C -0.76596 -1.14916 -1.14723 C 0.62573 -1.35023 0.68528 O 1.12422 -1.62499 1.74054 C 0.58009 -0.62203 -1.45298 O 1.03485 -0.18952 -2.47462 H -1.33346 -2.39836 0.58942

	H -1.38695 -1.53571 -1.94263		H -1.38705 -1.53599 -1.94270
	O 1.33483 -0.67068 -0.29177		O 1.33481 -0.67106 -0.29188
TSac	C -4.21113 -0.06655 -1.44765	**TSba**	N 0.80316 0.36568 0.60281
$ClCH_2CH_2Cl$	C -3.07638 0.19216 -0.64919	**$CHCl_3$**	C 0.05814 1.47273 0.24154
	C -1.87956 0.79473 -1.15579		C 0.07115 -0.36592 1.54829
	C -3.04560 -0.26366 0.68794		N -1.13761 0.34151 1.77899
	C -1.81979 -0.07979 1.40650		N -1.16918 1.39210 1.00719
	C -0.97628 1.02728 1.08123		O 0.35727 2.37652 -0.50024
	C -1.00736 1.48424 -0.25796		O 0.41863 -1.37813 2.10785
	C -5.29246 -0.72813 -0.91128		C 2.09545 0.03325 0.11255
	C -4.14999 -0.97216 1.20795		C 2.37951 -1.28738 -0.23082
	H -1.73880 -0.50784 2.40442		C 3.06224 1.02794 -0.02028
	C -0.03803 1.57817 1.98378		C 3.64558 -1.61095 -0.70616
	C -0.10070 2.48591 -0.67410		C 4.31994 0.69389 -0.51172
	C 0.77914 3.03245 0.23002		C 4.61638 -0.62337 -0.85228
	C 0.81079 2.57587 1.56609		H 1.61998 -2.05223 -0.11413
	H -0.00366 1.20896 3.00517		H 2.82922 2.05160 0.24982
	H -0.11548 2.81927 -1.70823		H 3.86957 -2.64105 -0.96698
	H 1.46253 3.81611 -0.08346		H 5.07312 1.46865 -0.62002
	H 1.51836 3.01363 2.26402		H 5.60178 -0.87935 -1.23015
	C -5.26163 -1.18372 0.42419		C -2.51354 -1.07549 0.64622
	H -4.22444 0.27295 -2.48034		C -3.44691 0.06321 0.22282
	H -1.84557 1.06481 -2.21010		C -2.56503 -0.80062 -1.66563
	H -6.17506 -0.90809 -1.51809		C -1.92106 -1.52214 -0.49457
	H -4.11571 -1.33510 2.23214		H -2.48930 -1.55336 1.61405
	H -6.12083 -1.70940 0.83040		H -1.11009 -2.23589 -0.58131
	C -0.73782 -1.60268 0.17160		C -3.97655 -0.53460 -1.10870
	C -0.76586 -1.15293 -1.14977		H -4.54766 0.18106 -1.70966
	C 0.62477 -1.35929 0.68085		H -4.55391 -1.45292 -0.95985
	O 1.13308 -1.63729 1.73238		C -2.51302 1.15473 -0.35295
	C 0.57880 -0.63109 -1.45616		H -2.75055 2.21036 -0.33365
	O 1.04292 -0.20310 -2.47735		C -1.92152 0.53963 -1.45938
	H -1.33543 -2.40160 0.58829		H -1.13478 0.95489 -2.07832
	H -1.38943 -1.53856 -1.94441		H -4.17020 0.40038 0.96242
	O 1.33508 -0.67779 -0.29509		H -2.44693 -1.25562 -2.64664
TSba	N 0.79978 0.36801 0.59571	**TSba**	N 0.80567 0.35525 0.61662
THF	C 0.05672 1.47724 0.23911	**1,4-dioxane**	C 0.06006 1.46428 0.25796
	C 0.07258 -0.35909 1.54740		C 0.06330 -0.39200 1.54331
	N -1.13370 0.34961 1.78242		N -1.14859 0.31487 1.77264
	N -1.16819 1.39897 1.00814		N -1.17314 1.37403 1.01302
	O 0.35624 2.38103 -0.50305		O 0.36056 2.37331 -0.47544
	O 0.42392 -1.36917 2.10954		O 0.39943 -1.41555 2.08613
	C 2.09260 0.03599 0.10637		C 2.09712 0.02660 0.12233
	C 2.36926 -1.28025 -0.25835		C 2.39822 -1.29910 -0.18627

	C	3.06634	1.02663	-0.00333	C	3.04704	1.03125	-0.05358
	C	3.63629	-1.60451	-0.73101	C	3.66249	-1.61640	-0.67007
	C	4.32503	0.69252	-0.49252	C	4.30299	0.70174	-0.55180
	C	4.61459	-0.62095	-0.85347	C	4.61606	-0.61972	-0.85831
	H	1.60242	-2.04111	-0.16290	H	1.65450	-2.07237	-0.03405
	H	2.83840	2.04693	0.28408	H	2.80012	2.05900	0.18524
	H	3.85493	-2.63133	-1.00896	H	3.89873	-2.65022	-0.90352
	H	5.08420	1.46382	-0.58290	H	5.04207	1.48453	-0.69299
	H	5.60080	-0.87729	-1.22923	H	5.59988	-0.87135	-1.24260
	C	-2.51935	-1.07068	0.65638	C	-2.51346	-1.07526	0.63948
	C	-3.44813	0.06745	0.22071	C	-3.44640	0.06629	0.22162
	C	-2.56101	-0.81416	-1.65764	C	-2.56266	-0.78451	-1.67159
	C	-1.92357	-1.52795	-0.47847	C	-1.92028	-1.51365	-0.50557
	H	-2.49991	-1.54138	1.62793	H	-2.49572	-1.56464	1.60141
	H	-1.11404	-2.24447	-0.55700	H	-1.10616	-2.22327	-0.59401
	C	-3.97387	-0.53949	-1.10832	C	-3.97462	-0.52199	-1.11464
	H	-4.54064	0.17344	-1.71657	H	-4.54384	0.19853	-1.71164
	H	-4.55476	-1.45485	-0.95475	H	-4.55316	-1.44069	-0.97285
	C	-2.50891	1.15123	-0.35992	C	-2.50939	1.16102	-0.34288
	H	-2.74171	2.20816	-0.35025	H	-2.74638	2.21625	-0.31425
	C	-1.91465	0.52565	-1.45892	C	-1.91847	0.55398	-1.45498
	H	-1.12441	0.93336	-2.07872	H	-1.12754	0.97350	-2.06507
	H	-4.17398	0.41209	0.95449	H	-4.16986	0.39875	0.96295
	H	-2.43999	-1.27633	-2.63492	H	-2.44527	-1.23335	-2.65552
TSba $PhCH_3$	N	0.80568	0.35593	0.61594	**TSba** $ClCH_2CH_2Cl$	N	0.79912	0.37102	0.59406
	C	0.06013	1.46475	0.25685		C	0.05629	1.47954	0.23613
	C	0.06375	-0.39013	1.54374		C	0.07358	-0.35301	1.54892
	N	-1.14783	0.31693	1.77303		N	-1.13182	0.35631	1.78436
	N	-1.17253	1.37564	1.01274		N	-1.16748	1.40364	1.00715
	O	0.36083	2.37326	-0.47726		O	0.35589	2.38175	-0.50820
	O	0.40027	-1.41316	2.08764		O	0.42664	-1.36118	2.11396
	C	2.09719	0.02693	0.12189		C	2.09145	0.03767	0.10416
	C	2.39702	-1.29837	-0.18971		C	2.36331	-1.27643	-0.27137
	C	3.04836	1.03096	-0.05061		C	3.06929	1.02536	0.00565
	C	3.66140	-1.61598	-0.67307		C	3.63035	-1.60204	-0.74327
	C	4.30442	0.70127	-0.54848		C	4.32792	0.69032	-0.48323
	C	4.61622	-0.61984	-0.85794		C	4.61293	-0.62132	-0.85452
	H	1.65204	-2.07106	-0.04041		H	1.59280	-2.03488	-0.18554
	H	2.80244	2.05838	0.19084		H	2.84446	2.04399	0.30180
	H	3.89671	-2.64947	-0.90898		H	3.84553	-2.62727	-1.02973
	H	5.04457	1.48355	-0.68704		H	5.09053	1.45922	-0.56511
	H	5.60014	-0.87163	-1.24196		H	5.59918	-0.87860	-1.22967
	C	-2.51333	-1.07472	0.64009		C	-2.51839	-1.06966	0.65971
	C	-3.44650	0.06640	0.22162		C	-3.44788	0.06684	0.22103

	C	-2.56313	-0.78587	-1.67119		C	-2.55940	-0.81894	-1.65489
	C	-1.92024	-1.51387	-0.50466		C	-1.92196	-1.52963	-0.47349
	H	-2.49554	-1.56343	1.60241		H	-2.49894	-1.53808	1.63244
	H	-1.10652	-2.22401	-0.59298		H	-1.11253	-2.24649	-0.55052
	C	-3.97499	-0.52321	-1.11402		C	-3.97267	-0.54368	-1.10678
	H	-4.54469	0.19658	-1.71143		H	-4.53967	0.16764	-1.71671
	H	-4.55316	-1.44199	-0.97122		H	-4.55327	-1.45888	-0.95117
	C	-2.50995	1.16066	-0.34429		C	-2.50947	1.14965	-0.36214
	H	-2.74637	2.21604	-0.31593		H	-2.74238	2.20665	-0.35513
	C	-1.91898	0.55282	-1.45572		C	-1.91421	0.52178	-1.45920
	H	-1.12850	0.97188	-2.06679		H	-1.12414	0.92827	-2.08013
	H	-4.16993	0.39936	0.96277		H	-4.17442	0.41260	0.95367
	H	-2.44568	-1.23549	-2.65475		H	-2.43737	-1.28304	-2.63113
TSbb $CHCl_3$	C	0.88806	-0.20195	-1.90388	**TSbb** **THF**	C	0.88494	-0.20113	-1.90690
	C	0.90656	1.04632	-1.22524		C	0.90434	1.04704	-1.22977
	C	2.21127	1.03847	0.32076		C	2.21252	1.03850	0.32684
	C	2.06962	-0.31656	1.05659		C	2.07190	-0.31823	1.05911
	C	4.25096	-0.12715	0.49799		C	4.25241	-0.12576	0.49871
	C	3.54942	1.06131	-0.08230		C	3.54956	1.06488	-0.07635
	H	1.77898	1.96328	0.70145		H	1.77516	1.96203	0.70513
	H	4.01607	1.81398	-0.71134		H	4.01651	1.82171	-0.70041
	C	3.43735	-0.33143	1.79553		C	3.44035	-0.33298	1.79705
	H	3.65266	-1.28973	2.27751		H	3.65713	-1.29196	2.27710
	H	3.54941	0.48904	2.51203		H	3.55204	0.48648	2.51478
	C	2.36255	-1.38095	-0.00125		C	2.36550	-1.38175	0.00043
	H	1.69540	-2.17927	-0.29806		H	1.69855	-2.18002	-0.29749
	C	3.64183	-1.20712	-0.39204		C	3.64402	-1.20684	-0.39096
	H	4.15702	-1.66815	-1.22617		H	4.16081	-1.66942	-1.22336
	H	1.16443	-0.44389	1.64840		H	1.16744	-0.44723	1.65180
	H	5.33695	-0.08097	0.53752		H	5.33846	-0.07831	0.53716
	C	-0.29519	1.36722	-0.47524		C	-0.29636	1.36940	-0.47950
	N	-1.23074	1.62077	0.15626		N	-1.23398	1.62193	0.14934
	C	1.46399	2.18630	-1.92934		C	1.46603	2.18500	-1.93261
	N	1.94084	3.09312	-2.46750		N	1.94462	3.08966	-2.47285
	C	1.85110	-0.46391	-2.91169		C	1.84531	-0.46564	-2.91662
	N	2.67229	-0.65696	-3.71077		N	2.66157	-0.66048	-3.72026
	C	-0.14754	-1.14803	-1.68185		C	-0.15053	-1.14666	-1.68245
	N	-0.98444	-1.93106	-1.49179		N	-0.98942	-1.92755	-1.49231
TSbb **1,4-dioxane**	C	0.89792	-0.20433	-1.89487	**TSbb** $PhCH_3$	C	0.89683	-0.20396	-1.89653
	C	0.91058	1.04481	-1.21322		C	0.91035	1.04490	-1.21478
	C	2.20906	1.03959	0.30632		C	2.20922	1.03947	0.30774
	C	2.06457	-0.31009	1.05264		C	2.06492	-0.31061	1.05317
	C	4.24670	-0.13251	0.49350		C	4.24708	-0.13195	0.49422
	C	3.54895	1.05101	-0.09976		C	3.54897	1.05198	-0.09787

	H 1.79055 1.96833 0.69217 H 4.01420 1.79180 -0.74306 C 3.43205 -0.32739 1.79077 H 3.64302 -1.28412 2.27766 H 3.54823 0.49583 2.50340 C 2.35118 -1.37776 -0.00335 H 1.68125 -2.17497 -0.29539 C 3.63212 -1.20894 -0.39534 H 4.14005 -1.66622 -1.23571 H 1.15871 -0.43113 1.64441 H 5.33270 -0.09114 0.53342 C -0.29358 1.35939 -0.46265 N -1.22374 1.61240 0.17700 C 1.45627 2.18991 -1.92084 N 1.93000 3.10206 -2.45279 C 1.87014 -0.45803 -2.89594 N 2.70788 -0.64251 -3.67984 C -0.13870 -1.15230 -1.68414 N -0.97122 -1.94101 -1.49879		H 1.78942 1.96793 0.69289 H 4.01450 1.79399 -0.73966 C 3.43245 -0.32758 1.79150 H 3.64383 -1.28438 2.27810 H 3.54815 0.49549 2.50439 C 2.35234 -1.37817 -0.00280 H 1.68269 -2.17556 -0.29524 C 3.63314 -1.20903 -0.39451 H 4.14192 -1.66700 -1.23400 H 1.15910 -0.43227 1.64489 H 5.33309 -0.09008 0.53411 C -0.29392 1.35999 -0.46477 N -1.22501 1.61306 0.17349 C 1.45730 2.18967 -1.92168 N 1.93150 3.10135 -2.45399 C 1.86839 -0.45883 -2.89794 N 2.70466 -0.64412 -3.68320 C -0.13955 -1.15179 -1.68419 N -0.97247 -1.93982 -1.49771
TSbb $ClCH_2CH_2Cl$	C 0.88253 -0.20100 -1.90793 C 0.90341 1.04747 -1.23246 C 2.21280 1.03830 0.33020 C 2.07279 -0.32018 1.05920 C 4.25337 -0.12414 0.49992 C 3.54962 1.06785 -0.07162 H 1.77216 1.96079 0.70742 H 4.01684 1.82826 -0.69125 C 3.44103 -0.33479 1.79778 H 3.65885 -1.29444 2.27608 H 3.55145 0.48353 2.51700 C 2.36837 -1.38190 -0.00080 H 1.70247 -2.18047 -0.30049 C 3.64670 -1.20505 -0.39136 H 4.16523 -1.66709 -1.22303 H 1.16820 -0.45119 1.65133 H 5.33938 -0.07547 0.53886 C -0.29659 1.37221 -0.48254 N -1.23528 1.62558 0.14435 C 1.46854 2.18338 -1.93526 N 1.94912 3.08625 -2.47672 C 1.84032 -0.46805 -2.91947 N 2.65245 -0.66575 -3.72655 C -0.15277 -1.14577 -1.67973 N -0.99210 -1.92565 -1.48731	**TSbc** $CHCl_3$	O 0.67679 0.24661 0.47542 C 0.04515 1.48276 0.48366 C 0.05048 -0.58927 1.39119 C -1.16876 0.08720 1.85403 C -1.17466 1.35742 1.29478 O 0.49714 2.41266 -0.12792 O 0.50808 -1.66787 1.65673 C -2.52143 -1.03015 0.60358 C -3.47188 0.11322 0.19667 C -2.62624 -0.72061 -1.71996 C -1.94910 -1.44161 -0.58564 H -2.65843 -1.69167 1.45050 H -1.13164 -2.14435 -0.70222 C -4.02449 -0.46537 -1.13400 H -4.60223 0.26427 -1.71104 H -4.60244 -1.38480 -0.99387 C -2.52220 1.19185 -0.36281 H -2.66693 2.26221 -0.27717 C -1.95045 0.60121 -1.47538 H -1.13472 0.99585 -2.07082 H -4.18777 0.44071 0.94959 H -2.52499 -1.15281 -2.71284 H -1.64378 2.23397 1.71996 H -1.63659 -0.19841 2.78595

TSbc **THF**				**TSbc** **1,4-dioxane**			
	O	0.67660	0.24698	0.47608	O	0.67658	0.24510	0.47321
	C	0.04454	1.48315	0.48481	C	0.04637	1.48149	0.48043
	C	0.04991	-0.58857	1.39226	C	0.05136	-0.59160	1.38803
	C	-1.16846	0.08751	1.85495	C	-1.16992	0.08619	1.85155
	C	-1.17449	1.35792	1.29547	C	-1.17491	1.35627	1.29340
	O	0.49888	2.41262	-0.12671	O	0.49224	2.41206	-0.13203
	O	0.50989	-1.66682	1.65749	O	0.50247	-1.67134	1.65381
	C	-2.52118	-1.03062	0.60284	C	-2.52170	-1.02828	0.60581
	C	-3.47121	0.11320	0.19679	C	-3.47350	0.11350	0.19633
	C	-2.62689	-0.72090	-1.72059	C	-2.62418	-0.71979	-1.71819
	C	-1.94889	-1.44165	-0.58662	C	-1.94908	-1.44098	-0.58284
	H	-2.65833	-1.69174	1.45018	H	-2.65887	-1.69096	1.45148
	H	-1.13236	-2.14538	-0.70448	H	-1.12896	-2.14083	-0.69590
	C	-4.02466	-0.46518	-1.13368	C	-4.02376	-0.46619	-1.13468
	H	-4.60254	0.26471	-1.71025	H	-4.60138	0.26248	-1.71307
	H	-4.60288	-1.38438	-0.99319	H	-4.60067	-1.38638	-0.99521
	C	-2.52176	1.19152	-0.36346	C	-2.52353	1.19303	-0.36135
	H	-2.66675	2.26191	-0.27735	H	-2.66748	2.26325	-0.27622
	C	-1.95010	0.60040	-1.47591	C	-1.95127	0.60363	-1.47406
	H	-1.13531	0.99479	-2.07295	H	-1.13304	0.99901	-2.06514
	H	-4.18626	0.44100	0.95034	H	-4.19162	0.44020	0.94759
	H	-2.52593	-1.15306	-2.71355	H	-2.52214	-1.15223	-2.71080
	H	-1.64514	2.23414	1.71984	H	-1.64025	2.23359	1.72064
	H	-1.63779	-0.19853	2.78608	H	-1.63387	-0.19820	2.78559
TSbc **$PhCH_3$**				**TSbc** **$ClCH_2CH_2Cl$**			
	O	0.67664	0.24531	0.47349	O	0.67661	0.24663	0.47648
	C	0.04625	1.48166	0.48082	C	0.04457	1.48301	0.48592
	C	0.05130	-0.59129	1.38842	C	0.04958	-0.58850	1.39290
	C	-1.16977	0.08631	1.85184	C	-1.16854	0.08737	1.85539
	C	-1.17490	1.35640	1.29353	C	-1.17360	1.35822	1.29685
	O	0.49284	2.41218	-0.13148	O	0.50043	2.41227	-0.12533
	O	0.50318	-1.67088	1.65421	O	0.51075	-1.66647	1.65820
	C	-2.52169	-1.02854	0.60553	C	-2.52063	-1.02999	0.60244
	C	-3.47331	0.11345	0.19637	C	-3.47109	0.11361	0.19647
	C	-2.62444	-0.71989	-1.71840	C	-2.62744	-0.72085	-1.72120
	C	-1.94912	-1.44108	-0.58318	C	-1.94863	-1.44089	-0.58727
	H	-2.65880	-1.69108	1.45136	H	-2.65795	-1.69107	1.44983
	H	-1.12933	-2.14130	-0.69667	H	-1.13275	-2.14529	-0.70595
	C	-4.02386	-0.46607	-1.13461	C	-4.02493	-0.46585	-1.13335
	H	-4.60148	0.26273	-1.71283	H	-4.60334	0.26356	-1.70988
	H	-4.60092	-1.38617	-0.99508	H	-4.60280	-1.38523	-0.99219
	C	-2.52336	1.19287	-0.36151	C	-2.52224	1.19175	-0.36470
	H	-2.66740	2.26311	-0.27636	H	-2.66689	2.26218	-0.27798
	C	-1.95117	0.60332	-1.47421	C	-1.95034	0.60036	-1.47683
	H	-1.13325	0.99862	-2.06582	H	-1.13585	0.99462	-2.07446

	H	-4.19117	0.44025	0.94783	H	-4.18553	0.44131	0.95062
	H	-2.52249	-1.15230	-2.71105	H	-2.52658	-1.15343	-2.71401
	H	-1.64067	2.23362	1.72054	H	-1.64491	2.23448	1.72044
	H	-1.63417	-0.19822	2.78563	H	-1.63896	-0.19878	2.78599
TSca $CHCl_3$	C	-0.69980	1.20512	1.59824	C	-0.70721	1.22804	1.60788
	C	-1.39627	0.99357	0.41106	C	-1.40684	1.00203	0.42579
	C	-0.26250	2.54241	1.63234	C	-0.26317	2.56356	1.62095
	C	-0.68261	3.18026	0.46980	C	-0.68047	3.18546	0.44846
	C	-1.74311	2.33329	-0.17012	C	-1.74432	2.33338	-0.17854
	H	-0.50761	4.22112	0.22788	H	-0.50308	4.22261	0.19218
	H	-1.87246	0.06481	0.12314	H	-1.88697	0.07113	0.15105
	N	0.32591	0.97107	-0.88248	N	0.32454	0.95604	-0.87467
	N	0.73894	2.20625	-0.86619	N	0.74097	2.19036	-0.86852
	C	1.24474	0.14928	-0.12840	C	1.23924	0.13964	-0.11181
	O	1.17293	-1.04666	-0.00379	O	1.16717	-1.05585	0.02107
	C	1.95829	2.29097	-0.09906	C	1.95867	2.27862	-0.09919
	O	2.61914	3.28536	0.05959	O	2.62454	3.27176	0.04902
	N	2.24540	0.99849	0.32965	N	2.23946	0.99031	0.34315
	H	0.39053	2.97323	2.38254	H	0.39025	3.00350	2.36572
	H	-0.43537	0.43685	2.31557	H	-0.44733	0.47017	2.33796
	H	-2.71895	2.64174	0.23512	H	-2.71888	2.65452	0.22020
	H	-1.78806	2.37654	-1.25724	H	-1.78897	2.35876	-1.26625
	C	3.36565	0.61512	1.11671	C	3.36418	0.60846	1.12479
	C	3.71030	1.37434	2.23288	C	3.69356	1.34878	2.25781
	C	4.10330	-0.51270	0.76415	C	4.12148	-0.49804	0.74778
	C	4.81161	1.00296	2.99628	C	4.80119	0.98057	3.01390
	C	5.19337	-0.88293	1.54479	C	5.21766	-0.86620	1.52089
	C	5.55253	-0.12650	2.65754	C	5.56240	-0.12762	2.65032
	H	3.12714	2.25131	2.49241	H	3.09238	2.20746	2.53766
	H	3.82157	-1.09466	-0.10618	H	3.85071	-1.06426	-0.13665
	H	5.08650	1.59725	3.86252	H	5.06486	1.56006	3.89362
	H	5.76881	-1.76330	1.27467	H	5.80910	-1.72989	1.23197
	H	6.40991	-0.41520	3.25818	H	6.42476	-0.41396	3.24506
TSca **1,4-dioxane**	C	-0.70894	1.17717	1.58220	C	-0.70796	1.17906	1.58296
	C	-1.39001	0.98032	0.38388	C	-1.38964	0.98130	0.38493
	C	-0.28353	2.51772	1.64421	C	-0.28221	2.51947	1.64364
	C	-0.69647	3.17162	0.48856	C	-0.69585	3.17259	0.48779
	C	-1.74651	2.32807	-0.17455	C	-1.74602	2.32867	-0.17440
	H	-0.52453	4.21658	0.26441	H	-0.52378	4.21736	0.26265
	H	-1.85326	0.05238	0.07426	H	-1.85388	0.05331	0.07682
	N	0.33570	0.99666	-0.88776	N	0.33482	0.99435	-0.88690
	N	0.73803	2.23366	-0.84747	N	0.73843	2.23124	-0.84959
	C	1.25885	0.16714	-0.14474	C	1.25737	0.16573	-0.14229
	O	1.19063	-1.02970	-0.03823	O	1.18866	-1.03101	-0.03351

	C	1.95494	2.31567	-0.07350	C	1.95529	2.31364	-0.07612
	O	2.59967	3.31461	0.11203	O	2.60176	3.31213	0.10660
	N	2.25414	1.01598	0.32942	N	2.25306	1.01472	0.33009
	H	0.36268	2.93904	2.40515	H	0.36421	2.94137	2.40413
	H	-0.44146	0.39764	2.28570	H	-0.44067	0.40013	2.28723
	H	-2.72682	2.61887	0.23244	H	-2.72639	2.61995	0.23211
	H	-1.78287	2.39138	-1.26090	H	-1.78260	2.39118	-1.26081
	C	3.37246	0.62646	1.11589	C	3.37176	0.62581	1.11630
	C	3.75565	1.41175	2.20154	C	3.75224	1.40914	2.20427
	C	4.07108	-0.53581	0.79536	C	4.07316	-0.53397	0.79305
	C	4.85319	1.03102	2.96528	C	4.85030	1.02906	2.96765
	C	5.15801	-0.91305	1.57645	C	5.16055	-0.91076	1.57377
	C	5.55453	-0.13194	2.65863	C	5.55455	-0.13144	2.65820
	H	3.20772	2.31757	2.43461	H	3.20153	2.31274	2.43965
	H	3.75915	-1.14004	-0.04836	H	3.76300	-1.13659	-0.05257
	H	5.15702	1.64600	3.80691	H	5.15215	1.64244	3.81116
	H	5.70162	-1.82019	1.33048	H	5.70645	-1.81599	1.32580
	H	6.40917	-0.42715	3.25973	H	6.40956	-0.42623	3.25903
TSca $ClCH_2CH_2Cl$	C	-0.71612	1.24351	1.61342	**TScb** $CHCl_3$	C	2.49594	0.21971	-0.50996
	C	-1.41600	1.00960	0.43341		C	1.59785	-0.07382	-1.54183
	C	-0.26547	2.57717	1.61394		C	2.35622	-0.73724	0.49762
	C	-0.67835	3.18960	0.43505		C	1.36695	-1.65202	0.12035
	C	-1.74462	2.33620	-0.18588		C	1.13221	-1.48505	-1.35022
	H	-0.49654	4.22378	0.16972		H	1.10803	-2.54603	0.67812
	H	-1.89971	0.07829	0.16611		H	1.54631	0.45899	-2.48566
	N	0.32228	0.94303	-0.86677		C	-0.42308	-0.31251	0.54043
	N	0.74183	2.17594	-0.87084		C	-0.28141	0.66772	-0.48939
	C	1.23387	0.13128	-0.09562		H	2.85033	-0.71336	1.46190
	O	1.15972	-1.06309	0.04730		H	3.11606	1.10680	-0.45448
	C	1.95923	2.26776	-0.10129		H	1.83671	-2.14567	-1.87931
	O	2.62844	3.26008	0.03829		H	0.13482	-1.72885	-1.72062
	N	2.23497	0.98333	0.35378		C	-0.12956	0.05540	1.89876
	H	0.38789	3.02145	2.35629		N	0.12156	0.34776	2.99135
	H	-0.46119	0.49171	2.35155		C	0.15284	1.99190	-0.13697
	H	-2.71832	2.66548	0.20853		N	0.51731	3.05489	0.14504
	H	-1.78690	2.35064	-1.27389		C	-1.12453	0.58770	-1.65040
	C	3.36388	0.60341	1.13078		N	-1.78469	0.50663	-2.59938
	C	3.68251	1.32983	2.27560		C	-1.40522	-1.35032	0.38561
	C	4.13567	-0.48669	0.73605		N	-2.17722	-2.20349	0.24771
	C	4.79516	0.96472	3.02608					
	C	5.23686	-0.85241	1.50326					
	C	5.57128	-0.12700	2.64445					
	H	3.06818	2.17459	2.56955					
	H	3.87270	-1.04166	-0.15813					

	H 5.05094 1.53320 3.91531 H 5.84012 -1.70321 1.20086 H 6.43753 -0.41111 3.23469		
TScb **THF**	C 2.49707 0.21938 -0.51061 C 1.60116 -0.07547 -1.54360 C 2.35699 -0.73747 0.49742 C 1.36940 -1.65349 0.11956 C 1.13343 -1.48552 -1.35050 H 1.11067 -2.54751 0.67769 H 1.54961 0.45755 -2.48748 C -0.42431 -0.31158 0.54097 C -0.28320 0.66874 -0.48833 H 2.85257 -0.71473 1.46113 H 3.11892 1.10549 -0.45632 H 1.83712 -2.14707 -1.87985 H 0.13590 -1.72894 -1.72087 C -0.13135 0.05635 1.89922 N 0.11759 0.35082 2.99176 C 0.15091 1.99264 -0.13582 N 0.51329 3.05585 0.14823 C -1.12558 0.58825 -1.64948 N -1.78743 0.50668 -2.59727 C -1.40594 -1.34954 0.38579 N -2.17937 -2.20128 0.24706	**TScb** **1,4-dioxane**	C 2.49096 0.22043 -0.50660 C 1.58557 -0.06824 -1.53473 C 2.35473 -0.73914 0.49816 C 1.36335 -1.65184 0.12122 C 1.12887 -1.48443 -1.34970 H 1.10179 -2.54535 0.67777 H 1.53345 0.46489 -2.47797 C -0.42316 -0.31203 0.54012 C -0.27588 0.66493 -0.49263 H 2.84591 -0.71375 1.46353 H 3.10561 1.11070 -0.44738 H 1.84099 -2.13675 -1.87824 H 0.13282 -1.73241 -1.72007 C -0.12441 0.05447 1.89780 N 0.13430 0.34015 2.99039 C 0.15887 1.99058 -0.14227 N 0.52835 3.05366 0.13233 C -1.12118 0.58590 -1.65340 N -1.77620 0.50605 -2.60592 C -1.40505 -1.35040 0.38604 N -2.17222 -2.20829 0.25023
TScb **$PhCH_3$**	C 2.49205 0.22038 -0.50745 C 1.58782 -0.06921 -1.53613 C 2.35508 -0.73853 0.49796 C 1.36392 -1.65151 0.12117 C 1.12950 -1.48447 -1.34978 H 1.10281 -2.54512 0.67784 H 1.53590 0.46331 -2.47974 C -0.42278 -0.31261 0.54004 C -0.27640 0.66511 -0.49235 H 2.84574 -0.71218 1.46362 H 3.10689 1.11056 -0.44815 H 1.83902 -2.13936 -1.87868 H 0.13287 -1.73077 -1.71987 C -0.12543 0.05473 1.89779 N 0.13273 0.34297 2.98984 C 0.15816 1.99033 -0.14079 N 0.52762 3.05269 0.13666 C -1.12183 0.58592 -1.65282 N -1.77835 0.50514 -2.60425 C -1.40471 -1.35084 0.38537	**TScb** **$ClCH_2CH_2Cl$**	C 2.49746 0.21925 -0.51079 C 1.60254 -0.07618 -1.54431 C 2.35739 -0.73771 0.49734 C 1.37086 -1.65449 0.11906 C 1.13406 -1.48579 -1.35066 H 1.11211 -2.54852 0.67732 H 1.55102 0.45692 -2.48824 C -0.42513 -0.31095 0.54132 C -0.28395 0.66919 -0.48788 H 2.85358 -0.71548 1.46082 H 3.11995 1.10502 -0.45693 H 1.83746 -2.14757 -1.88026 H 0.13644 -1.72908 -1.72094 C -0.13216 0.05695 1.89944 N 0.11597 0.35255 2.99187 C 0.15013 1.99298 -0.13537 N 0.51153 3.05625 0.14973 C -1.12609 0.58845 -1.64905 N -1.78880 0.50641 -2.59620 C -1.40641 -1.34902 0.38588

	N	-2.17315	-2.20740	0.24840		
TScc	C	1.79725	1.49117	0.82834	**TScc**	
$CHCl_3$	C	1.78581	1.35666	-0.55950	**THF**	
	C	2.14087	0.25898	1.40214		
	C	2.35117	-0.67112	0.38476		
	C	2.54733	0.10227	-0.89051		
	H	2.71761	-1.67943	0.54220		
	H	1.64216	2.17712	-1.25373		
	C	-0.10807	0.18495	-0.81744		
	C	0.23203	-1.03411	-0.24891		
	C	-0.96579	0.89448	0.14797		
	O	-1.55798	1.93475	0.06419		
	C	-0.41081	-1.09413	1.07565		
	O	-0.46655	-1.97530	1.88826		
	H	-0.15943	0.42268	-1.87139		
	H	0.50045	-1.94465	-0.76738		
	O	-1.01503	0.13423	1.30911		
	H	2.12512	0.03328	2.46237		
	H	1.47353	2.37011	1.37420		
	H	3.61431	0.36321	-0.96876		
	H	2.26177	-0.40642	-1.81211		
TScc	C	1.79645	1.49049	0.82774	**TScc**	
1,4-dioxane	C	1.78348	1.35548	-0.55990	**$PhCH_3$**	
	C	2.14013	0.25840	1.40143		
	C	2.34893	-0.67180	0.38405		
	C	2.54859	0.10269	-0.89045		
	H	2.71525	-1.67980	0.54254		
	H	1.63961	2.17653	-1.25309		
	C	-0.10733	0.18467	-0.81790		
	C	0.23253	-1.03398	-0.24954		
	C	-0.96484	0.89648	0.14958		
	O	-1.55086	1.93841	0.06275		
	C	-0.40946	-1.09344	1.07804		
	O	-0.45832	-1.97488	1.88878		
	H	-0.16131	0.42274	-1.87142		
	H	0.49867	-1.94561	-0.76683		
	O	-1.01326	0.13504	1.30947		
	H	2.11954	0.03127	2.46096		
	H	1.46799	2.36755	1.37317		
	H	3.61537	0.36433	-0.96719		
	H	2.26460	-0.40584	-1.81271		
TScc	C	1.79702	1.49129	0.82885	**TSfa**	
$ClCH_2CH_2Cl$	C	1.78581	1.35679	-0.55931	**$PhCH_3$**	
	C	2.14057	0.25924	1.40262		

	N	-2.18053	-2.20005	0.24654		
TScc	C	1.79701	1.49120	0.82864		
THF	C	1.78576	1.35670	-0.55943		
	C	2.14057	0.25914	1.40242		
	C	2.35107	-0.67109	0.38488		
	C	2.54647	0.10201	-0.89053		
	H	2.71766	-1.67953	0.54189		
	H	1.64231	2.17697	-1.25411		
	C	-0.10782	0.18534	-0.81739		
	C	0.23242	-1.03417	-0.24867		
	C	-0.96554	0.89407	0.14722		
	O	-1.55994	1.93376	0.06490		
	C	-0.41063	-1.09443	1.07477		
	O	-0.46890	-1.97524	1.88830		
	H	-0.15798	0.42316	-1.87151		
	H	0.50199	-1.94434	-0.76749		
	O	-1.01475	0.13418	1.30895		
	H	2.12679	0.03407	2.46292		
	H	1.47525	2.37087	1.37469		
	H	3.61351	0.36284	-0.96905		
	H	2.26050	-0.40676	-1.81194		
TScc	C	1.79660	1.49058	0.82783		
$PhCH_3$	C	1.78363	1.35557	-0.55986		
	C	2.14026	0.25850	1.40152		
	C	2.34902	-0.67176	0.38410		
	C	2.54849	0.10268	-0.89042		
	H	2.71533	-1.67979	0.54252		
	H	1.63976	2.17660	-1.25312		
	C	-0.10741	0.18471	-0.81789		
	C	0.23251	-1.03403	-0.24947		
	C	-0.96491	0.89627	0.14938		
	O	-1.55162	1.93803	0.06289		
	C	-0.40955	-1.09351	1.07779		
	O	-0.45918	-1.97492	1.88874		
	H	-0.16120	0.42270	-1.87146		
	H	0.49879	-1.94557	-0.76690		
	O	-1.01334	0.13498	1.30943		
	H	2.12015	0.03149	2.46112		
	H	1.46863	2.36784	1.37330		
	H	3.61528	0.36422	-0.96733		
	H	2.26453	-0.40584	-1.81270		
TSfa	C	-3.73697	1.17725	-1.07487		
$PhCH_3$	C	-2.69210	0.61584	-0.33162		
	C	-1.51497	1.38504	0.05295		

	C 2.35113 -0.67103 0.38501 C 2.54613 0.10196 -0.89044 H 2.71772 -1.67956 0.54179 H 1.64236 2.17694 -1.25420 C -0.10803 0.18531 -0.81753 C 0.23226 -1.03435 -0.24874 C -0.96542 0.89384 0.14682 O -1.56077 1.93335 0.06527 C -0.41054 -1.09454 1.07432 O -0.46990 -1.97510 1.88842 H -0.15766 0.42299 -1.87177 H 0.50225 -1.94431 -0.76783 O -1.01453 0.13420 1.30887 H 2.12774 0.03440 2.46324 H 1.47616 2.37132 1.37496 H 3.61320 0.36278 -0.96900 H 2.26027 -0.40678 -1.81187		C -2.66633 -0.77194 -0.10333 C -1.53259 -1.32425 0.58329 C -0.66503 -0.50988 1.35217 C -0.70416 0.89190 1.15191 C -4.76828 0.38047 -1.52880 C -3.69777 -1.57851 -0.61732 C 0.27873 -1.05491 2.26165 C 0.16106 1.72226 1.89605 C 1.01462 1.17376 2.82088 C 1.08311 -0.22606 2.99627 H 0.36172 -2.13116 2.35288 H 0.16963 2.78692 1.70092 H 1.66410 1.81940 3.40376 H 1.79212 -0.64491 3.70307 C -4.74667 -1.00291 -1.29926 H -3.71221 2.23434 -1.31162 H -5.58539 0.82194 -2.09050 H -3.64376 -2.65364 -0.49630 H -5.54723 -1.62632 -1.68480 N 1.75111 0.01924 -1.02066 C 1.01909 1.19173 -0.98478 C 0.87237 -1.03925 -1.31506 N -0.40905 -0.48805 -1.49797 N -0.33972 0.81540 -1.31085 O 1.40978 2.31622 -0.79686 O 1.17026 -2.20316 -1.44648 C 3.15514 -0.09123 -0.82416 C 3.88468 -1.01955 -1.56433 C 3.79358 0.73270 0.10007 C 5.25586 -1.12279 -1.36893 C 5.16761 0.62709 0.27539 C 5.90323 -0.30028 -0.45360 H 3.37713 -1.66214 -2.27165 H 3.21827 1.45463 0.66448 H 5.82077 -1.85009 -1.94393 H 5.66354 1.27471 0.99201 H 6.97622 -0.38147 -0.30969 O -1.56263 2.73876 -0.14606 C -2.35922 3.46319 0.79045 H -3.40917 3.15902 0.74203 H -1.99770 3.32999 1.81435 H -2.26921 4.51177 0.50632 O -1.42737 -2.67047 0.67855 C -2.12022 -3.28620 1.76975

			H -1.75150 -2.91290 2.72965 H -3.19726 -3.10642 1.70161 H -1.91877 -4.35381 1.68701

Table s2 The optimized geometries(in Å) for transtition states of substituted antharacene with **2a**,**2b** and **2c**, obtained with CAM-B3LYP+IDSCRF/6-31G(d)

Species	Cartesian coordinates	Species	Cartesian coordinates
TSda **PhCH$_3$**	C -4.11691 -0.11153 -1.47642 C -3.01901 0.13395 -0.63750 C -1.80115 0.72080 -1.11674 C -3.04313 -0.29111 0.70752 C -1.86234 -0.07890 1.50869 C -0.98620 0.99393 1.15326 C -0.98056 1.43599 -0.19407 C -5.24547 -0.72089 -0.97542 C -4.19861 -0.93756 1.19068 C -0.08199 1.59208 2.06766 C -0.09168 2.45753 -0.59730 C 0.74176 3.04581 0.31988 C 0.74624 2.60663 1.66150 H -0.06349 1.26268 3.09995 H -0.08858 2.77231 -1.63599 H 1.40495 3.84949 0.01562 H 1.41506 3.07560 2.37614 C -5.28560 -1.12970 0.36744 H -4.06852 0.19698 -2.51651 H -1.73331 0.97654 -2.16947 H -6.10423 -0.88942 -1.61752 H -4.24655 -1.26511 2.22257 H -6.17889 -1.60677 0.75823 N 1.42147 -0.85605 -0.37581 C 0.61462 -0.51585 -1.44909 C 0.61120 -1.45761 0.59467 N -0.70043 -1.54927 0.05792 N -0.70592 -0.99952 -1.13552 O 0.92590 0.03028 -2.47890 O 0.96610 -1.88270 1.66974 C 2.82241 -0.62746 -0.27283 C 3.62576 -1.55981 0.38046 C 3.38284 0.51673 -0.83582 C 4.99335 -1.33629 0.47393 C 4.75409 0.72032 -0.74539 C 5.56347 -0.20030 -0.08979 H 3.17934 -2.44161 0.82117	**TSea** **PhCH$_3$**	C -4.19644 -0.06986 -1.43228 C -3.03520 0.14580 -0.66958 C -1.84592 0.76673 -1.21616 C -2.99356 -0.30478 0.66593 C -1.77756 -0.10467 1.41965 C -0.95426 1.00803 1.05593 C -1.00190 1.47121 -0.28508 C -5.29712 -0.68410 -0.87588 C -4.11630 -0.96030 1.20469 C -0.05241 1.61994 1.96120 C -0.16269 2.54164 -0.67355 C 0.66960 3.14296 0.23735 C 0.72871 2.67501 1.56503 H -0.00252 1.26982 2.98531 H -0.19626 2.90540 -1.69327 H 1.28563 3.98383 -0.06585 H 1.39384 3.15351 2.27674 C -5.25599 -1.13269 0.45094 H -4.23935 0.27061 -2.45975 H -6.19684 -0.82121 -1.46739 H -4.09674 -1.31153 2.22942 H -6.12414 -1.61727 0.88662 N 1.43808 -0.87753 -0.35181 C 0.66462 -0.52406 -1.44820 C 0.60396 -1.48938 0.58216 N -0.70384 -1.53171 0.01853 N -0.66969 -0.98125 -1.17765 O 1.03925 0.00184 -2.46963 O 0.93021 -1.96143 1.64647 C 2.83816 -0.66877 -0.21391 C 3.62569 -1.64959 0.38405 C 3.41112 0.50991 -0.68440 C 4.99263 -1.44083 0.51492 C 4.78152 0.69951 -0.55927 C 5.57586 -0.27056 0.04175 H 3.16709 -2.55792 0.75349 H 2.78753 1.26259 -1.14893

	H 2.75090 1.23056 -1.34666 H 5.61623 -2.06250 0.98701 H 5.18947 1.60996 -1.19013 H 6.63392 -0.03394 -0.01925 C -1.73832 -0.73211 2.85001 H -2.15937 -0.09281 3.63585 H -2.25774 -1.68991 2.86982 H -0.69047 -0.92610 3.08458		H 5.60466 -2.20430 0.98516 H 5.22827 1.61627 -0.93172 H 6.64576 -0.11542 0.14076 C -1.63523 -0.74882 2.76490 H -2.17820 -0.17365 3.52511 H -2.03554 -1.76304 2.74928 H -0.59010 -0.82200 3.06178 C -1.82190 1.12570 -2.67353 H -0.80323 1.28870 -3.02072 H -2.24281 0.31716 -3.27173 H -2.41043 2.03363 -2.85146
TSfa **$PhCH_3$**	C -4.20254 -0.01466 -1.48590 C -3.03005 0.09423 -0.71927 C -1.82869 0.72770 -1.21844 C -3.02752 -0.37230 0.61248 C -1.82340 -0.18555 1.39265 C -0.95998 0.90744 1.05753 C -0.96722 1.37917 -0.27643 C -5.33973 -0.57439 -0.94547 C -4.19875 -0.93690 1.14585 C -0.04584 1.45647 1.98474 C -0.06821 2.39978 -0.65871 C 0.78195 2.94533 0.27006 C 0.79555 2.46869 1.59842 H -0.03272 1.06736 2.99517 H -0.07510 2.74017 -1.68680 H 1.45589 3.74574 -0.01900 H 1.48281 2.90343 2.31720 C -5.33761 -1.03778 0.37681 H -4.22522 0.38514 -2.49201 H -6.24644 -0.63387 -1.53895 H -4.22018 -1.25388 2.18071 H -6.24262 -1.45590 0.80582 N 1.44093 -0.93654 -0.33015 C 0.64515 -0.69777 -1.44834 C 0.62302 -1.47827 0.66038 N -0.67277 -1.62770 0.09583 N -0.66083 -1.17186 -1.13825 O 0.98923 -0.22572 -2.50869 O 0.94705 -1.81247 1.77796 C 2.83198 -0.66676 -0.21342 C 3.63693 -1.51326 0.54690 C 3.38555 0.43284 -0.86610 C 4.99607 -1.24899 0.65658	**TSga** **$PhCH_3$**	C -3.86762 1.05120 -1.02526 C -2.73298 0.54757 -0.36531 C -1.57773 1.37330 -0.04890 C -2.65395 -0.83347 -0.09307 C -1.44480 -1.34861 0.51106 C -0.66013 -0.45718 1.30930 C -0.74919 0.93560 1.05450 C -4.91519 0.22174 -1.36201 C -3.71828 -1.67005 -0.48150 C 0.26653 -0.91675 2.28026 C 0.06709 1.82226 1.79527 C 0.91425 1.35098 2.76703 C 1.01997 -0.03240 3.00743 H 0.36977 -1.97892 2.46343 H 0.02136 2.88582 1.60017 H 1.51334 2.04737 3.34547 H 1.70469 -0.39922 3.76533 C -4.83970 -1.14878 -1.08694 H -3.93123 2.10383 -1.26904 H -5.79379 0.63122 -1.85038 H -3.66551 -2.73559 -0.29755 H -5.66051 -1.80430 -1.36049 N 1.76225 -0.07909 -0.99698 C 0.97809 1.05086 -1.16874 C 0.93871 -1.19911 -1.13462 N -0.36621 -0.73361 -1.43181 N -0.34748 0.58771 -1.46959 O 1.33686 2.20500 -1.14672 O 1.28061 -2.35856 -1.07624 C 3.16135 -0.09512 -0.74131 C 3.95845 -1.07529 -1.32836 C 3.72495 0.87178 0.08754 C 5.32412 -1.08616 -1.07532

	C 4.74879 0.67711 -0.75726 C 5.55861 -0.15756 0.00433 H 3.19665 -2.35929 1.05809 H 2.75356 1.07946 -1.45940 H 5.61866 -1.90844 1.25350 H 5.17750 1.53187 -1.27163 H 6.62260 0.04095 0.08876 O -1.72634 1.13573 -2.48614 C -1.90734 0.20868 -3.56786 H -0.92986 0.05641 -4.02450 H -2.28574 -0.74689 -3.20845 H -2.60349 0.66012 -4.27769 O -1.69990 -0.66738 2.63055 C -1.92099 -2.05968 2.90210 H -2.21588 -2.59095 1.99842 H -0.97449 -2.46268 3.26011 H -2.69142 -2.14036 3.67203		C 5.09429 0.85668 0.32085 C 5.89772 -0.12094 -0.25505 H 3.50800 -1.82715 -1.96336 H 3.09557 1.62991 0.53487 H 5.94282 -1.85348 -1.53035 H 5.53291 1.61465 0.96264 H 6.96667 -0.13056 -0.06582 C -1.25513 -2.83680 0.62721 H -1.60491 -3.30766 -0.29434 H -0.18797 -3.06022 0.67428 C -1.62086 2.84017 -0.40813 H -0.60204 3.22713 -0.43242 H -1.99066 2.93383 -1.43181 C -2.48481 3.67752 0.54530 H -2.11652 3.63081 1.57358 H -2.47189 4.72566 0.23276 H -3.52543 3.34340 0.55833 C -1.97651 -3.45095 1.83792 H -3.05536 -3.27860 1.79987 H -1.80733 -4.53122 1.86242 H -1.61340 -3.03157 2.77993
TSha **$PhCH_3$**	C 2.86315 -3.21458 -0.63922 C 2.09026 -2.18116 -0.09420 C 0.74810 -2.39619 0.37935 C 2.57009 -0.85377 -0.09904 C 1.74343 0.18822 0.45362 C 0.67843 -0.15007 1.33456 C 0.22522 -1.49723 1.36667 C 4.11590 -2.94696 -1.14772 C 3.84804 -0.60063 -0.64314 C 0.01483 0.80177 2.15921 C -0.80143 -1.87630 2.25901 C -1.36977 -0.94644 3.09165 C -0.96920 0.40700 3.02504 H 0.30284 1.84398 2.10417 H -1.13211 -2.90940 2.27063 H -2.14161 -1.24517 3.79422 H -1.45211 1.14068 3.66256 C 4.60815 -1.63216 -1.14594 H 2.46544 -4.22511 -0.64908 H 0.37667 -3.41607 0.38714 H 4.72227 -3.75123 -1.55237 H 4.23416 0.41139 -0.64951 H 5.59587 -1.42677 -1.54657	**TSdb** **$ClCH_2CH_2Cl$**	C 2.47626 -0.42784 -1.63044 C 1.25037 -0.64023 -0.98207 C 0.00907 0.03809 -1.35305 C 1.23694 -1.47127 0.16803 C 0.00352 -1.71740 0.80371 C -1.22721 -1.46868 0.16384 C -1.23496 -0.63765 -0.98631 C 3.63191 -1.01821 -1.15472 C 2.43685 -2.02425 0.66812 C -2.42996 -2.01915 0.65983 C -2.45816 -0.42275 -1.63891 C -3.61667 -1.01070 -1.16714 C -3.61078 -1.80150 -0.00779 H -2.39851 -2.63039 1.55683 H -2.50743 0.19076 -2.52948 H -4.54851 -0.84982 -1.70065 H -4.53539 -2.23760 0.35606 C 3.62040 -1.80905 0.00457 H 2.52986 0.18561 -2.52082 H 4.56592 -0.85923 -1.68501 H 2.40105 -2.63547 1.56497 H 4.54284 -2.24708 0.37157 C 0.00526 0.94908 1.44286

	N -2.01035 -0.35826 -0.93704 C -1.61723 -1.66256 -0.72356 C -0.89603 0.35816 -1.41148 N 0.17907 -0.54692 -1.52292 N -0.23282 -1.73122 -1.13678 O -2.26835 -2.60007 -0.33227 O -0.88133 1.52125 -1.74168 C -3.31680 0.16537 -0.72891 C -3.82685 1.11685 -1.60917 C -4.07843 -0.28388 0.34701 C -5.10397 1.62192 -1.40188 C -5.35912 0.22062 0.53420 C -5.87550 1.17509 -0.33487 H -3.22119 1.46595 -2.43534 H -3.67164 -1.02608 1.02142 H -5.49818 2.36694 -2.08610 H -5.95390 -0.13451 1.37020 H -6.87534 1.56918 -0.18141 C 2.19533 1.59725 0.30953 C 2.74119 2.28142 1.40066 C 2.13157 2.23447 -0.93207 C 3.20937 3.58133 1.25339 C 2.58984 3.53903 -1.07099 C 3.13055 4.21441 0.01756 H 2.81402 1.78560 2.36415 H 1.69395 1.71097 -1.77342 H 3.63839 4.09811 2.10648 H 2.52239 4.02895 -2.03748 H 3.49140 5.23215 -0.09654		C 0.00803 1.47734 0.09522 C -1.20886 0.82484 2.16293 N -2.21040 0.70811 2.73731 C 1.21673 0.82229 2.16692 N 2.21612 0.70337 2.74460 C 1.20685 2.20645 -0.27064 N 2.16639 2.77088 -0.57913 C -1.18807 2.20893 -0.27458 N -2.14541 2.77532 -0.58628 H 0.00134 -2.27440 1.73917 C 0.01203 0.81951 -2.65063 H -0.86548 1.45945 -2.74373 H 0.89145 1.45721 -2.74108 H 0.01242 0.12473 -3.49689
TSeb $ClCH_2CH_2Cl$	C -4.25345 0.01808 -1.35581 C -3.08291 0.21345 -0.60142 C -1.89567 0.83667 -1.15021 C -3.02705 -0.26946 0.72640 C -1.78595 -0.11158 1.45711 C -0.97204 1.03729 1.11519 C -1.02805 1.52029 -0.21262 C -5.34833 -0.60677 -0.79678 C -4.14315 -0.93484 1.26398 C -0.09193 1.64154 2.03046 C -0.20247 2.59453 -0.58928 C 0.62801 3.19414 0.33402 C 0.68348 2.71600 1.64837 H -0.03904 1.28523 3.05192 H -0.23538 2.97805 -1.60169	**TSfb** $ClCH_2CH_2Cl$	C -2.18454 -1.62986 -1.11616 C -1.11640 -0.72992 -0.99340 C 0.23121 -1.19955 -0.71797 C -1.37047 0.66476 -1.04764 C -0.25142 1.55303 -0.89091 C 1.08985 1.07463 -1.08015 C 1.33265 -0.31488 -1.05556 C -3.46267 -1.17051 -1.35661 C -2.68598 1.10726 -1.30968 C 2.16228 1.97328 -1.24921 C 2.64614 -0.78136 -1.21100 C 3.67854 0.11100 -1.41841 C 3.43796 1.49232 -1.43538 H 1.96651 3.03815 -1.24331 H 2.84508 -1.84403 -1.14955

	H 1.24060 4.04004 0.03845 H 1.33909 3.19145 2.37109 C -5.29298 -1.08490 0.51759 H -4.31329 0.38431 -2.37338 H -6.25578 -0.72769 -1.37996 H -4.11729 -1.30848 2.28029 H -6.15753 -1.57628 0.95266 C -0.62497 -1.55738 0.17912 C -0.68198 -1.06013 -1.18755 C 0.62636 -1.46278 0.87365 N 1.61569 -1.35937 1.46504 C -1.37816 -2.73674 0.49370 N -2.00999 -3.66369 0.77789 C -1.48740 -1.78237 -2.12922 N -2.16306 -2.32727 -2.89458 C 0.51662 -0.50777 -1.74908 N 1.46194 -0.02208 -2.20701 C -1.66899 -0.70548 2.83336 H -2.09915 -1.70676 2.87691 H -0.62939 -0.76948 3.15668 H -2.20618 -0.07864 3.55470 C -1.89713 1.26741 -2.59064 H -0.88630 1.45255 -2.95590 H -2.35727 0.51673 -3.23423 H -2.46799 2.19701 -2.69919		H 4.68917 -0.26158 -1.55438 H 4.26110 2.18353 -1.58456 C -3.71007 0.20269 -1.47289 H -1.99348 -2.69100 -1.01753 H -4.27793 -1.87892 -1.46555 H -2.90081 2.15896 -1.42899 H -4.71147 0.55890 -1.69106 C -0.01931 0.37036 1.74616 C 0.24349 -0.99071 1.34191 C 1.03749 1.26952 2.02139 N 1.90083 2.01753 2.23178 C -1.33243 0.77246 2.08773 N -2.41361 1.11027 2.34708 C -0.77701 -1.96072 1.67912 N -1.60501 -2.72248 1.94120 C 1.56917 -1.49658 1.62630 N 2.63293 -1.88854 1.84830 O 0.45734 -2.55478 -0.80038 C 0.53310 -3.09893 -2.12333 H -0.40693 -2.95531 -2.66298 H 1.34892 -2.64337 -2.69088 H 0.72421 -4.16420 -1.99528 O -0.32714 2.85494 -0.73100 C -1.41897 3.58113 -0.14016 H -2.03057 4.02267 -0.92870 H -2.01275 2.94172 0.51089 H -0.94641 4.37322 0.43996
TShb $ClCH_2CH_2Cl$	C -4.15777 -0.07132 -1.30219 C -3.02347 0.13613 -0.51306 C -1.80426 0.69661 -1.06750 C -2.99691 -0.33883 0.82628 C -1.86791 -0.03657 1.64797 C -0.87940 0.89947 1.20698 C -0.89429 1.34444 -0.14044 C -5.24257 -0.76181 -0.79522 C -4.09085 -1.11131 1.29057 C 0.08041 1.44596 2.09318 C 0.01917 2.31404 -0.56287 C 0.93511 2.84238 0.32717 C 0.96957 2.40090 1.65700 H 0.09500 1.12749 3.12774 H -0.00309 2.65406 -1.59333 H 1.62987 3.60732 -0.00592 H 1.69229 2.82199 2.34831	**TSdc** 1,4-dioxane	C -4.18713 -0.06160 -1.42224 C -3.05431 0.16558 -0.61647 C -1.84597 0.74108 -1.12655 C -3.03991 -0.28013 0.72436 C -1.81995 -0.10661 1.47624 C -0.97713 1.00544 1.12279 C -1.00108 1.45207 -0.21924 C -5.29981 -0.67414 -0.89684 C -4.18796 -0.92766 1.23335 C -0.07287 1.61351 2.02442 C -0.12636 2.47748 -0.63576 C 0.71763 3.07367 0.26815 C 0.74061 2.63881 1.60728 H -0.03468 1.28299 3.05582 H -0.13926 2.79170 -1.67499 H 1.37474 3.87720 -0.04890 H 1.41356 3.11374 2.31422

	C -5.19712 -1.30423 0.49619 H -4.17689 0.31060 -2.31794 H -1.91671 1.19358 -2.03120 H -6.12547 -0.90506 -1.41069 H -4.05803 -1.54821 2.27965 H -6.03466 -1.88473 0.86903 C -0.49865 -1.75988 -0.48727 C -0.82317 -0.88160 -1.60161 C 0.74805 -1.64891 0.16338 N 1.77101 -1.54086 0.70552 C -1.35695 -2.82275 -0.13593 N -2.08004 -3.68556 0.15406 C -1.71216 -1.46703 -2.59483 N -2.42517 -1.91381 -3.38547 C 0.33302 -0.29486 -2.26451 N 1.23792 0.19090 -2.79204 C -1.80143 -0.55100 3.03769 C -2.79019 -0.20487 3.96643 C -0.73287 -1.35614 3.44524 C -2.71207 -0.66260 5.27517 C -0.67374 -1.83051 4.74936 C -1.65991 -1.48396 5.66671 H -3.60885 0.44274 3.66775 H 0.05003 -1.61426 2.74068 H -3.47795 -0.37660 5.98950 H 0.15220 -2.46798 5.04950 H -1.60566 -1.84877 6.68796		C -5.29950 -1.10420 0.44283 H -4.17515 0.27181 -2.45623 H -6.18119 -0.82480 -1.51231 H -4.20810 -1.26375 2.26373 H -6.18421 -1.57907 0.85540 C -0.69483 -1.63127 0.10299 C -0.76954 -1.12868 -1.19567 C 0.66703 -1.38641 0.58981 O 1.19841 -1.67616 1.62656 C 0.57498 -0.60447 -1.52999 O 0.99716 -0.15172 -2.55590 H -1.29191 -2.42605 0.52420 H -1.39456 -1.51674 -1.98770 O 1.35732 -0.68164 -0.39336 C -1.68556 -0.72082 2.84225 H -0.63657 -0.90580 3.08187 H -2.10118 -0.05854 3.61140 H -2.21009 -1.67556 2.90516 H -1.82198 1.03372 -2.17382
TSec **1,4-dioxane**	C -4.21431 -0.04438 -1.42824 C -3.04431 0.15361 -0.66376 C -1.84662 0.75138 -1.20606 C -3.01378 -0.30272 0.67489 C -1.78682 -0.14354 1.42001 C -0.96588 0.98677 1.06858 C -0.99620 1.44325 -0.27172 C -5.32171 -0.64678 -0.87907 C -4.15410 -0.94275 1.20642 C -0.07642 1.59711 1.98167 C -0.13599 2.49600 -0.65797 C 0.69474 3.09386 0.25778 C 0.72473 2.64087 1.58809 H -0.04093 1.25270 3.00831 H -0.14682 2.84991 -1.68194 H 1.33299 3.91698 -0.04758 H 1.38604 3.11555 2.30606	**TSfc** **1,4-dioxane**	C -4.21587 -0.09608 -1.45844 C -3.03262 0.03792 -0.70687 C -1.83636 0.66355 -1.22754 C -3.00655 -0.41694 0.62993 C -1.78486 -0.22515 1.38131 C -0.96809 0.90994 1.04101 C -0.99431 1.36463 -0.29464 C -5.33439 -0.67085 -0.89910 C -4.16458 -0.99517 1.18447 C -0.09047 1.51382 1.96475 C -0.14250 2.41700 -0.68856 C 0.68179 3.01265 0.23512 C 0.70790 2.55904 1.56773 H -0.06872 1.14288 2.98183 H -0.16103 2.74361 -1.72081 H 1.32366 3.83483 -0.06543 H 1.36970 3.03492 2.28458

	C -5.29134 -1.09987 0.44958 H -4.25574 0.31081 -2.45110 H -6.22315 -0.76595 -1.47203 H -4.14865 -1.28674 2.23393 H -6.16930 -1.56898 0.88261 C -0.68447 -1.64536 0.15473 C -0.71535 -1.19740 -1.16550 C 0.68034 -1.41108 0.65832 O 1.18924 -1.69525 1.70759 C 0.63001 -0.68560 -1.47968 O 1.09028 -0.26544 -2.50551 H -1.27881 -2.44615 0.56995 H -1.33904 -1.58759 -1.95646 O 1.39017 -0.73317 -0.32095 C -1.79886 1.13155 -2.66231 H -0.76925 1.18754 -3.01857 H -2.31713 0.39903 -3.28333 H -2.27377 2.10614 -2.82698 C -1.67470 -0.73036 2.80224 H -0.63073 -0.88861 3.07653 H -2.12953 -0.06587 3.54658 H -2.17682 -1.69706 2.86738		C -5.30861 -1.12289 0.42998 H -4.25795 0.30573 -2.46352 H -6.24923 -0.74737 -1.47826 H -4.16727 -1.28989 2.22684 H -6.20362 -1.54731 0.87384 C -0.61638 -1.70675 0.13684 C -0.64262 -1.25904 -1.18510 C 0.73177 -1.43189 0.65923 O 1.23517 -1.69929 1.71619 C 0.68913 -0.70687 -1.48058 O 1.15172 -0.27062 -2.49931 H -1.17979 -2.54460 0.51834 H -1.23034 -1.69963 -1.97598 O 1.43568 -0.73687 -0.31232 O -1.83177 1.16426 -2.49185 C -1.83151 0.29570 -3.62364 H -0.82318 -0.08981 -3.78692 H -2.54035 -0.52878 -3.51056 H -2.13599 0.91188 -4.47057 O -1.72944 -0.59918 2.68763 C -1.70562 -1.97704 3.05628 H -2.42581 -2.56908 2.48563 H -0.69708 -2.37329 2.92243 H -1.97855 -2.00655 4.11193
TShc **$PhCH_3$**	C -4.17693 0.05671 -1.42816 C -3.05106 0.22998 -0.60322 C -1.79120 0.70993 -1.10625 C -3.07717 -0.21602 0.73609 C -1.87747 -0.06380 1.52446 C -0.93395 0.95806 1.15311 C -0.91633 1.39072 -0.19235 C -5.31815 -0.52605 -0.92864 C -4.24861 -0.85049 1.21293 C 0.00173 1.51144 2.05888 C 0.02053 2.35540 -0.60942 C 0.89755 2.90183 0.29700 C 0.88693 2.47391 1.63794 H 0.00376 1.17915 3.09022 H 0.03552 2.66202 -1.65091 H 1.60617 3.65975 -0.02162 H 1.58894 2.90527 2.34458 C -5.34878 -0.98700 0.40017 H -4.13461 0.39762 -2.45892 H -1.76117 1.03238 -2.14530	**TSfa-1** **$PhCH_3$**	C -3.73697 1.17725 -1.07487 C -2.69210 0.61584 -0.33162 C -1.51497 1.38504 0.05295 C -2.66633 -0.77194 -0.10333 C -1.53259 -1.32425 0.58329 C -0.66503 -0.50988 1.35217 C -0.70416 0.89190 1.15191 C -4.76828 0.38047 -1.52880 C -3.69777 -1.57851 -0.61732 C 0.27873 -1.05491 2.26165 C 0.16106 1.72226 1.89605 C 1.01462 1.17376 2.82088 C 1.08311 -0.22606 2.99627 H 0.36172 -2.13116 2.35288 H 0.16963 2.78692 1.70092 H 1.66410 1.81940 3.40376 H 1.79212 -0.64491 3.70307 C -4.74667 -1.00291 -1.29926 H -3.71221 2.23434 -1.31162 H -5.58539 0.82194 -2.09050

	H -6.19405 -0.63811 -1.56011 H -4.27924 -1.21962 2.23080 H -6.24748 -1.45851 0.78535 C -0.77385 -1.69513 0.02394 C -0.90501 -1.09920 -1.24147 C 0.63501 -1.60938 0.40084 O 1.23996 -2.04365 1.34376 C 0.46668 -0.68759 -1.65372 O 0.84713 -0.22236 -2.69007 H -1.41012 -2.45990 0.44240 H -1.56798 -1.46682 -2.01463 O 1.31220 -0.89132 -0.58998 C -1.90695 -0.51956 2.95265 C -2.71819 0.18950 3.84755 C -1.15052 -1.58744 3.43300 C -2.77980 -0.16907 5.18754 C -1.21779 -1.94638 4.77658 C -2.03113 -1.24407 5.65612 H -3.30359 1.03018 3.48619 H -0.48353 -2.12552 2.77072 H -3.41412 0.39381 5.86570 H -0.62142 -2.78058 5.13361 H -2.07856 -1.52755 6.70318		H -3.64376 -2.65364 -0.49630 H -5.54723 -1.62632 -1.68480 N 1.75111 0.01924 -1.02066 C 1.01909 1.19173 -0.98478 C 0.87237 -1.03925 -1.31506 N -0.40905 -0.48805 -1.49797 N -0.33972 0.81540 -1.31085 O 1.40978 2.31622 -0.79686 O 1.17026 -2.20316 -1.44648 C 3.15514 -0.09123 -0.82416 C 3.88468 -1.01955 -1.56433 C 3.79358 0.73270 0.10007 C 5.25586 -1.12279 -1.36893 C 5.16761 0.62709 0.27539 C 5.90323 -0.30028 -0.45360 H 3.37713 -1.66214 -2.27165 H 3.21827 1.45463 0.66448 H 5.82077 -1.85009 -1.94393 H 5.66354 1.27471 0.99201 H 6.97622 -0.38147 -0.30969 O -1.56263 2.73876 -0.14606 C -2.35922 3.46319 0.79045 H -3.40917 3.15902 0.74203 H -1.99770 3.32999 1.81435 H -2.26921 4.51177 0.50632 O -1.42737 -2.67047 0.67855 C -2.12022 -3.28620 1.76975 H -1.75150 -2.91290 2.72965 H -3.19726 -3.10642 1.70161 H -1.91877 -4.35381 1.68701
TSfb-1 $ClCH_2CH_2Cl$	C 2.58510 0.88786 -1.33702 C 1.32752 0.32571 -1.11873 C 0.14221 1.14148 -0.80446 C 1.21019 -1.07849 -1.00582 C -0.08417 -1.64126 -0.81139 C -1.27678 -0.87632 -0.95974 C -1.17026 0.52879 -1.07127 C 3.69799 0.07115 -1.45817 C 2.36224 -1.88902 -1.06391 C -2.54543 -1.49090 -0.97639 C -2.32783 1.28695 -1.24524 C -3.56126 0.66042 -1.32514 C -3.67362 -0.72685 -1.17777 H -2.62325 -2.55987 -0.81902	**TSfc-1** 1,4-dioxane	C -4.21266 -0.14605 -1.42713 C -3.09729 0.17617 -0.62890 C -1.90348 0.79109 -1.15994 C -3.05049 -0.26490 0.70686 C -1.81343 -0.06039 1.42262 C -0.96916 1.05248 1.06991 C -1.01596 1.49446 -0.26877 C -5.27128 -0.83895 -0.88742 C -4.11960 -1.02243 1.22492 C 0.00288 1.58507 1.94288 C -0.08924 2.46115 -0.71284 C 0.80905 3.01023 0.17021 C 0.85523 2.56999 1.50530 H 0.09037 1.18874 2.94698

	H -2.26158 2.36702 -1.29413		H -0.07217 2.74090 -1.75895
	H -4.45407 1.25896 -1.47793		H 1.50959 3.76520 -0.17212
	H -4.65074 -1.19776 -1.20528		H 1.59095 2.98818 2.18483
	C 3.59080 -1.31625 -1.30830		C -5.22433 -1.28006 0.44695
	H 2.69185 1.96459 -1.38790		H -4.21853 0.13674 -2.47310
	H 4.66943 0.51837 -1.64518		H -6.13714 -1.06777 -1.50074
	H 2.27314 -2.95672 -0.90399		H -4.05357 -1.41824 2.23140
	H 4.47784 -1.93827 -1.36763		H -6.05414 -1.84727 0.85675
	C 0.08376 -0.18702 1.67438		C -0.76875 -1.54656 0.19804
	C 0.17892 1.14997 1.06896		C -0.81345 -1.10213 -1.13314
	C -1.16523 -0.69549 2.08784		C 0.61758 -1.35482 0.66999
	N -2.20391 -1.11517 2.39844		O 1.13917 -1.65536 1.70491
	C 1.25109 -0.88661 2.04492		C 0.54650 -0.63860 -1.47756
	N 2.22109 -1.46520 2.32018		O 0.99866 -0.24880 -2.51537
	C 1.43048 1.83996 1.37039		H -1.36019 -2.34406 0.62508
	N 2.42300 2.37599 1.61494		H -1.44221 -1.49914 -1.91764
	C -0.93475 2.02906 1.41581		O 1.32385 -0.69643 -0.32856
	N -1.81957 2.71502 1.69651		O -1.89459 1.12846 -2.48839
	O 0.24716 2.49576 -1.06957		C -2.57986 2.33523 -2.82854
	C 0.25157 2.86682 -2.45119		H -3.64398 2.27182 -2.58180
	H 1.09679 2.41770 -2.97951		H -2.14757 3.19838 -2.31478
	H -0.67883 2.57182 -2.94370		H -2.46007 2.45388 -3.90562
	H 0.34552 3.95245 -2.46492		O -1.71094 -0.57879 2.68723
	O -0.18832 -2.95878 -0.59911		C -2.35192 0.17153 3.72059
	C -0.27217 -3.82595 -1.74798		H -1.94672 1.18510 3.78758
	H -0.33838 -4.83573 -1.34721		H -3.43226 0.23140 3.55798
	H -1.16399 -3.59392 -2.33535		H -2.15030 -0.36427 4.64838
	H 0.62141 -3.72427 -2.36863		

Table s3 The optimized geometries(in Å) for transtition states, obtained with CAM-B3LYP+IDSCRF/6-311++G(d,p) and BMK+IDSCRF/6-311++G(d,p)

Species	Cartesian coordinates	Species	Cartesian coordinates
TSaa	C -4.14956 -0.09787 -1.47237	**TSaa**	C -4.17488 -0.06702 -1.47844
THF	C -3.03923 0.18744 -0.66343	**THF**	C -3.05323 0.19672 -0.66406
CAM	C -1.84630 0.80429 -1.15907	**BMK**	C -1.84689 0.80476 -1.16103
	C -3.02475 -0.23561 0.67776		C -3.04111 -0.24303 0.68180
	C -1.81651 -0.01128 1.41287		C -1.82211 -0.04403 1.42114
	C -0.98305 1.09201 1.07940		C -0.95619 1.04440 1.08970
	C -1.00108 1.52160 -0.26746		C -0.97430 1.49431 -0.26100
	C -5.23405 -0.75213 -0.93535		C -5.27346 -0.71552 -0.94086
	C -4.12096 -0.93939 1.19806		C -4.15193 -0.94056 1.20189
	H -1.72582 -0.44953 2.40112		H -1.73053 -0.50398 2.40316
	C -0.09327 1.69845 1.99212		C -0.02151 1.60134 2.00213
	C -0.13543 2.55762 -0.68002		C -0.06855 2.50574 -0.67520

	C 0.68309 3.16511 0.23625 C 0.70675 2.73132 1.57824 H -0.06869 1.35402 3.01969 H -0.14464 2.87763 -1.71582 H 1.32469 3.98315 -0.07054 H 1.36855 3.21891 2.28450 C -5.21970 -1.17401 0.40396 H -4.14753 0.20959 -2.51220 H -1.77945 1.01640 -2.22092 H -6.10327 -0.95370 -1.55056 H -4.09691 -1.28414 2.22584 H -6.07803 -1.69714 0.80930 N 1.40071 -0.85672 -0.27476 C 0.59789 -0.62749 -1.38481 C 0.59366 -1.31997 0.75586 N -0.72470 -1.44455 0.22243 N -0.72213 -1.03986 -1.03013 O 0.94095 -0.22433 -2.46431 O 0.93165 -1.62051 1.86990 C 2.81341 -0.67899 -0.20967 C 3.60786 -1.71871 0.25636 C 3.38008 0.52055 -0.61772 C 4.98306 -1.54867 0.32072 C 4.75792 0.67566 -0.56289 C 5.56072 -0.35434 -0.09071 H 3.15138 -2.64939 0.56883 H 2.74806 1.32108 -0.97781 H 5.60474 -2.35688 0.68778 H 5.20372 1.60913 -0.88613 H 6.63605 -0.22713 -0.04459		C 0.79388 3.06779 0.24285 C 0.82162 2.61009 1.58647 H 0.00328 1.23954 3.02649 H -0.07889 2.83851 -1.70967 H 1.46572 3.86504 -0.06247 H 1.51694 3.05989 2.28914 C -5.26234 -1.15275 0.40285 H -4.17016 0.25086 -2.51768 H -1.77811 1.02630 -2.22422 H -6.14869 -0.89964 -1.55721 H -4.13013 -1.29399 2.22944 H -6.12920 -1.66884 0.80554 N 1.37391 -0.84608 -0.29054 C 0.57314 -0.61845 -1.40317 C 0.57217 -1.35500 0.72434 N -0.74875 -1.49191 0.19035 N -0.74859 -1.06034 -1.06664 O 0.91181 -0.19328 -2.47267 O 0.91092 -1.67592 1.82984 C 2.77779 -0.63573 -0.21068 C 3.58582 -1.62575 0.35719 C 3.33596 0.54453 -0.70883 C 4.96454 -1.42525 0.42990 C 4.71835 0.72789 -0.64168 C 5.53452 -0.25143 -0.07067 H 3.13587 -2.53557 0.73974 H 2.69634 1.30130 -1.14788 H 5.59272 -2.19250 0.87290 H 5.15499 1.64207 -1.03313 H 6.60915 -0.10288 -0.01932
TSda **$PhCH_3$** **CAM**	C -4.09917 -0.15945 -1.47475 C -3.01118 0.12359 -0.63732 C -1.80801 0.72798 -1.12494 C -3.02928 -0.28149 0.71084 C -1.85654 -0.03674 1.51108 C -0.99980 1.04358 1.13995 C -1.00052 1.46546 -0.21162 C -5.21143 -0.78877 -0.96896 C -4.16739 -0.95072 1.19936 C -0.12015 1.68236 2.04822 C -0.14735 2.51111 -0.62402 C 0.65576 3.14147 0.28820 C 0.67071 2.71966 1.63325 H -0.09376 1.36962 3.08341	**TSda** **$PhCH_3$** **BMK**	C -4.12504 -0.13307 -1.48439 C -3.02351 0.13087 -0.64464 C -1.80729 0.71951 -1.13990 C -3.04582 -0.27617 0.71338 C -1.86042 -0.05456 1.51534 C -0.96646 1.00164 1.13498 C -0.96858 1.43375 -0.22452 C -5.25538 -0.74171 -0.97079 C -4.20265 -0.92625 1.20885 C -0.03861 1.59764 2.03804 C -0.07299 2.45067 -0.64679 C 0.77336 3.04475 0.26297 C 0.79435 2.60844 1.61291 H -0.00936 1.27439 3.07252

	H -0.15033 2.81393 -1.66442		H -0.07576 2.75446 -1.68962
	H 1.28819 3.96481 -0.02237		H 1.43550 3.84580 -0.05198
	H 1.31685 3.22125 2.34372		H 1.47481 3.07775 2.31681
	C -5.24497 -1.18037 0.37744		C -5.29365 -1.13352 0.38475
	H -4.05536 0.13217 -2.51785		H -4.07670 0.15634 -2.53044
	H -1.74933 0.97469 -2.17842		H -1.74206 0.96027 -2.19771
	H -6.06222 -0.98797 -1.60959		H -6.11487 -0.92291 -1.60906
	H -4.20833 -1.27041 2.23188		H -4.24848 -1.24203 2.24496
	H -6.12529 -1.67482 0.77068		H -6.18477 -1.61057 0.78156
	N 1.43168 -0.84817 -0.35335		N 1.40648 -0.85950 -0.35845
	C 0.63616 -0.51235 -1.43325		C 0.61329 -0.54446 -1.44787
	C 0.61734 -1.44389 0.61534		C 0.59574 -1.47110 0.60514
	N -0.69093 -1.52304 0.07399		N -0.71500 -1.57399 0.05946
	N -0.68811 -0.98269 -1.11986		N -0.71374 -1.02971 -1.14524
	O 0.96013 0.01268 -2.46320		O 0.93472 -0.02138 -2.47659
	O 0.96706 -1.86928 1.68482		O 0.94188 -1.88801 1.67627
	C 2.83965 -0.65831 -0.25863		C 2.80418 -0.62675 -0.24810
	C 3.63680 -1.68506 0.23277		C 3.62841 -1.61630 0.29866
	C 3.40507 0.54214 -0.66847		C 3.34680 0.57927 -0.70274
	C 5.00859 -1.50105 0.31906		C 5.00099 -1.38688 0.39898
	C 4.77991 0.71006 -0.59006		C 4.72332 0.79028 -0.60949
	C 5.58419 -0.30678 -0.09387		C 5.55331 -0.18680 -0.05570
	H 3.18443 -2.61389 0.55269		H 3.20101 -2.54952 0.64497
	H 2.77349 1.33075 -1.05274		H 2.69918 1.33314 -1.13266
	H 5.62984 -2.30013 0.70569		H 5.63922 -2.15385 0.82693
	H 5.22249 1.64374 -0.91641		H 5.14452 1.72358 -0.97076
	H 6.65721 -0.16997 -0.03084		H 6.62321 -0.01735 0.01791
	C -1.73256 -0.66584 2.86070		C -1.74199 -0.69789 2.87068
	H -2.23839 -0.05456 3.61599		H -2.25584 -0.08771 3.62604
	H -2.17675 -1.65879 2.86871		H -2.18925 -1.69290 2.86410
	H -0.68778 -0.77316 3.14530		H -0.69545 -0.80432 3.15937

Table s3 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions, without and with correction of cavities for all studied bimolecular reactions, obtained with CAM-B3LYP+IDSCRF/6-31G(d).

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
$CHCl_3$						
1a	-539.21038	-539.00318	-539.04677	-539.03510	91.7	67.2
	-539.21038	-539.00318	-539.04677	-539.03594	91.7	68.9
2a	-622.24185	-622.10431	-622.15042	-622.13831	97.0	71.6
	-622.24185	-622.10431	-622.15042	-622.13958	97.0	74.2
TSaa	-1161.43514	-1161.08950	-1161.15844	-1161.14687	145.1	120.7
	10.72	11.29	24.32	16.65	-43.7	-18.0

	10.72	11.29	24.32	17.97	-43.7	-22.4
1a	-539.21038	-539.00318	-539.04677	-539.03510	91.7	67.2
	-539.21038	-539.00318	-539.04677	-539.03532	91.7	67.6
2b	-447.30123	-447.24337	-447.28703	-447.27488	91.9	66.3
	-447.30123	-447.24337	-447.28703	-447.27636	91.9	69.4
TSab	-986.49377	-986.22802	-986.29490	-986.28275	140.8	115.2
	11.19	11.63	24.41	17.09	-42.9	-18.3
	11.19	11.63	24.41	18.15	-42.9	-21.9
1a	-539.21038	-539.00318	-539.04677	-539.03510	91.7	67.2
	-539.21038	-539.00318	-539.04677	-539.03532	91.7	67.6
2c	-379.14266	-379.07984	-379.11429	-379.10198	72.5	46.6
	-379.14266	-379.07984	-379.11429	-379.10351	72.5	49.8
TSac	-918.32508	-918.05406	-918.11151	-918.09951	120.9	95.7
	17.55	18.17	31.09	23.58	-43.3	-18.1
	17.55	18.17	31.09	24.67	-43.3	-21.8
1b	-271.31563	-271.17928	-271.21242	-271.20079	69.7	45.3
	-271.31563	-271.17928	-271.21242	-271.20175	69.7	47.3
2a	-622.24185	-622.10431	-622.15042	-622.13831	97.0	71.6
	-622.24185	-622.10431	-622.15042	-622.13855	97.0	72.1
TSba	-893.53578	-893.26093	-893.31983	-893.30804	124.0	99.2
	13.62	14.22	26.99	19.49	-42.8	-17.7
	13.62	14.22	26.99	20.24	-42.8	-20.2
1b	-271.31563	-271.17928	-271.21242	-271.20079	69.7	45.3
	-271.31563	-271.17928	-271.21242	-271.20164	69.7	47.1
2b	-447.30123	-447.24337	-447.28703	-447.27488	91.9	66.3
	-447.30123	-447.24337	-447.28703	-447.27608	91.9	68.8
TSbb	-718.58770	-718.39319	-718.45025	-718.43843	120.1	95.2
	18.30	18.49	30.87	23.37	-41.6	-16.4
	18.30	18.49	30.87	24.66	-41.6	-20.7
1b	-271.31563	-271.17928	-271.21242	-271.20079	69.7	45.3
	-271.31563	-271.17928	-271.21242	-271.20147	69.7	46.7
2c	-379.14266	-379.07984	-379.11429	-379.10198	72.5	46.6
	-379.14266	-379.07984	-379.11429	-379.10318	72.5	49.1
TSbc	-650.41795	-650.21809	-650.26583	-650.25374	100.5	75.0
	25.31	25.75	38.20	30.77	-41.8	-16.8
	25.31	25.75	38.20	31.95	-41.8	-20.8
1c	-193.98109	-193.88206	-193.91302	-193.90143	65.2	40.8
	-193.98109	-193.88206	-193.91302	-193.90243	65.2	42.9
2a	-622.24185	-622.10431	-622.15042	-622.13831	97.0	71.6
	-622.24185	-622.10431	-622.15042	-622.13855	97.0	72.1
TSca	-816.22278	-815.98439	-816.04045	-816.02877	118.0	93.4
	0.10	1.24	14.43	6.88	-44.2	-18.9
	0.10	1.24	14.43	7.66	-44.2	-21.5

1c	-193.98109	-193.88206	-193.91302	-193.90143	65.2	40.8
	-193.98109	-193.88206	-193.91302	-193.90231	65.2	42.6
2b	-447.30123	-447.24337	-447.28703	-447.27488	91.9	66.3
	-447.30123	-447.24337	-447.28703	-447.27519	91.9	67.0
TScb	-641.27392	-641.11559	-641.16933	-641.15725	113.1	87.7
	5.27	6.17	19.28	11.96	-44.0	-19.4
	5.27	6.17	19.28	12.71	-44.0	-21.9
1c	-193.98109	-193.88206	-193.91302	-193.90143	65.2	40.8
	-193.98109	-193.88206	-193.91302	-193.90213	65.2	42.2
2c	-379.14266	-379.07984	-379.11429	-379.10198	72.5	46.6
	-379.14266	-379.07984	-379.11429	-379.10307	72.5	48.9
TScc	-573.10761	-572.94404	-572.98854	-572.97653	93.7	68.4
	10.13	11.21	24.33	16.87	-44.0	-19.0
	10.13	11.21	24.33	17.99	-44.0	-22.8
THF						
1a	-539.21096	-539.00377	-539.04736	-539.03580	91.8	67.4
	-539.21096	-539.00377	-539.04736	-539.03667	91.8	69.3
2a	-622.24297	-622.10545	-622.15158	-622.13976	97.1	72.2
	-622.24297	-622.10545	-622.15158	-622.14097	97.1	74.8
TSaa	-1161.43702	-1161.09146	-1161.16040	-1161.14879	145.1	120.7
	10.61	11.14	24.18	16.80	-43.7	-19.0
	10.61	11.14	24.18	18.10	-43.7	-23.3
1a	-539.21096	-539.00377	-539.04736	-539.03580	91.8	67.4
	-539.21096	-539.00377	-539.04736	-539.03602	91.8	67.9
2b	-447.30244	-447.24458	-447.28824	-447.27590	91.9	65.9
	-447.30244	-447.24458	-447.28824	-447.27748	91.9	69.2
TSab	-986.49598	-986.23029	-986.29758	-986.28571	141.6	116.6
	10.93	11.33	23.86	16.31	-42.0	-16.7
	10.93	11.33	23.86	17.44	-42.0	-20.5
1a	-539.21096	-539.00377	-539.04736	-539.03580	91.8	67.4
	-539.21096	-539.00377	-539.04736	-539.03602	91.8	67.9
2c	-379.14371	-379.08093	-379.11538	-379.10311	72.5	46.7
	-379.14371	-379.08093	-379.11538	-379.10466	72.5	49.9
TSac	-918.32677	-918.05582	-918.11327	-918.10128	120.9	95.7
	17.51	18.12	31.04	23.61	-43.4	-18.4
	17.51	18.12	31.04	24.73	-43.4	-22.2
1b	-271.31580	-271.17948	-271.21262	-271.20083	69.7	44.9
	-271.31580	-271.17948	-271.21262	-271.20190	69.7	47.2
2a	-622.24297	-622.10545	-622.15158	-622.13976	97.1	72.2
	-622.24297	-622.10545	-622.15158	-622.14000	97.1	72.7
TSba	-893.53735	-893.26257	-893.32140	-893.30972	123.8	99.2
	13.44	14.03	26.86	19.37	-43.0	-17.9
	13.44	14.03	26.86	20.20	-43.0	-20.7

1b	-271.31580	-271.17948	-271.21262	-271.20083	69.7	44.9
	-271.31580	-271.17948	-271.21262	-271.20167	69.7	46.7
2b	-447.30244	-447.24458	-447.28824	-447.27590	91.9	65.9
	-447.30244	-447.24458	-447.28824	-447.27711	91.9	68.5
TSbb	-718.58974	-718.39528	-718.45238	-718.44045	120.2	95.1
	17.88	18.06	30.42	22.77	-41.5	-15.8
	17.88	18.06	30.42	24.06	-41.5	-20.1
1b	-271.31580	-271.17948	-271.21262	-271.20083	69.7	44.9
	-271.31580	-271.17948	-271.21262	-271.20097	69.7	45.2
2c	-379.14371	-379.08093	-379.11538	-379.10311	72.5	46.7
	-379.14371	-379.08093	-379.11538	-379.10425	72.5	49.1
TSbc	-650.41945	-650.21967	-650.26754	-650.25545	100.8	75.3
	25.14	25.56	37.94	30.43	-41.5	-16.3
	25.14	25.56	37.94	31.23	-41.5	-19.0
1c	-193.98128	-193.88228	-193.91324	-193.90177	65.2	41.0
	-193.98128	-193.88228	-193.91324	-193.90281	65.2	43.2
2a	-622.24297	-622.10545	-622.15158	-622.13976	97.1	72.2
	-622.24297	-622.10545	-622.15158	-622.14000	97.1	72.7
TSca	-816.22433	-815.98603	-816.04220	-816.03067	118.2	93.9
	-0.05	1.07	14.19	6.81	-44.0	-19.3
	-0.05	1.07	14.19	7.62	-44.0	-22.0
1c	-193.98128	-193.88228	-193.91324	-193.90177	65.2	41.0
	-193.98128	-193.88228	-193.91324	-193.90258	65.2	42.7
2b	-447.30244	-447.24458	-447.28824	-447.27590	91.9	65.9
	-447.30244	-447.24458	-447.28824	-447.27621	91.9	66.6
TScb	-641.27579	-641.11751	-641.17128	-641.15942	113.2	88.2
	4.98	5.87	18.95	11.45	-43.9	-18.7
	4.98	5.87	18.95	12.15	-43.9	-21.1
1c	-193.98128	-193.88228	-193.91324	-193.90177	65.2	41.0
	-193.98128	-193.88228	-193.91324	-193.90245	65.2	42.5
2c	-379.14371	-379.08093	-379.11538	-379.10311	72.5	46.7
	-379.14371	-379.08093	-379.11538	-379.10422	72.5	49.0
TScc	-573.10914	-572.94563	-572.99015	-572.97790	93.7	67.9
	9.95	11.03	24.14	16.93	-44.0	-19.8
	9.95	11.03	24.14	18.06	-44.0	-23.6
1,4-dioxane						
1a	-539.20904	-539.00175	-539.04534	-539.03369	91.7	67.2
	-539.20904	-539.00175	-539.04534	-539.03450	91.7	68.9
2a	-622.23913	-622.10150	-622.14753	-622.13532	96.9	71.2
	-622.23913	-622.10150	-622.14753	-622.13662	96.9	73.9
TSaa	-1161.43060	-1161.08478	-1161.15379	-1161.14202	145.3	120.5
	11.03	11.59	24.52	16.94	-43.4	-17.9
	11.03	11.59	24.52	18.26	-43.4	-22.4

1a	-539.20904	-539.00175	-539.04534	-539.03369	91.7	67.2
	-539.20904	-539.00175	-539.04534	-539.03391	91.7	67.7
2b	-447.29824	-447.24040	-447.28401	-447.27171	91.8	65.9
	-447.29824	-447.24040	-447.28401	-447.27325	91.8	69.1
TSab	-986.48824	-986.22240	-986.28906	-986.27704	140.3	115.0
	11.95	12.39	25.28	17.80	-43.2	-18.1
	11.95	12.39	25.28	18.90	-43.2	-21.8
1a	-539.20904	-539.00175	-539.04534	-539.03369	91.7	67.2
	-539.20904	-539.00175	-539.04534	-539.03391	91.7	67.7
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10075	72.5	49.9
TSac	-918.32085	-918.04967	-918.10715	-918.09507	121.0	95.6
	17.64	18.27	31.17	23.76	-43.3	-18.4
	17.64	18.27	31.17	24.85	-43.3	-22.1
1b	-271.31521	-271.17877	-271.21191	-271.20019	69.7	45.1
	-271.31521	-271.17877	-271.21191	-271.20114	69.7	47.1
2a	-622.23913	-622.10150	-622.14753	-622.13532	96.9	71.2
	-622.23913	-622.10150	-622.14753	-622.13556	96.9	71.7
TSba	-893.53191	-893.25684	-893.31571	-893.30403	123.9	99.3
	14.08	14.70	27.44	19.75	-42.7	-16.9
	14.08	14.70	27.44	20.51	-42.7	-19.5
1b	-271.31521	-271.17877	-271.21191	-271.20019	69.7	45.1
	-271.31521	-271.17877	-271.21191	-271.20102	69.7	46.8
2b	-447.29824	-447.24040	-447.28401	-447.27171	91.8	65.9
	-447.29824	-447.24040	-447.28401	-447.27293	91.8	68.5
TSbb	-718.58237	-718.38775	-718.44475	-718.43277	120.0	94.7
	19.50	19.72	32.11	24.55	-41.6	-16.2
	19.50	19.72	32.11	25.85	-41.6	-20.6
1b	-271.31521	-271.17877	-271.21191	-271.20019	69.7	45.1
	-271.31521	-271.17877	-271.21191	-271.20033	69.7	45.4
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10040	72.5	49.2
TSbc	-650.41410	-650.21406	-650.26157	-650.24895	100.0	73.4
	25.75	26.19	38.79	31.68	-42.3	-18.4
	25.75	26.19	38.79	32.49	-42.3	-21.1
1c	-193.98061	-193.88151	-193.91247	-193.90093	65.2	40.9
	-193.98061	-193.88151	-193.91247	-193.90189	65.2	42.9
2a	-622.23913	-622.10150	-622.14753	-622.13532	96.9	71.2
	-622.23913	-622.10150	-622.14753	-622.13556	96.9	71.7
TSca	-816.21896	-815.98036	-816.03636	-816.02471	117.9	93.3
	0.49	1.66	14.83	7.24	-44.2	-18.7
	0.49	1.66	14.83	8.00	-44.2	-21.2
1c	-193.98061	-193.88151	-193.91247	-193.90093	65.2	40.9

	-193.98061	-193.88151	-193.91247	-193.90177	65.2	42.6
2b	-447.29824	-447.24040	-447.28401	-447.27171	91.8	65.9
	-447.29824	-447.24040	-447.28401	-447.27202	91.8	66.5
TScb	-641.26903	-641.11059	-641.16421	-641.15233	112.9	87.9
	6.16	7.10	20.25	12.74	-44.1	-18.9
	6.16	7.10	20.25	13.46	-44.1	-21.3
1c	-193.98061	-193.88151	-193.91247	-193.90093	65.2	40.9
	-193.98061	-193.88151	-193.91247	-193.90163	65.2	42.3
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10033	72.5	49.0
TScc	-573.10364	-572.93992	-572.98441	-572.97229	93.6	68.1
	10.60	11.68	24.81	17.50	-44.0	-19.5
	10.60	11.68	24.81	18.62	-44.0	-23.3
toluene						
1a	-539.20918	-539.00191	-539.04550	-539.03396	91.7	67.5
	-539.20918	-539.00191	-539.04550	-539.03477	91.7	69.2
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13706	96.9	74.2
TSaa	-1161.43110	-1161.08530	-1161.15433	-1161.14243	145.3	120.2
	10.99	11.57	24.49	17.12	-43.3	-18.7
	10.99	11.57	24.49	18.45	-43.3	-23.1
1a	-539.20918	-539.00191	-539.04550	-539.03396	91.7	67.5
	-539.20918	-539.00191	-539.04550	-539.03418	91.7	67.9
2b	-447.29858	-447.24073	-447.28435	-447.27206	91.8	65.9
	-447.29858	-447.24073	-447.28435	-447.27363	91.8	69.2
TSab	-986.48887	-986.22304	-986.28972	-986.27775	140.3	115.2
	11.85	12.30	25.18	17.74	-43.2	-18.2
	11.85	12.30	25.18	18.86	-43.2	-22.0
1a	-539.20918	-539.00191	-539.04550	-539.03396	91.7	67.5
	-539.20918	-539.00191	-539.04550	-539.03418	91.7	67.9
2c	-379.14023	-379.07736	-379.11180	-379.09963	72.5	46.9
	-379.14023	-379.07736	-379.11180	-379.10115	72.5	50.1
TSac	-918.32133	-918.05017	-918.10765	-918.09579	121.0	96.0
	17.62	18.26	31.16	23.72	-43.3	-18.3
	17.62	18.26	31.16	24.81	-43.3	-22.0
1b	-271.31525	-271.17883	-271.21196	-271.20016	69.7	44.9
	-271.31525	-271.17883	-271.21196	-271.20116	69.7	47.0
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13600	96.9	72.0
TSba	-893.53234	-893.25730	-893.31622	-893.30449	124.0	99.3
	14.02	14.65	27.35	19.72	-42.6	-17.0
	14.02	14.65	27.35	20.51	-42.6	-19.7
1b	-271.31525	-271.17883	-271.21196	-271.20016	69.7	44.9

	-271.31525	-271.17883	-271.21196	-271.20102	69.7	46.7
2b	-447.29858	-447.24073	-447.28435	-447.27206	91.8	65.9
	-447.29858	-447.24073	-447.28435	-447.27326	91.8	68.5
TSbb	-718.58299	-718.38839	-718.44539	-718.43351	120.0	95.0
	19.35	19.56	31.95	24.29	-41.6	-15.9
	19.35	19.56	31.95	25.58	-41.6	-20.2
1b	-271.31525	-271.17883	-271.21196	-271.20016	69.7	44.9
	-271.31525	-271.17883	-271.21196	-271.20030	69.7	45.2
2c	-379.14023	-379.07736	-379.11180	-379.09963	72.5	46.9
	-379.14023	-379.07736	-379.11180	-379.10073	72.5	49.2
TSbc	-650.41455	-650.21453	-650.26206	-650.24977	100.0	74.2
	25.68	26.14	38.72	31.39	-42.2	-17.6
	25.68	26.14	38.72	32.17	-42.2	-20.2
1c	-193.98066	-193.88158	-193.91253	-193.90104	65.2	41.0
	-193.98066	-193.88158	-193.91253	-193.90202	65.2	43.0
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13600	96.9	72.0
TSca	-816.21939	-815.98082	-816.03682	-816.02497	117.9	92.9
	0.44	1.62	14.78	7.42	-44.2	-19.5
	0.44	1.62	14.78	8.19	-44.2	-22.0
1c	-193.98066	-193.88158	-193.91253	-193.90104	65.2	41.0
	-193.98066	-193.88158	-193.91253	-193.90187	65.2	42.7
2b	-447.29858	-447.24073	-447.28435	-447.27206	91.8	65.9
	-447.29858	-447.24073	-447.28435	-447.27237	91.8	66.6
TScb	-641.26960	-641.11117	-641.16481	-641.15310	112.9	88.2
	6.05	6.99	20.12	12.55	-44.1	-18.7
	6.05	6.99	20.12	13.26	-44.1	-21.1
1c	-193.98066	-193.88158	-193.91253	-193.90104	65.2	41.0
	-193.98066	-193.88158	-193.91253	-193.90175	65.2	42.4
2c	-379.14023	-379.07736	-379.11180	-379.09963	72.5	46.9
	-379.14023	-379.07736	-379.11180	-379.10071	72.5	49.1
TScc	-573.10410	-572.94040	-572.98489	-572.97251	93.6	67.6
	10.54	11.63	24.75	17.67	-44.0	-20.3
	10.54	11.63	24.75	18.79	-44.0	-24.0
1,2-dichloroethane						
1a	-539.21126	-539.00410	-539.04768	-539.03611	91.7	67.4
	-539.21126	-539.00410	-539.04768	-539.03693	91.7	69.1
2a	-622.24354	-622.10604	-622.15218	-622.14009	97.1	71.7
	-622.24354	-622.10604	-622.15218	-622.14138	97.1	74.4
TSaa	-1161.43798	-1161.09246	-1161.16142	-1161.14972	145.1	120.5
	10.55	11.09	24.12	16.62	-43.7	-18.5
	10.55	11.09	24.12	17.94	-43.7	-23.0
1a	-539.21126	-539.00410	-539.04768	-539.03611	91.7	67.4

	-539.21126	-539.00410	-539.04768	-539.03633	91.7	67.8
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27815	91.9	69.4
TSab	-986.49711	-986.23144	-986.29894	-986.28716	142.1	117.3
	10.79	11.19	23.59	16.03	-41.6	-16.2
	10.79	11.19	23.59	17.14	-41.6	-19.9
1a	-539.21126	-539.00410	-539.04768	-539.03611	91.7	67.4
	-539.21126	-539.00410	-539.04768	-539.03633	91.7	67.8
2c	-379.14424	-379.08147	-379.11591	-379.10365	72.5	46.7
	-379.14424	-379.08147	-379.11591	-379.10520	72.5	49.9
TSac	-918.32763	-918.05671	-918.11415	-918.10204	120.9	95.4
	17.49	18.11	31.02	23.67	-43.3	-18.7
	17.49	18.11	31.02	24.78	-43.3	-22.4
1b	-271.31589	-271.17959	-271.21273	-271.20106	69.7	45.2
	-271.31589	-271.17959	-271.21273	-271.20203	69.7	47.2
2a	-622.24354	-622.10604	-622.15218	-622.14009	97.1	71.7
	-622.24354	-622.10604	-622.15218	-622.14033	97.1	72.2
TSba	-893.53814	-893.26340	-893.32219	-893.31059	123.7	99.3
	13.36	13.95	26.81	19.18	-43.1	-17.5
	13.36	13.95	26.81	19.94	-43.1	-20.1
1b	-271.31589	-271.17959	-271.21273	-271.20106	69.7	45.2
	-271.31589	-271.17959	-271.21273	-271.20189	69.7	47.0
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27782	91.9	68.7
TSbb	-718.59074	-718.39631	-718.45345	-718.44163	120.3	95.4
	17.70	17.86	30.21	22.61	-41.4	-15.9
	17.70	17.86	30.21	23.90	-41.4	-20.3
1b	-271.31589	-271.17959	-271.21273	-271.20106	69.7	45.2
	-271.31589	-271.17959	-271.21273	-271.20176	69.7	46.7
2c	-379.14424	-379.08147	-379.11591	-379.10365	72.5	46.7
	-379.14424	-379.08147	-379.11591	-379.10482	72.5	49.2
TSbc	-650.42019	-650.22045	-650.26842	-650.25614	101.0	75.1
	25.06	25.48	37.79	30.48	-41.3	-16.8
	25.06	25.48	37.79	31.65	-41.3	-20.7
1c	-193.98138	-193.88239	-193.91336	-193.90184	65.2	40.9
	-193.98138	-193.88239	-193.91336	-193.90282	65.2	43.0
2a	-622.24354	-622.10604	-622.15218	-622.14009	97.1	71.7
	-622.24354	-622.10604	-622.15218	-622.14033	97.1	72.2
TSca	-816.22512	-815.98686	-816.04309	-816.03155	118.3	94.0
	-0.13	0.99	14.09	6.51	-43.9	-18.5
	-0.13	0.99	14.09	7.28	-43.9	-21.1
1c	-193.98138	-193.88239	-193.91336	-193.90184	65.2	40.9
	-193.98138	-193.88239	-193.91336	-193.90268	65.2	42.7

2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27691	91.9	66.8
TScb	-641.27673	-641.11847	-641.17226	-641.16024	113.2	87.9
	4.83	5.71	18.80	11.42	-43.9	-19.1
	4.83	5.71	18.80	12.14	-43.9	-21.5
1c	-193.98138	-193.88239	-193.91336	-193.90184	65.2	40.9
	-193.98138	-193.88239	-193.91336	-193.90253	65.2	42.4
2c	-379.14424	-379.08147	-379.11591	-379.10365	72.5	46.7
	-379.14424	-379.08147	-379.11591	-379.10475	72.5	49.0
TScc	-573.10990	-572.94643	-572.99096	-572.97897	93.7	68.5
	9.86	10.94	24.04	16.64	-43.9	-19.1
	9.86	10.94	24.04	17.77	-43.9	-22.9

Table s4 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions, without and with correction of cavities for all studied bimolecular reactions, obtained with BMK+IDSCRF/6-31G(d).

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
$CHCl_3$						
1a	-539.15447	-538.94825	-538.99192	-538.98031	91.9	67.5
	-539.15447	-538.94825	-538.99192	-538.98116	91.9	69.3
2a	-622.18697	-622.04901	-622.09401	-622.08205	94.7	69.5
	-622.18697	-622.04901	-622.09401	-622.08329	94.7	72.1
TSaa	-1161.32696	-1160.98264	-1161.05005	-1161.03838	141.9	117.3
	9.09	9.17	22.52	15.05	-44.8	-19.7
	9.09	9.17	22.52	16.36	-44.8	-24.1
1a	-539.15447	-538.94825	-538.99192	-538.98031	91.9	67.5
	-539.15447	-538.94825	-538.99192	-538.98053	91.9	67.9
2b	-447.26663	-447.20930	-447.25312	-447.24086	92.2	66.4
	-447.26663	-447.20930	-447.25312	-447.24239	92.2	69.7
TSab	-986.40964	-986.14593	-986.21252	-986.20053	140.2	114.9
	7.19	7.29	20.41	12.95	-44.0	-19.0
	7.19	7.29	20.41	14.05	-44.0	-22.7
1a	-539.15447	-538.94825	-538.99192	-538.98031	91.9	67.5
	-539.15447	-538.94825	-538.99192	-538.98053	91.9	67.9
2c	-379.11368	-379.05082	-379.08530	-379.07308	72.6	46.9
	-379.11368	-379.05082	-379.08530	-379.07459	72.6	50.0
TSac	-918.24262	-917.97314	-918.03238	-918.02032	124.7	99.3
	16.02	16.27	28.14	20.75	-39.8	-15.0
	16.02	16.27	28.14	21.84	-39.8	-18.7
1b	-271.28908	-271.15332	-271.18653	-271.17487	69.9	45.4
	-271.28908	-271.15332	-271.18653	-271.17587	69.9	47.5
2a	-622.18697	-622.04901	-622.09401	-622.08205	94.7	69.5

	-622.18697	-622.04901	-622.09401	-622.08229	94.7	70.1
TSba	-893.45948	-893.18531	-893.24270	-893.23094	120.8	96.1
	10.40	10.68	23.74	16.30	-43.8	-18.9
	10.40	10.68	23.74	17.08	-43.8	-21.5
1b	-271.28908	-271.15332	-271.18653	-271.17487	69.9	45.4
	-271.28908	-271.15332	-271.18653	-271.17570	69.9	47.1
2b	-447.26663	-447.20930	-447.25312	-447.24086	92.2	66.4
	-447.26663	-447.20930	-447.25312	-447.24208	92.2	69.0
TSbb	-718.53398	-718.34069	-718.39932	-718.38747	123.4	98.5
	13.64	13.76	25.31	17.73	-38.7	-13.4
	13.64	13.76	25.31	19.02	-38.7	-17.7
1b	-271.28908	-271.15332	-271.18653	-271.17487	69.9	45.4
	-271.28908	-271.15332	-271.18653	-271.17557	69.9	46.9
2c	-379.11368	-379.05082	-379.08530	-379.07308	72.6	46.9
	-379.11368	-379.05082	-379.08530	-379.07424	72.6	49.3
TSbc	-650.36842	-650.16942	-650.21696	-650.20485	100.1	74.6
	21.55	21.79	34.43	27.05	-42.4	-17.6
	21.55	21.79	34.43	28.22	-42.4	-21.6
1c	-193.95777	-193.85944	-193.89047	-193.87902	65.3	41.2
	-193.95777	-193.85944	-193.89047	-193.88002	65.3	43.3
2a	-622.18697	-622.04901	-622.09401	-622.08205	94.7	69.5
	-622.18697	-622.04901	-622.09401	-622.08229	94.7	70.1
TSca	-816.14814	-815.90986	-815.96422	-815.95254	114.4	89.8
	-2.13	-0.88	12.71	5.35	-45.6	-20.9
	-2.13	-0.88	12.71	6.13	-45.6	-23.6
1c	-193.95777	-193.85944	-193.89047	-193.87902	65.3	41.2
	-193.95777	-193.85944	-193.89047	-193.87984	65.3	43.0
2b	-447.26663	-447.20930	-447.25312	-447.24086	92.2	66.4
	-447.26663	-447.20930	-447.25312	-447.24117	92.2	67.1
TScb	-641.22206	-641.06435	-641.11771	-641.10576	112.3	87.1
	1.47	2.75	16.24	8.86	-45.2	-20.5
	1.47	2.75	16.24	9.57	-45.2	-22.9
1c	-193.95777	-193.85944	-193.89047	-193.87902	65.3	41.2
	-193.95777	-193.85944	-193.89047	-193.87971	65.3	42.7
2c	-379.11368	-379.05082	-379.08530	-379.07308	72.6	46.9
	-379.11368	-379.05082	-379.08530	-379.07419	72.6	49.2
TScc	-573.05919	-572.89623	-572.94078	-572.92878	93.8	68.5
	7.69	8.80	21.96	14.63	-44.1	-19.6
	7.69	8.80	21.96	15.76	-44.1	-23.4
THF						
1a	-539.15516	-538.94898	-538.99265	-538.98103	91.9	67.5
	-539.15516	-538.94898	-538.99265	-538.98190	91.9	69.3
2a	-622.18811	-622.05015	-622.09513	-622.08328	94.7	69.7

	-622.18811	-622.05015	-622.09513	-622.08449	94.7	72.3
TSaa	-1161.32897	-1160.98469	-1161.05236	-1161.04087	142.4	118.2
	8.97	9.06	22.23	14.71	-44.1	-18.9
	8.97	9.06	22.23	16.01	-44.1	-23.3
1a	-539.15516	-538.94898	-538.99265	-538.98103	91.9	67.5
	-539.15516	-538.94898	-538.99265	-538.98125	91.9	67.9
2b	-447.26782	-447.21048	-447.25429	-447.24191	92.2	66.2
	-447.26782	-447.21048	-447.25429	-447.24349	92.2	69.5
TSab	-986.41226	-986.14858	-986.21532	-986.20337	140.5	115.3
	6.73	6.83	19.84	12.28	-43.6	-18.3
	6.73	6.83	19.84	13.41	-43.6	-22.1
1a	-539.15516	-538.94898	-538.99265	-538.98103	91.9	67.5
	-539.15516	-538.94898	-538.99265	-538.98125	91.9	67.9
2c	-379.11479	-379.05196	-379.08643	-379.07421	72.6	46.8
	-379.11479	-379.05196	-379.08643	-379.07573	72.6	50.0
TSac	-918.24444	-917.97507	-918.03461	-918.02286	125.3	100.6
	16.01	16.23	27.91	20.32	-39.1	-13.7
	16.01	16.23	27.91	21.41	-39.1	-17.4
1b	-271.28929	-271.15356	-271.18677	-271.17515	69.9	45.5
	-271.28929	-271.15356	-271.18677	-271.17617	69.9	47.6
2a	-622.18811	-622.05015	-622.09513	-622.08328	94.7	69.7
	-622.18811	-622.05015	-622.09513	-622.08352	94.7	70.2
TSba	-893.46106	-893.18674	-893.24398	-893.23243	120.5	96.2
	10.25	10.65	23.80	16.32	-44.1	-19.0
	10.25	10.65	23.80	17.11	-44.1	-21.7
1b	-271.28929	-271.15356	-271.18677	-271.17515	69.9	45.5
	-271.28929	-271.15356	-271.18677	-271.17595	69.9	47.1
2b	-447.26782	-447.21048	-447.25429	-447.24191	92.2	66.2
	-447.26782	-447.21048	-447.25429	-447.24318	92.2	68.8
TSbb	-718.53593	-718.34270	-718.40228	-718.39030	125.4	100.2
	13.29	13.39	24.33	16.79	-36.7	-11.4
	13.29	13.39	24.33	18.09	-36.7	-15.8
1b	-271.28929	-271.15356	-271.18677	-271.17515	69.9	45.5
	-271.28929	-271.15356	-271.18677	-271.17584	69.9	46.9
2c	-379.11479	-379.05196	-379.08643	-379.07421	72.6	46.8
	-379.11479	-379.05196	-379.08643	-379.07539	72.6	49.3
TSbc	-650.37001	-650.17108	-650.21860	-650.20640	100.0	74.4
	21.38	21.61	34.26	26.96	-42.4	-17.9
	21.38	21.61	34.26	28.13	-42.4	-21.9
1c	-193.95800	-193.85970	-193.89073	-193.87935	65.3	41.4
	-193.95800	-193.85970	-193.89073	-193.88036	65.3	43.5
2a	-622.18811	-622.05015	-622.09513	-622.08328	94.7	69.7
	-622.18811	-622.05015	-622.09513	-622.08352	94.7	70.2

TSca	-816.14979	-815.91172	-815.96612	-815.95453	114.5	90.1
	-2.31	-1.17	12.39	5.08	-45.5	-21.0
	-2.31	-1.17	12.39	5.87	-45.5	-23.6
1c	-193.95800	-193.85970	-193.89073	-193.87935	65.3	41.4
	-193.95800	-193.85970	-193.89073	-193.88013	65.3	43.0
2b	-447.26782	-447.21048	-447.25429	-447.24191	92.2	66.2
	-447.26782	-447.21048	-447.25429	-447.24222	92.2	66.8
TScb	-641.22394	-641.06629	-641.11966	-641.10780	112.3	87.4
	1.18	2.44	15.91	8.45	-45.2	-20.2
	1.18	2.44	15.91	9.13	-45.2	-22.5
1c	-193.95800	-193.85970	-193.89073	-193.87935	65.3	41.4
	-193.95800	-193.85970	-193.89073	-193.88002	65.3	42.8
2c	-379.11479	-379.05196	-379.08643	-379.07421	72.6	46.8
	-379.11479	-379.05196	-379.08643	-379.07534	72.6	49.2
TScc	-573.06081	-572.89786	-572.94237	-572.93027	93.7	68.2
	7.52	8.66	21.83	14.61	-44.2	-20.0
	7.52	8.66	21.83	15.75	-44.2	-23.8
1,4-dioxane						
1a	-539.15284	-538.94655	-538.99021	-538.97867	91.9	67.6
	-539.15284	-538.94655	-538.99021	-538.97943	91.9	69.2
2a	-622.18415	-622.04661	-622.09203	-622.07962	95.6	69.5
	-622.18415	-622.04661	-622.09203	-622.08103	95.6	72.4
TSaa	-1161.32188	-1160.97750	-1161.04489	-1161.03340	141.8	117.6
	9.48	9.83	23.44	15.62	-45.7	-19.4
	9.48	9.83	23.44	16.97	-45.7	-24.0
1a	-539.15284	-538.94655	-538.99021	-538.97867	91.9	67.6
	-539.15284	-538.94655	-538.99021	-538.97889	91.9	68.1
2b	-447.26368	-447.20635	-447.25020	-447.23804	92.3	66.7
	-447.26368	-447.20635	-447.25020	-447.23956	92.3	69.9
TSab	-986.40305	-986.13915	-986.20604	-986.19425	140.8	116.0
	8.45	8.63	21.57	14.09	-43.4	-18.3
	8.45	8.63	21.57	15.19	-43.4	-22.0
1a	-539.15284	-538.94655	-538.99021	-538.97867	91.9	67.6
	-539.15284	-538.94655	-538.99021	-538.97889	91.9	68.1
2c	-379.11080	-379.04787	-379.08235	-379.07016	72.6	46.9
	-379.11080	-379.04787	-379.08235	-379.07169	72.6	50.1
TSac	-918.23804	-917.96855	-918.02784	-918.01594	124.8	99.7
	16.06	16.23	28.06	20.64	-39.7	-14.8
	16.06	16.23	28.06	21.74	-39.7	-18.5
1b	-271.28858	-271.15272	-271.18593	-271.17433	69.9	45.5
	-271.28858	-271.15272	-271.18593	-271.17521	69.9	47.3
2a	-622.18415	-622.04661	-622.09203	-622.07962	95.6	69.5
	-622.18415	-622.04661	-622.09203	-622.07986	95.6	70.0

TSba	-893.45542	-893.18142	-893.23921	-893.22773	121.6	97.5
	10.86	11.24	24.32	16.45	-43.9	-17.5
	10.86	11.24	24.32	17.16	-43.9	-19.9
1b	-271.28858	-271.15272	-271.18593	-271.17433	69.9	45.5
	-271.28858	-271.15272	-271.18593	-271.17517	69.9	47.3
2b	-447.26368	-447.20635	-447.25020	-447.23804	92.3	66.7
	-447.26368	-447.20635	-447.25020	-447.23925	92.3	69.2
TSbb	-718.52887	-718.33640	-718.39146	-718.37959	115.9	90.9
	14.68	14.23	28.03	20.57	-46.3	-21.3
	14.68	14.23	28.03	21.86	-46.3	-25.6
1b	-271.28858	-271.15272	-271.18593	-271.17433	69.9	45.5
	-271.28858	-271.15272	-271.18593	-271.17503	69.9	46.9
2c	-379.11080	-379.04787	-379.08235	-379.07016	72.6	46.9
	-379.11080	-379.04787	-379.08235	-379.07133	72.6	49.4
TSbc	-650.36435	-650.16515	-650.21278	-650.20043	100.3	74.3
	21.98	22.24	34.83	27.65	-42.2	-18.1
	21.98	22.24	34.83	28.82	-42.2	-22.1
1c	-193.95719	-193.85879	-193.88982	-193.87841	65.3	41.3
	-193.95719	-193.85879	-193.88982	-193.87929	65.3	43.1
2a	-622.18415	-622.04661	-622.09203	-622.07962	95.6	69.5
	-622.18415	-622.04661	-622.09203	-622.07986	95.6	70.0
TSca	-816.14401	-815.90556	-815.96009	-815.94843	114.8	90.2
	-1.68	-0.10	13.65	6.02	-46.1	-20.5
	-1.68	-0.10	13.65	6.73	-46.1	-22.9
1c	-193.95719	-193.85879	-193.88982	-193.87841	65.3	41.3
	-193.95719	-193.85879	-193.88982	-193.87925	65.3	43.1
2b	-447.26368	-447.20635	-447.25020	-447.23804	92.3	66.7
	-447.26368	-447.20635	-447.25020	-447.23835	92.3	67.3
TScb	-641.21714	-641.05934	-641.11274	-641.10076	112.4	87.2
	2.34	3.64	17.12	9.85	-45.2	-20.8
	2.34	3.64	17.12	10.56	-45.2	-23.2
1c	-193.95719	-193.85879	-193.88982	-193.87841	65.3	41.3
	-193.95719	-193.85879	-193.88982	-193.87909	65.3	42.7
2c	-379.11080	-379.04787	-379.08235	-379.07016	72.6	46.9
	-379.11080	-379.04787	-379.08235	-379.07127	72.6	49.2
TScc	-573.05501	-572.89187	-572.93639	-572.92424	93.7	68.1
	8.15	9.28	22.45	15.27	-44.2	-20.1
	8.15	9.28	22.45	16.39	-44.2	-23.8
toluene						
1a	-539.15302	-538.94673	-538.99040	-538.97876	91.9	67.4
	-539.15302	-538.94673	-538.99040	-538.97963	91.9	69.2
2a	-622.18447	-622.04696	-622.09241	-622.08052	95.7	70.6
	-622.18447	-622.04696	-622.09241	-622.08173	95.7	73.2

TSaa	-1161.32263	-1160.97832	-1161.04552	-1161.03400	141.4	117.2
	9.32	9.64	23.40	15.86	-46.1	-20.9
	9.32	9.64	23.40	17.17	-46.1	-25.3
1a	-539.15302	-538.94673	-538.99040	-538.97876	91.9	67.4
	-539.15302	-538.94673	-538.99040	-538.97898	91.9	67.9
2b	-447.26401	-447.20671	-447.25054	-447.23828	92.3	66.5
	-447.26401	-447.20671	-447.25054	-447.23981	92.3	69.7
TSab	-986.40370	-986.13982	-986.20683	-986.19498	141.0	116.1
	8.36	8.55	21.40	13.84	-43.1	-17.8
	8.36	8.55	21.40	14.94	-43.1	-21.5
1a	-539.15302	-538.94673	-538.99040	-538.97876	91.9	67.4
	-539.15302	-538.94673	-538.99040	-538.97898	91.9	67.9
2c	-379.11114	-379.04822	-379.08269	-379.07033	72.6	46.5
	-379.11114	-379.04822	-379.08269	-379.07190	72.6	49.8
TSac	-918.23857	-917.96908	-918.02864	-918.01658	125.3	100.0
	16.06	16.23	27.89	20.40	-39.1	-14.0
	16.06	16.23	27.89	21.52	-39.1	-17.7
1b	-271.28863	-271.15279	-271.18600	-271.17433	69.9	45.3
	-271.28863	-271.15279	-271.18600	-271.17535	69.9	47.5
2a	-622.18447	-622.04696	-622.09241	-622.08052	95.7	70.6
	-622.18447	-622.04696	-622.09241	-622.08076	95.7	71.2
TSba	-893.45589	-893.18184	-893.23946	-893.22763	121.3	96.4
	10.80	11.24	24.44	17.08	-44.3	-19.6
	10.80	11.24	24.44	17.88	-44.3	-22.3
1b	-271.28863	-271.15279	-271.18600	-271.17433	69.9	45.3
	-271.28863	-271.15279	-271.18600	-271.17516	69.9	47.1
2b	-447.26401	-447.20671	-447.25054	-447.23828	92.3	66.5
	-447.26401	-447.20671	-447.25054	-447.23950	92.3	69.0
TSbb	-718.52947	-718.33702	-718.39208	-718.38036	115.9	91.2
	14.54	14.11	27.90	20.24	-46.3	-20.6
	14.54	14.11	27.90	21.53	-46.3	-24.9
1b	-271.28863	-271.15279	-271.18600	-271.17433	69.9	45.3
	-271.28863	-271.15279	-271.18600	-271.17447	69.9	45.6
2c	-379.11114	-379.04822	-379.08269	-379.07033	72.6	46.5
	-379.11114	-379.04822	-379.08269	-379.07154	72.6	49.1
TSbc	-650.36482	-650.16564	-650.21323	-650.20101	100.2	74.5
	21.93	22.20	34.80	27.39	-42.3	-17.4
	21.93	22.20	34.80	28.24	-42.3	-20.3
1c	-193.95726	-193.85886	-193.88990	-193.87850	65.3	41.3
	-193.95726	-193.85886	-193.88990	-193.87951	65.3	43.4
2a	-622.18447	-622.04696	-622.09241	-622.08052	95.7	70.6
	-622.18447	-622.04696	-622.09241	-622.08076	95.7	71.2
TSca	-816.14452	-815.90645	-815.96179	-815.95020	116.5	92.1

	-1.75	-0.40	12.88	5.53	-44.5	-19.9
	-1.75	-0.40	12.88	6.32	-44.5	-22.5
1c	-193.95726	-193.85886	-193.88990	-193.87850	65.3	41.3
	-193.95726	-193.85886	-193.88990	-193.87931	65.3	43.0
2b	-447.26401	-447.20671	-447.25054	-447.23828	92.3	66.5
	-447.26401	-447.20671	-447.25054	-447.23859	92.3	67.1
TScb	-641.21772	-641.05993	-641.11332	-641.10143	112.4	87.3
	2.23	3.54	17.02	9.63	-45.2	-20.4
	2.23	3.54	17.02	10.34	-45.2	-22.8
1c	-193.95726	-193.85886	-193.88990	-193.87850	65.3	41.3
	-193.95726	-193.85886	-193.88990	-193.87915	65.3	42.7
2c	-379.11114	-379.04822	-379.08269	-379.07033	72.6	46.5
	-379.11114	-379.04822	-379.08269	-379.07150	72.6	49.0
TScc	-573.05550	-572.89237	-572.93689	-572.92457	93.7	67.8
	8.09	9.23	22.40	15.22	-44.2	-20.1
	8.09	9.23	22.40	16.37	-44.2	-23.9
1,2-dichloroethane						
1a	-539.15552	-538.94935	-538.99301	-538.98148	91.9	67.6
	-539.15552	-538.94935	-538.99301	-538.98232	91.9	69.4
2a	-622.18868	-622.05077	-622.09576	-622.08382	94.7	69.6
	-622.18868	-622.05077	-622.09576	-622.08508	94.7	72.2
TSaa	-1161.33000	-1160.98543	-1161.05297	-1161.04131	142.1	117.6
	8.91	9.22	22.46	15.05	-44.5	-19.6
	8.91	9.22	22.46	16.37	-44.5	-24.0
1a	-539.15552	-538.94935	-538.99301	-538.98148	91.9	67.6
	-539.15552	-538.94935	-538.99301	-538.98170	91.9	68.1
2b	-447.26843	-447.21108	-447.25488	-447.24265	92.2	66.4
	-447.26843	-447.21108	-447.25488	-447.24420	92.2	69.7
TSab	-986.41358	-986.15002	-986.21695	-986.20500	140.9	115.7
	6.51	6.53	19.42	12.00	-43.2	-18.4
	6.51	6.53	19.42	13.12	-43.2	-22.1
1a	-539.15552	-538.94935	-538.99301	-538.98148	91.9	67.6
	-539.15552	-538.94935	-538.99301	-538.98170	91.9	68.1
2c	-379.11534	-379.05253	-379.08765	-379.07520	73.9	47.7
	-379.11534	-379.05253	-379.08765	-379.07685	73.9	51.2
TSac	-918.24536	-917.97606	-918.03573	-918.02387	125.6	100.6
	16.00	16.20	28.19	20.59	-40.2	-14.7
	16.00	16.20	28.19	21.76	-40.2	-18.7
1b	-271.28940	-271.15368	-271.18690	-271.17525	69.9	45.4
	-271.28940	-271.15368	-271.18690	-271.17625	69.9	47.5
2a	-622.18868	-622.05077	-622.09576	-622.08382	94.7	69.6
	-622.18868	-622.05077	-622.09576	-622.08406	94.7	70.1
TSba	-893.46188	-893.18816	-893.24610	-893.23440	121.9	97.3

	10.17	10.22	22.94	15.48	-42.7	-17.6
	10.17	10.22	22.94	16.26	-42.7	-20.3
1b	-271.28940	-271.15368	-271.18690	-271.17525	69.9	45.4
	-271.28940	-271.15368	-271.18690	-271.17608	69.9	47.2
2b	-447.26843	-447.21108	-447.25488	-447.24265	92.2	66.4
	-447.26843	-447.21108	-447.25488	-447.24387	92.2	69.0
TSbb	-718.53688	-718.34368	-718.40216	-718.39024	123.1	98.0
	13.15	13.23	24.86	17.36	-39.0	-13.9
	13.15	13.23	24.86	18.65	-39.0	-18.2
1b	-271.28940	-271.15368	-271.18690	-271.17525	69.9	45.4
	-271.28940	-271.15368	-271.18690	-271.17591	69.9	46.8
2c	-379.11534	-379.05253	-379.08765	-379.07520	73.9	47.7
	-379.11534	-379.05253	-379.08765	-379.07645	73.9	50.3
TSbc	-650.37080	-650.17190	-650.21943	-650.20724	100.0	74.4
	21.30	21.53	34.59	27.11	-43.8	-18.7
	21.30	21.53	34.59	28.31	-43.8	-22.7
1c	-193.95812	-193.85983	-193.89087	-193.87937	65.3	41.1
	-193.95812	-193.85983	-193.89087	-193.88039	65.3	43.3
2a	-622.18868	-622.05077	-622.09576	-622.08382	94.7	69.6
	-622.18868	-622.05077	-622.09576	-622.08406	94.7	70.1
TSca	-816.15061	-815.91266	-815.96714	-815.95553	114.7	90.2
	-2.39	-1.29	12.23	4.81	-45.4	-20.5
	-2.39	-1.29	12.23	5.60	-45.4	-23.1
1c	-193.95812	-193.85983	-193.89087	-193.87937	65.3	41.1
	-193.95812	-193.85983	-193.89087	-193.88021	65.3	42.9
2b	-447.26843	-447.21108	-447.25488	-447.24265	92.2	66.4
	-447.26843	-447.21108	-447.25488	-447.24296	92.2	67.1
TScb	-641.22486	-641.06723	-641.12060	-641.10876	112.3	87.4
	1.06	2.31	15.78	8.32	-45.2	-20.2
	1.06	2.31	15.78	9.04	-45.2	-22.6
1c	-193.95812	-193.85983	-193.89087	-193.87937	65.3	41.1
	-193.95812	-193.85983	-193.89087	-193.88002	65.3	42.5
2c	-379.11534	-379.05253	-379.08765	-379.07520	73.9	47.7
	-379.11534	-379.05253	-379.08765	-379.07637	73.9	50.2
TScc	-573.06161	-572.89870	-572.94321	-572.93097	93.7	67.9
	7.44	8.57	22.16	14.81	-45.6	-20.9
	7.44	8.57	22.16	15.95	-45.6	-24.7

Table s5 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions, without and with correction of cavities for all studied bimolecular reactions, obtained with M06-2x+IDSCRF/6-31G(d).

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)

$CHCl_3$						
1a	-539.29764	-539.09159	-539.13547	-539.12396	92.4	68.1
	-539.29764	-539.09159	-539.13547	-539.12475	92.4	69.8
2a	-622.28911	-622.15173	-622.19769	-622.18551	96.7	71.1
	-622.28911	-622.15173	-622.19769	-622.18685	96.7	73.9
TSaa	-1161.58375	-1161.23861	-1161.30646	-1161.29481	142.8	118.3
	1.88	2.96	16.75	9.20	-46.3	-20.9
	1.88	2.96	16.75	10.54	-46.3	-25.4
1a	-539.29764	-539.09159	-539.13547	-539.12396	92.4	68.1
	-539.29764	-539.09159	-539.13547	-539.12418	92.4	68.6
2b	-447.36192	-447.30407	-447.34791	-447.33572	92.3	66.6
	-447.36192	-447.30407	-447.34791	-447.33727	92.3	69.9
TSab	-986.66145	-986.39672	-986.46377	-986.45185	141.1	116.0
	-1.19	-0.67	12.31	4.91	-43.5	-18.7
	-1.19	-0.67	12.31	6.02	-43.5	-22.4
1a	-539.29764	-539.09159	-539.13547	-539.12396	92.4	68.1
	-539.29764	-539.09159	-539.13547	-539.12418	92.4	68.6
2c	-379.15037	-379.08764	-379.12214	-379.10992	72.6	46.9
	-379.15037	-379.08764	-379.12214	-379.11148	72.6	50.2
TSac	-918.43612	-918.16594	-918.22280	-918.21085	119.7	94.5
	7.46	8.34	21.84	14.45	-45.3	-20.5
	7.46	8.34	21.84	15.57	-45.3	-24.2
1b	-271.35551	-271.21976	-271.25297	-271.24131	69.9	45.4
	-271.35551	-271.21976	-271.25297	-271.24226	69.9	47.4
2a	-622.28911	-622.15173	-622.19769	-622.18551	96.7	71.1
	-622.28911	-622.15173	-622.19769	-622.18575	96.7	71.6
TSba	-893.63232	-893.35797	-893.41626	-893.40475	122.7	98.5
	7.72	8.48	21.59	13.85	-43.9	-18.0
	7.72	8.48	21.59	14.60	-43.9	-20.5
1b	-271.35551	-271.21976	-271.25297	-271.24131	69.9	45.4
	-271.35551	-271.21976	-271.25297	-271.24216	69.9	47.1
2b	-447.36192	-447.30407	-447.34791	-447.33572	92.3	66.6
	-447.36192	-447.30407	-447.34791	-447.33693	92.3	69.1
TSbb	-718.70091	-718.50680	-718.56496	-718.55302	122.4	97.3
	10.37	10.69	22.54	15.07	-39.8	-14.7
	10.37	10.69	22.54	16.35	-39.8	-19.0
1b	-271.35551	-271.21976	-271.25297	-271.24131	69.9	45.4
	-271.35551	-271.21976	-271.25297	-271.24201	69.9	46.8
2c	-379.15037	-379.08764	-379.12214	-379.10992	72.6	46.9
	-379.15037	-379.08764	-379.12214	-379.11108	72.6	49.3
TSbc	-650.47831	-650.27878	-650.32559	-650.31358	98.5	73.2
	17.30	17.96	31.07	23.63	-44.0	-19.0
	17.30	17.96	31.07	24.80	-44.0	-22.9

1c	-194.00602	-193.90709	-193.93809	-193.92665	65.2	41.2
	-194.00602	-193.90709	-193.93809	-193.92759	65.2	43.1
2a	-622.28911	-622.15173	-622.19769	-622.18551	96.7	71.1
	-622.28911	-622.15173	-622.19769	-622.18575	96.7	71.6
TSca	-816.30449	-816.06659	-816.12234	-816.11076	117.3	93.0
	-5.87	-4.88	8.43	0.88	-44.6	-19.3
	-5.87	-4.88	8.43	1.62	-44.6	-21.8
1c	-194.00602	-193.90709	-193.93809	-193.92665	65.2	41.2
	-194.00602	-193.90709	-193.93809	-193.92748	65.2	42.9
2b	-447.36192	-447.30407	-447.34791	-447.33572	92.3	66.6
	-447.36192	-447.30407	-447.34791	-447.33603	92.3	67.3
TScb	-641.37455	-641.21648	-641.26990	-641.25805	112.4	87.5
	-4.15	-3.34	10.10	2.71	-45.1	-20.3
	-4.15	-3.34	10.10	3.43	-45.1	-22.7
1c	-194.00602	-193.90709	-193.93809	-193.92665	65.2	41.2
	-194.00602	-193.90709	-193.93809	-193.92734	65.2	42.6
2c	-379.15037	-379.08764	-379.12214	-379.10992	72.6	46.9
	-379.15037	-379.08764	-379.12214	-379.11103	72.6	49.2
TScc	-573.15284	-572.98955	-573.03372	-573.02153	93.0	67.3
	2.23	3.25	16.64	9.44	-44.9	-20.8
	2.23	3.25	16.64	10.56	-44.9	-24.5
THF						
1a	-539.29831	-539.09229	-539.13617	-539.12448	92.4	67.7
	-539.29831	-539.09229	-539.13617	-539.12534	92.4	69.6
2a	-622.28675	-622.14943	-622.19533	-622.18332	96.6	71.3
	-622.28675	-622.14943	-622.19533	-622.18455	96.6	73.9
TSaa	-1161.58564	-1161.24046	-1161.30816	-1161.29647	142.5	117.9
	-0.36	0.79	14.65	7.11	-46.5	-21.2
	-0.36	0.79	14.65	8.42	-46.5	-25.6
1a	-539.29831	-539.09229	-539.13617	-539.12448	92.4	67.7
	-539.29831	-539.09229	-539.13617	-539.12470	92.4	68.2
2b	-447.36301	-447.30515	-447.34902	-447.33698	92.3	67.0
	-447.36301	-447.30515	-447.34902	-447.33841	92.3	70.0
TSab	-986.66356	-986.39888	-986.46602	-986.45423	141.3	116.5
	-1.41	-0.90	12.03	4.54	-43.4	-18.3
	-1.41	-0.90	12.03	5.57	-43.4	-21.7
1a	-539.29831	-539.09229	-539.13617	-539.12448	92.4	67.7
	-539.29831	-539.09229	-539.13617	-539.12470	92.4	68.2
2c	-379.15142	-379.08872	-379.12322	-379.11073	72.6	46.3
	-379.15142	-379.08872	-379.12322	-379.11233	72.6	49.7
TSac	-918.43783	-918.16773	-918.22462	-918.21272	119.7	94.7
	7.47	8.33	21.82	14.11	-45.2	-19.4
	7.47	8.33	21.82	15.25	-45.2	-23.2

1b	-271.35571	-271.21998	-271.25320	-271.24142	69.9	45.1
	-271.35571	-271.21998	-271.25320	-271.24244	69.9	47.3
2a	-622.28675	-622.14943	-622.19533	-622.18332	96.6	71.3
	-622.28675	-622.14943	-622.19533	-622.18356	96.6	71.8
TSba	-893.63396	-893.35975	-893.41777	-893.40622	122.1	97.8
	5.33	6.06	19.30	11.62	-44.4	-18.6
	5.33	6.06	19.30	12.41	-44.4	-21.3
1b	-271.35571	-271.21998	-271.25320	-271.24142	69.9	45.1
	-271.35571	-271.21998	-271.25320	-271.24233	69.9	47.0
2b	-447.36301	-447.30515	-447.34902	-447.33698	92.3	67.0
	-447.36301	-447.30515	-447.34902	-447.33811	92.3	69.4
TSbb	-718.70267	-718.50855	-718.56675	-718.55482	122.5	97.4
	10.07	10.40	22.26	14.80	-39.7	-14.7
	10.07	10.40	22.26	16.08	-39.7	-19.0
1b	-271.35571	-271.21998	-271.25320	-271.24142	69.9	45.1
	-271.35571	-271.21998	-271.25320	-271.24156	69.9	45.4
2c	-379.15142	-379.08872	-379.12322	-379.11073	72.6	46.3
	-379.15142	-379.08872	-379.12322	-379.11195	72.6	48.9
TSbc	-650.47980	-650.28035	-650.32718	-650.31499	98.6	72.9
	17.15	17.79	30.90	23.32	-44.0	-18.5
	17.15	17.79	30.90	24.17	-44.0	-21.4
1c	-194.00624	-193.90734	-193.93834	-193.92686	65.2	41.1
	-194.00624	-193.90734	-193.93834	-193.92785	65.2	43.2
2a	-622.28675	-622.14943	-622.19533	-622.18332	96.6	71.3
	-622.28675	-622.14943	-622.19533	-622.18356	96.6	71.8
TSca	-816.30603	-816.06825	-816.12421	-816.11254	117.8	93.2
	-8.18	-7.20	5.94	-1.48	-44.1	-19.2
	-8.18	-7.20	5.94	-0.70	-44.1	-21.8
1c	-194.00624	-193.90734	-193.93834	-193.92686	65.2	41.1
	-194.00624	-193.90734	-193.93834	-193.92774	65.2	42.9
2b	-447.36301	-447.30515	-447.34902	-447.33698	92.3	67.0
	-447.36301	-447.30515	-447.34902	-447.33729	92.3	67.6
TScb	-641.37627	-641.21823	-641.27170	-641.25968	112.5	87.2
	-4.41	-3.60	9.83	2.61	-45.0	-20.8
	-4.41	-3.60	9.83	3.36	-45.0	-23.3
1c	-194.00624	-193.90734	-193.93834	-193.92686	65.2	41.1
	-194.00624	-193.90734	-193.93834	-193.92750	65.2	42.4
2c	-379.15142	-379.08872	-379.12322	-379.11073	72.6	46.3
	-379.15142	-379.08872	-379.12322	-379.11191	72.6	48.8
TScc	-573.15437	-572.99115	-573.03533	-573.02315	93.0	67.3
	2.06	3.08	16.46	9.06	-44.9	-20.0
	2.06	3.08	16.46	10.21	-44.9	-23.9
1,4-dioxane						

1a	-539.29608	-539.08994	-539.13381	-539.12233	92.3	68.2
	-539.29608	-539.08994	-539.13381	-539.12315	92.3	69.9
2a	-622.28645	-622.14914	-622.19506	-622.18305	96.6	71.4
	-622.28645	-622.14914	-622.19506	-622.18434	96.6	74.1
TSaa	-1161.57913	-1161.23405	-1161.30197	-1161.29028	143.0	118.4
	2.13	3.16	16.88	9.48	-46.0	-21.2
	2.13	3.16	16.88	10.80	-46.0	-25.6
1a	-539.29608	-539.08994	-539.13381	-539.12233	92.3	68.2
	-539.29608	-539.08994	-539.13381	-539.12255	92.3	68.6
2b	-447.35925	-447.30139	-447.34516	-447.33292	92.1	66.4
	-447.35925	-447.30139	-447.34516	-447.33449	92.1	69.7
TSab	-986.65624	-986.39138	-986.45821	-986.44628	140.6	115.5
	-0.57	-0.03	13.03	5.63	-43.8	-19.0
	-0.57	-0.03	13.03	6.75	-43.8	-22.8
1a	-539.29608	-539.08994	-539.13381	-539.12233	92.3	68.2
	-539.29608	-539.08994	-539.13381	-539.12255	92.3	68.6
2c	-379.14765	-379.08484	-379.11935	-379.10694	72.6	46.5
	-379.14765	-379.08484	-379.11935	-379.10858	72.6	50.0
TSac	-918.43187	-918.16148	-918.21831	-918.20637	119.6	94.5
	7.44	8.35	21.87	14.37	-45.3	-20.2
	7.44	8.35	21.87	15.54	-45.3	-24.1
1b	-271.35503	-271.21919	-271.25240	-271.24087	69.9	45.6
	-271.35503	-271.21919	-271.25240	-271.24183	69.9	47.6
2a	-622.28645	-622.14914	-622.19506	-622.18305	96.6	71.4
	-622.28645	-622.14914	-622.19506	-622.18329	96.6	71.9
TSba	-893.62844	-893.35400	-893.41243	-893.40085	123.0	98.6
	8.18	8.99	21.98	14.48	-43.6	-18.4
	8.18	8.99	21.98	15.23	-43.6	-20.9
1b	-271.35503	-271.21919	-271.25240	-271.24087	69.9	45.6
	-271.35503	-271.21919	-271.25240	-271.24168	69.9	47.3
2b	-447.35925	-447.30139	-447.34516	-447.33292	92.1	66.4
	-447.35925	-447.30139	-447.34516	-447.33417	92.1	69.0
TSbb	-718.69634	-718.50216	-718.55989	-718.54802	121.5	96.5
	11.26	11.56	23.64	16.17	-40.5	-15.5
	11.26	11.56	23.64	17.47	-40.5	-19.8
1b	-271.35503	-271.21919	-271.25240	-271.24087	69.9	45.6
	-271.35503	-271.21919	-271.25240	-271.24152	69.9	47.0
2c	-379.14765	-379.08484	-379.11935	-379.10694	72.6	46.5
	-379.14765	-379.08484	-379.11935	-379.10821	72.6	49.2
TSbc	-650.47447	-650.27476	-650.32154	-650.30895	98.4	72.0
	17.70	18.37	31.51	24.39	-44.1	-20.2
	17.70	18.37	31.51	25.59	-44.1	-24.2
1c	-194.00547	-193.90648	-193.93747	-193.92604	65.2	41.2

	-194.00547	-193.90648	-193.93747	-193.92702	65.2	43.2
2a	-622.28645	-622.14914	-622.19506	-622.18305	96.6	71.4
	-622.28645	-622.14914	-622.19506	-622.18329	96.6	71.9
TSca	-816.30070	-816.06256	-816.11817	-816.10659	117.0	92.7
	-5.51	-4.35	9.01	1.57	-44.8	-19.9
	-5.51	-4.35	9.01	2.34	-44.8	-22.5
1c	-194.00547	-193.90648	-193.93747	-193.92604	65.2	41.2
	-194.00547	-193.90648	-193.93747	-193.92686	65.2	42.9
2b	-447.35925	-447.30139	-447.34516	-447.33292	92.1	66.4
	-447.35925	-447.30139	-447.34516	-447.33323	92.1	67.0
TScb	-641.37007	-641.21189	-641.26522	-641.25348	112.2	87.5
	-3.36	-2.52	10.92	3.44	-45.1	-20.0
	-3.36	-2.52	10.92	4.15	-45.1	-22.4
1c	-194.00547	-193.90648	-193.93747	-193.92604	65.2	41.2
	-194.00547	-193.90648	-193.93747	-193.92669	65.2	42.5
2c	-379.14765	-379.08484	-379.11935	-379.10694	72.6	46.5
	-379.14765	-379.08484	-379.11935	-379.10811	72.6	49.0
TScc	-573.14891	-572.98547	-573.02963	-573.01750	92.9	67.4
	2.64	3.67	17.06	9.71	-44.9	-20.3
	2.64	3.67	17.06	10.86	-44.9	-24.1
toluene						
1a	-539.29625	-539.09012	-539.13399	-539.12232	92.3	67.8
	-539.29625	-539.09012	-539.13399	-539.12319	92.3	69.6
2a	-622.28675	-622.14943	-622.19533	-622.18338	96.6	71.5
	-622.28675	-622.14943	-622.19533	-622.18460	96.6	74.0
TSaa	-1161.57964	-1161.23455	-1161.30247	-1161.29072	142.9	118.2
	2.11	3.14	16.85	9.40	-46.0	-21.0
	2.11	3.14	16.85	10.71	-46.0	-25.4
1a	-539.29625	-539.09012	-539.13399	-539.12232	92.3	67.8
	-539.29625	-539.09012	-539.13399	-539.12254	92.3	68.3
2b	-447.35955	-447.30169	-447.34547	-447.33305	92.1	66.0
	-447.35955	-447.30169	-447.34547	-447.33462	92.1	69.3
TSab	-986.65683	-986.39199	-986.45883	-986.44692	140.7	115.6
	-0.65	-0.11	12.95	5.30	-43.8	-18.2
	-0.65	-0.11	12.95	6.43	-43.8	-21.9
1a	-539.29625	-539.09012	-539.13399	-539.12232	92.3	67.8
	-539.29625	-539.09012	-539.13399	-539.12254	92.3	68.3
2c	-379.14797	-379.08516	-379.11967	-379.10746	72.6	46.9
	-379.14797	-379.08516	-379.11967	-379.10895	72.6	50.1
TSac	-918.43236	-918.16199	-918.21882	-918.20667	119.6	94.0
	7.44	8.34	21.86	14.50	-45.4	-20.7
	7.44	8.34	21.86	15.57	-45.4	-24.3
1b	-271.35508	-271.21925	-271.25247	-271.24093	69.9	45.6

	-271.35508	-271.21925	-271.25247	-271.24190	69.9	47.7
2a	-622.28675	-622.14943	-622.19533	-622.18338	96.6	71.5
	-622.28675	-622.14943	-622.19533	-622.18362	96.6	72.0
TSba	-893.62887	-893.35442	-893.41288	-893.40121	123.0	98.5
	8.13	8.95	21.91	14.50	-43.5	-18.6
	8.13	8.95	21.91	15.26	-43.5	-21.2
1b	-271.35508	-271.21925	-271.25247	-271.24093	69.9	45.6
	-271.35508	-271.21925	-271.25247	-271.24171	69.9	47.2
2b	-447.35955	-447.30169	-447.34547	-447.33305	92.1	66.0
	-447.35955	-447.30169	-447.34547	-447.33435	92.1	68.7
TSbb	-718.69687	-718.50271	-718.56049	-718.54867	121.6	96.7
	11.14	11.44	23.50	15.88	-40.4	-14.9
	11.14	11.44	23.50	17.19	-40.4	-19.3
1b	-271.35508	-271.21925	-271.25247	-271.24093	69.9	45.6
	-271.35508	-271.21925	-271.25247	-271.24161	69.9	47.0
2c	-379.14797	-379.08516	-379.11967	-379.10746	72.6	46.9
	-379.14797	-379.08516	-379.11967	-379.10866	72.6	49.4
TSbc	-650.47491	-650.27523	-650.32201	-650.30988	98.5	72.9
	17.66	18.31	31.46	24.17	-44.1	-19.6
	17.66	18.31	31.46	25.34	-44.1	-23.6
1c	-194.00554	-193.90655	-193.93754	-193.92607	65.2	41.1
	-194.00554	-193.90655	-193.93754	-193.92708	65.2	43.2
2a	-622.28675	-622.14943	-622.19533	-622.18338	96.6	71.5
	-622.28675	-622.14943	-622.19533	-622.18362	96.6	72.0
TSca	-816.30113	-816.06301	-816.11860	-816.10684	117.0	92.2
	-5.55	-4.41	8.95	1.64	-44.8	-20.3
	-5.55	-4.41	8.95	2.42	-44.8	-22.9
1c	-194.00554	-193.90655	-193.93754	-193.92607	65.2	41.1
	-194.00554	-193.90655	-193.93754	-193.92687	65.2	42.8
2b	-447.35955	-447.30169	-447.34547	-447.33305	92.1	66.0
	-447.35955	-447.30169	-447.34547	-447.33336	92.1	66.7
TScb	-641.37059	-641.21243	-641.26577	-641.25390	112.3	87.3
	-3.45	-2.63	10.82	3.28	-45.1	-19.8
	-3.45	-2.63	10.82	3.97	-45.1	-22.1
1c	-194.00554	-193.90655	-193.93754	-193.92607	65.2	41.1
	-194.00554	-193.90655	-193.93754	-193.92676	65.2	42.5
2c	-379.14797	-379.08516	-379.11967	-379.10746	72.6	46.9
	-379.14797	-379.08516	-379.11967	-379.10856	72.6	49.2
TScc	-573.14937	-572.98594	-573.03011	-573.01797	92.9	67.4
	2.60	3.62	17.01	9.76	-44.9	-20.6
	2.60	3.62	17.01	10.89	-44.9	-24.4
1,2-dichloroethane						
1a	-539.29866	-539.09265	-539.13653	-539.12492	92.3	67.9

	-539.29866	-539.09265	-539.13653	-539.12580	92.3	69.8
2a	-622.29074	-622.15325	-622.19911	-622.18731	96.5	71.7
	-622.29074	-622.15325	-622.19911	-622.18850	96.5	74.2
TSaa	-1161.58660	-1161.24142	-1161.30906	-1161.29757	142.4	118.2
	1.76	2.81	16.68	9.20	-46.5	-21.4
	1.76	2.81	16.68	10.50	-46.5	-25.8
1a	-539.29866	-539.09265	-539.13653	-539.12492	92.3	67.9
	-539.29866	-539.09265	-539.13653	-539.12514	92.3	68.4
2b	-447.36356	-447.30570	-447.34958	-447.33734	92.3	66.6
	-447.36356	-447.30570	-447.34958	-447.33886	92.3	69.8
TSab	-986.66464	-986.39998	-986.46716	-986.45519	141.4	116.2
	-1.52	-1.02	11.89	4.44	-43.3	-18.3
	-1.52	-1.02	11.89	5.53	-43.3	-22.0
1a	-539.29866	-539.09265	-539.13653	-539.12492	92.3	67.9
	-539.29866	-539.09265	-539.13653	-539.12514	92.3	68.4
2c	-379.15194	-379.08926	-379.12441	-379.11213	74.0	48.1
	-379.15194	-379.08926	-379.12441	-379.11367	74.0	51.4
TSac	-918.43870	-918.16863	-918.22555	-918.21356	119.8	94.6
	7.47	8.33	22.21	14.74	-46.6	-21.5
	7.47	8.33	22.21	15.84	-46.6	-25.2
1b	-271.35581	-271.22010	-271.25331	-271.24153	69.9	45.1
	-271.35581	-271.22010	-271.25331	-271.24261	69.9	47.4
2a	-622.29074	-622.15325	-622.19911	-622.18731	96.5	71.7
	-622.29074	-622.15325	-622.19911	-622.18755	96.5	72.2
TSba	-893.63479	-893.36062	-893.41856	-893.40682	122.0	97.3
	7.38	7.99	21.25	13.82	-44.5	-19.5
	7.38	7.99	21.25	14.65	-44.5	-22.3
1b	-271.35581	-271.22010	-271.25331	-271.24153	69.9	45.1
	-271.35581	-271.22010	-271.25331	-271.24240	69.9	46.9
2b	-447.36356	-447.30570	-447.34958	-447.33734	92.3	66.6
	-447.36356	-447.30570	-447.34958	-447.33853	92.3	69.1
TSbb	-718.70355	-718.50971	-718.56738	-718.55538	121.4	96.1
	9.93	10.10	22.28	14.74	-40.9	-15.6
	9.93	10.10	22.28	16.03	-40.9	-19.9
1b	-271.35581	-271.22010	-271.25331	-271.24153	69.9	45.1
	-271.35581	-271.22010	-271.25331	-271.24167	69.9	45.4
2c	-379.15194	-379.08926	-379.12441	-379.11213	74.0	48.1
	-379.15194	-379.08926	-379.12441	-379.11327	74.0	50.5
TSbc	-650.48054	-650.28114	-650.32798	-650.31571	98.6	72.8
	17.07	17.71	31.21	23.81	-45.3	-20.5
	17.07	17.71	31.21	24.62	-45.3	-23.2
1c	-194.00635	-193.90747	-193.93847	-193.92711	65.2	41.3
	-194.00635	-193.90747	-193.93847	-193.92812	65.2	43.5

2a	-622.29074	-622.15325	-622.19911	-622.18731	96.5	71.7
	-622.29074	-622.15325	-622.19911	-622.18755	96.5	72.2
TSca	-816.30680	-816.06906	-816.12511	-816.11329	118.0	93.1
	-6.09	-5.23	7.83	0.71	-43.8	-20.0
	-6.09	-5.23	7.83	1.50	-43.8	-22.6
1c	-194.00635	-193.90747	-193.93847	-193.92711	65.2	41.3
	-194.00635	-193.90747	-193.93847	-193.92792	65.2	43.0
2b	-447.36356	-447.30570	-447.34958	-447.33734	92.3	66.6
	-447.36356	-447.30570	-447.34958	-447.33765	92.3	67.2
TScb	-641.37712	-641.21910	-641.27259	-641.26066	112.6	87.5
	-4.52	-3.72	9.70	2.38	-45.0	-20.5
	-4.52	-3.72	9.70	3.08	-45.0	-22.8
1c	-194.00635	-193.90747	-193.93847	-193.92711	65.2	41.3
	-194.00635	-193.90747	-193.93847	-193.92777	65.2	42.7
2c	-379.15194	-379.08926	-379.12441	-379.11213	74.0	48.1
	-379.15194	-379.08926	-379.12441	-379.11328	74.0	50.6
TScc	-573.15512	-572.99195	-573.03613	-573.02387	93.0	67.2
	1.99	3.00	16.79	9.64	-46.3	-22.3
	1.99	3.00	16.79	10.78	-46.3	-26.1

Table s6 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions, without and with correction of cavities for all studied bimolecular reactions, obtained with wB97x+IDSCRF/6-31G(d).

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
$CHCl_3$						
1a	-539.37994	-539.17241	-539.21613	-539.20459	92.0	67.7
	-539.37994	-539.17241	-539.21613	-539.20543	92.0	69.5
2a	-622.37729	-622.23920	-622.28512	-622.27319	96.7	71.5
	-622.37729	-622.23920	-622.28512	-622.27444	96.7	74.2
TSaa	-1161.74292	-1161.39641	-1161.46510	-1161.45323	144.6	119.6
	8.98	9.54	22.68	15.41	-44.1	-19.7
	8.98	9.54	22.68	16.72	-44.1	-24.1
1a	-539.37994	-539.17241	-539.21613	-539.20459	92.0	67.7
	-539.37994	-539.17241	-539.21613	-539.20481	92.0	68.2
2b	-447.39891	-447.34089	-447.38455	-447.37229	91.9	66.1
	-447.39891	-447.34089	-447.38455	-447.37385	91.9	69.4
TSab	-986.76914	-986.50282	-986.57059	-986.55878	142.6	117.8
	6.09	6.58	18.88	11.36	-41.3	-16.0
	6.09	6.58	18.88	12.47	-41.3	-19.8
1a	-539.37994	-539.17241	-539.21613	-539.20459	92.0	67.7
	-539.37994	-539.17241	-539.21613	-539.20481	92.0	68.2
2c	-379.20433	-379.14129	-379.17575	-379.16289	72.5	45.5
	-379.20433	-379.14129	-379.17575	-379.16471	72.5	49.3

TSac	-918.56071	-918.28910	-918.34657	-918.33472	121.0	96.0
	14.78	15.44	28.43	20.56	-43.6	-17.2
	14.78	15.44	28.43	21.84	-43.6	-21.5
1b	-271.41149	-271.27474	-271.30789	-271.29619	69.8	45.1
	-271.41149	-271.27474	-271.30789	-271.29721	69.8	47.3
2a	-622.37729	-622.23920	-622.28512	-622.27319	96.7	71.5
	-622.37729	-622.23920	-622.28512	-622.27343	96.7	72.0
TSba	-893.76473	-893.48891	-893.54739	-893.53574	123.1	98.6
	15.09	15.71	28.63	21.11	-43.3	-18.1
	15.09	15.71	28.63	21.90	-43.3	-20.8
1b	-271.41149	-271.27474	-271.30789	-271.29619	69.8	45.1
	-271.41149	-271.27474	-271.30789	-271.29703	69.8	46.9
2b	-447.39891	-447.34089	-447.38455	-447.37229	91.9	66.1
	-447.39891	-447.34089	-447.38455	-447.37350	91.9	68.6
TSbb	-718.78438	-718.58927	-718.64633	-718.63448	120.1	95.1
	16.33	16.54	28.93	21.34	-41.6	-16.1
	16.33	16.54	28.93	22.63	-41.6	-20.4
1b	-271.41149	-271.27474	-271.30789	-271.29619	69.8	45.1
	-271.41149	-271.27474	-271.30789	-271.29680	69.8	46.4
2c	-379.20433	-379.14129	-379.17575	-379.16289	72.5	45.5
	-379.20433	-379.14129	-379.17575	-379.16426	72.5	48.4
TSbc	-650.57555	-650.37506	-650.42291	-650.41092	100.7	75.5
	25.27	25.71	38.11	30.22	-41.6	-15.1
	25.27	25.71	38.11	31.46	-41.6	-19.3
1c	-194.04638	-193.94717	-193.97816	-193.96678	65.2	41.3
	-194.04638	-193.94717	-193.97816	-193.96776	65.2	43.4
2a	-622.37729	-622.23920	-622.28512	-622.27319	96.7	71.5
	-622.37729	-622.23920	-622.28512	-622.27343	96.7	72.0
TSca	-816.42364	-816.18442	-816.24013	-816.22842	117.2	92.6
	0.02	1.22	14.53	7.25	-44.6	-20.2
	0.02	1.22	14.53	8.02	-44.6	-22.8
1c	-194.04638	-193.94717	-193.97816	-193.96678	65.2	41.3
	-194.04638	-193.94717	-193.97816	-193.96759	65.2	43.0
2b	-447.39891	-447.34089	-447.38455	-447.37229	91.9	66.1
	-447.39891	-447.34089	-447.38455	-447.37260	91.9	66.7
TScb	-641.44137	-641.28264	-641.33656	-641.32479	113.5	88.7
	2.46	3.40	16.41	8.96	-43.6	-18.7
	2.46	3.40	16.41	9.66	-43.6	-21.0
1c	-194.04638	-193.94717	-193.97816	-193.96678	65.2	41.3
	-194.04638	-193.94717	-193.97816	-193.96735	65.2	42.5
2c	-379.20433	-379.14129	-379.17575	-379.16289	72.5	45.5
	-379.20433	-379.14129	-379.17575	-379.16424	72.5	48.3
TScc	-573.23665	-573.07262	-573.11703	-573.10500	93.5	68.2

	8.82	9.94	23.14	15.48	-44.3	-18.6
	8.82	9.94	23.14	16.68	-44.3	-22.6
THF						
1a	-539.38059	-539.17309	-539.21680	-539.20508	92.0	67.3
	-539.38059	-539.17309	-539.21680	-539.20592	92.0	69.1
2a	-622.37842	-622.24035	-622.28624	-622.27412	96.6	71.1
	-622.37842	-622.24035	-622.28624	-622.27537	96.6	73.7
TSaa	-1161.74481	-1161.39825	-1161.46663	-1161.45489	143.9	119.2
	8.91	9.53	22.85	15.25	-44.7	-19.2
	8.91	9.53	22.85	16.57	-44.7	-23.6
1a	-539.38059	-539.17309	-539.21680	-539.20508	92.0	67.3
	-539.38059	-539.17309	-539.21680	-539.20530	92.0	67.8
2b	-447.40010	-447.34208	-447.38575	-447.37346	91.9	66.0
	-447.40010	-447.34208	-447.38575	-447.37497	91.9	69.2
TSab	-986.77136	-986.50604	-986.57057	-986.55871	135.8	110.8
	5.85	5.73	20.07	12.44	-48.1	-22.5
	5.85	5.73	20.07	13.53	-48.1	-26.2
1a	-539.38059	-539.17309	-539.21680	-539.20508	92.0	67.3
	-539.38059	-539.17309	-539.21680	-539.20530	92.0	67.8
2c	-379.20539	-379.14238	-379.17684	-379.16461	72.5	46.8
	-379.20539	-379.14238	-379.17684	-379.16609	72.5	49.9
TSac	-918.56243	-918.29088	-918.34835	-918.33630	121.0	95.6
	14.78	15.43	28.42	20.95	-43.6	-18.5
	14.78	15.43	28.42	22.02	-43.6	-22.1
1b	-271.41168	-271.27497	-271.30812	-271.29644	69.8	45.2
	-271.41168	-271.27497	-271.30812	-271.29741	69.8	47.2
2a	-622.37842	-622.24035	-622.28624	-622.27412	96.6	71.1
	-622.37842	-622.24035	-622.28624	-622.27436	96.6	71.6
TSba	-893.76636	-893.49065	-893.54913	-893.53730	123.1	98.2
	14.90	15.48	28.38	20.87	-43.3	-18.1
	14.90	15.48	28.38	21.63	-43.3	-20.6
1b	-271.41168	-271.27497	-271.30812	-271.29644	69.8	45.2
	-271.41168	-271.27497	-271.30812	-271.29727	69.8	46.9
2b	-447.40010	-447.34208	-447.38575	-447.37346	91.9	66.0
	-447.40010	-447.34208	-447.38575	-447.37469	91.9	68.6
TSbb	-718.78636	-718.59128	-718.64841	-718.63668	120.2	95.5
	15.95	16.17	28.53	20.85	-41.5	-15.7
	15.95	16.17	28.53	22.14	-41.5	-20.0
1b	-271.41168	-271.27497	-271.30812	-271.29644	69.8	45.2
	-271.41168	-271.27497	-271.30812	-271.29714	69.8	46.7
2c	-379.20539	-379.14238	-379.17684	-379.16461	72.5	46.8
	-379.20539	-379.14238	-379.17684	-379.16577	72.5	49.2
TSbc	-650.57703	-650.37662	-650.42469	-650.41231	101.2	75.1

	25.13	25.56	37.82	30.58	-41.1	-16.8
	25.13	25.56	37.82	31.75	-41.1	-20.8
1c	-194.04660	-193.94741	-193.97840	-193.96686	65.2	40.9
	-194.04660	-193.94741	-193.97840	-193.96784	65.2	43.0
2a	-622.37842	-622.24035	-622.28624	-622.27412	96.6	71.1
	-622.37842	-622.24035	-622.28624	-622.27436	96.6	71.6
TSca	-816.42523	-816.18622	-816.24227	-816.23067	118.0	93.5
	-0.13	0.97	14.04	6.47	-43.8	-18.5
	-0.13	0.97	14.04	7.24	-43.8	-21.0
1c	-194.04660	-193.94741	-193.97840	-193.96686	65.2	40.9
	-194.04660	-193.94741	-193.97840	-193.96770	65.2	42.7
2b	-447.40010	-447.34208	-447.38575	-447.37346	91.9	66.0
	-447.40010	-447.34208	-447.38575	-447.37377	91.9	66.7
TScb	-641.44319	-641.28452	-641.33852	-641.32649	113.6	88.3
	2.20	3.12	16.08	8.68	-43.5	-18.6
	2.20	3.12	16.08	9.40	-43.5	-21.0
1c	-194.04660	-193.94741	-193.97840	-193.96686	65.2	40.9
	-194.04660	-193.94741	-193.97840	-193.96756	65.2	42.4
2c	-379.20539	-379.14238	-379.17684	-379.16461	72.5	46.8
	-379.20539	-379.14238	-379.17684	-379.16569	72.5	49.1
TScc	-573.23818	-573.07421	-573.11864	-573.10640	93.5	67.8
	8.67	9.78	22.97	15.73	-44.2	-20.0
	8.67	9.78	22.97	16.85	-44.2	-23.7
1,4-dioxane						
1a	-539.37842	-539.17081	-539.21452	-539.20276	92.0	67.3
	-539.37842	-539.17081	-539.21452	-539.20362	92.0	69.1
2a	-622.37452	-622.23629	-622.28210	-622.27005	96.4	71.1
	-622.37452	-622.23629	-622.28210	-622.27127	96.4	73.6
TSaa	-1161.73837	-1161.39161	-1161.45975	-1161.44802	143.4	118.7
	9.14	9.72	23.14	15.56	-45.0	-19.6
	9.14	9.72	23.14	16.87	-45.0	-24.0
1a	-539.37842	-539.17081	-539.21452	-539.20276	92.0	67.3
	-539.37842	-539.17081	-539.21452	-539.20298	92.0	67.7
2b	-447.39596	-447.33795	-447.38156	-447.36924	91.8	65.9
	-447.39596	-447.33795	-447.38156	-447.37074	91.8	69.0
TSab	-986.76366	-986.49723	-986.56423	-986.55209	141.0	115.5
	6.73	7.24	19.99	12.49	-42.8	-17.7
	6.73	7.24	19.99	13.57	-42.8	-21.3
1a	-539.37842	-539.17081	-539.21452	-539.20276	92.0	67.3
	-539.37842	-539.17081	-539.21452	-539.20298	92.0	67.7
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16205	72.5	49.7
TSac	-918.55643	-918.28466	-918.34212	-918.33031	120.9	96.1

	14.78	15.44	28.44	20.69	-43.6	-17.6
	14.78	15.44	28.44	21.79	-43.6	-21.3
1b	-271.41101	-271.27418	-271.30732	-271.29560	69.7	45.1
	-271.41101	-271.27418	-271.30732	-271.29659	69.7	47.2
2a	-622.37452	-622.23629	-622.28210	-622.27005	96.4	71.1
	-622.37452	-622.23629	-622.28210	-622.27029	96.4	71.6
TSba	-893.76070	-893.48484	-893.54375	-893.53196	124.0	99.2
	15.58	16.08	28.66	21.14	-42.2	-17.0
	15.58	16.08	28.66	21.92	-42.2	-19.6
1b	-271.41101	-271.27418	-271.30732	-271.29560	69.7	45.1
	-271.41101	-271.27418	-271.30732	-271.29643	69.7	46.8
2b	-447.39596	-447.33795	-447.38156	-447.36924	91.8	65.9
	-447.39596	-447.33795	-447.38156	-447.37046	91.8	68.4
TSbb	-718.77919	-718.58398	-718.64103	-718.62913	120.1	95.0
	17.43	17.66	30.03	22.41	-41.5	-15.9
	17.43	17.66	30.03	23.70	-41.5	-20.3
1b	-271.41101	-271.27418	-271.30732	-271.29560	69.7	45.1
	-271.41101	-271.27418	-271.30732	-271.29574	69.7	45.4
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16172	72.5	49.0
TSbc	-650.57173	-650.37104	-650.41857	-650.40633	100.0	74.3
	25.63	26.10	38.70	31.24	-42.3	-17.3
	25.63	26.10	38.70	32.09	-42.3	-20.1
1c	-194.04584	-193.94656	-193.97755	-193.96610	65.2	41.1
	-194.04584	-193.94656	-193.97755	-193.96707	65.2	43.2
2a	-622.37452	-622.23629	-622.28210	-622.27005	96.4	71.1
	-622.37452	-622.23629	-622.28210	-622.27029	96.4	71.6
TSca	-816.41969	-816.18048	-816.23673	-816.22490	118.4	93.5
	0.42	1.49	14.38	7.06	-43.2	-18.7
	0.42	1.49	14.38	7.82	-43.2	-21.2
1c	-194.04584	-193.94656	-193.97755	-193.96610	65.2	41.1
	-194.04584	-193.94656	-193.97755	-193.96691	65.2	42.8
2b	-447.39596	-447.33795	-447.38156	-447.36924	91.8	65.9
	-447.39596	-447.33795	-447.38156	-447.36955	91.8	66.5
TScb	-641.43661	-641.27777	-641.33153	-641.31936	113.1	87.5
	3.26	4.23	17.31	10.03	-43.8	-19.5
	3.26	4.23	17.31	10.73	-43.8	-21.8
1c	-194.04584	-193.94656	-193.97755	-193.96610	65.2	41.1
	-194.04584	-193.94656	-193.97755	-193.96676	65.2	42.5
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16168	72.5	48.9
TScc	-573.23271	-573.06851	-573.11290	-573.10078	93.4	67.9
	9.22	10.35	23.58	16.21	-44.3	-19.7

	9.22	10.35	23.58	17.36	-44.3	-23.5
toluene						
1a	-539.37859	-539.17098	-539.21470	-539.20317	92.0	67.8
	-539.37859	-539.17098	-539.21470	-539.20403	92.0	69.6
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27172	96.3	74.0
TSaa	-1161.73888	-1161.39209	-1161.46008	-1161.44837	143.1	118.5
	9.12	9.71	23.18	15.87	-45.2	-20.7
	9.12	9.71	23.18	17.18	-45.2	-25.1
1a	-539.37859	-539.17098	-539.21470	-539.20317	92.0	67.8
	-539.37859	-539.17098	-539.21470	-539.20339	92.0	68.2
2b	-447.39628	-447.33832	-447.38203	-447.36984	92.0	66.3
	-447.39628	-447.33832	-447.38203	-447.37138	92.0	69.6
TSab	-986.76428	-986.49786	-986.56488	-986.55306	141.1	116.2
	6.65	7.18	19.99	12.52	-42.9	-17.9
	6.65	7.18	19.99	13.62	-42.9	-21.6
1a	-539.37859	-539.17098	-539.21470	-539.20317	92.0	67.8
	-539.37859	-539.17098	-539.21470	-539.20339	92.0	68.2
2c	-379.20189	-379.13878	-379.17325	-379.16103	72.5	46.8
	-379.20189	-379.13878	-379.17325	-379.16257	72.5	50.1
TSac	-918.55692	-918.28516	-918.34262	-918.33063	120.9	95.7
	14.78	15.44	28.45	21.07	-43.6	-18.9
	14.78	15.44	28.45	22.17	-43.6	-22.6
1b	-271.41106	-271.27424	-271.30738	-271.29582	69.7	45.4
	-271.41106	-271.27424	-271.30738	-271.29683	69.7	47.5
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27073	96.3	71.9
TSba	-893.76116	-893.48535	-893.54467	-893.53293	124.8	100.1
	15.52	15.98	28.26	20.95	-41.2	-16.7
	15.52	15.98	28.26	21.73	-41.2	-19.3
1b	-271.41106	-271.27424	-271.30738	-271.29582	69.7	45.4
	-271.41106	-271.27424	-271.30738	-271.29665	69.7	47.2
2b	-447.39628	-447.33832	-447.38203	-447.36984	92.0	66.3
	-447.39628	-447.33832	-447.38203	-447.37107	92.0	68.9
TSbb	-718.77980	-718.58461	-718.64168	-718.62976	120.1	95.0
	17.28	17.54	29.95	22.53	-41.6	-16.7
	17.28	17.54	29.95	23.82	-41.6	-21.0
1b	-271.41106	-271.27424	-271.30738	-271.29582	69.7	45.4
	-271.41106	-271.27424	-271.30738	-271.29651	69.7	46.9
2c	-379.20189	-379.13878	-379.17325	-379.16103	72.5	46.8
	-379.20189	-379.13878	-379.17325	-379.16222	72.5	49.3
TSbc	-650.57217	-650.37151	-650.41907	-650.40679	100.1	74.3
	25.59	26.05	38.63	31.41	-42.2	-18.0

	25.59	26.05	38.63	32.59	-42.2	-22.0
1c	-194.04591	-193.94663	-193.97762	-193.96623	65.2	41.3
	-194.04591	-193.94663	-193.97762	-193.96724	65.2	43.4
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27073	96.3	71.9
TSca	-816.42014	-816.18091	-816.23698	-816.22516	118.0	93.1
	0.38	1.44	14.41	7.25	-43.5	-19.5
	0.38	1.44	14.41	8.04	-43.5	-22.2
1c	-194.04591	-193.94663	-193.97762	-193.96623	65.2	41.3
	-194.04591	-193.94663	-193.97762	-193.96705	65.2	43.0
2b	-447.39628	-447.33832	-447.38203	-447.36984	92.0	66.3
	-447.39628	-447.33832	-447.38203	-447.37015	92.0	67.0
TScb	-641.43717	-641.27834	-641.33212	-641.32022	113.2	88.1
	3.15	4.15	17.28	9.95	-44.0	-19.4
	3.15	4.15	17.28	10.66	-44.0	-21.8
1c	-194.04591	-193.94663	-193.97762	-193.96623	65.2	41.3
	-194.04591	-193.94663	-193.97762	-193.96691	65.2	42.7
2c	-379.20189	-379.13878	-379.17325	-379.16103	72.5	46.8
	-379.20189	-379.13878	-379.17325	-379.16215	72.5	49.2
TScc	-573.23317	-573.06899	-573.11338	-573.10113	93.4	67.6
	9.18	10.30	23.53	16.40	-44.3	-20.5
	9.18	10.30	23.53	17.53	-44.3	-24.2
1,2-dichloroethane						
1a	-539.38093	-539.17344	-539.21715	-539.20584	92.0	68.2
	-539.38093	-539.17344	-539.21715	-539.20660	92.0	69.8
2a	-622.37899	-622.24099	-622.28709	-622.27495	97.0	71.5
	-622.37899	-622.24099	-622.28709	-622.27634	97.0	74.4
TSaa	-1161.74579	-1161.39923	-1161.46752	-1161.45602	143.7	119.5
	8.87	9.54	23.04	15.54	-45.3	-20.1
	8.87	9.54	23.04	16.89	-45.3	-24.7
1a	-539.38093	-539.17344	-539.21715	-539.20584	92.0	68.2
	-539.38093	-539.17344	-539.21715	-539.20606	92.0	68.7
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37583	91.9	69.8
TSab	-986.77250	-986.50623	-986.57375	-986.56196	142.1	117.3
	5.74	6.21	18.67	11.38	-41.8	-17.3
	5.74	6.21	18.67	12.51	-41.8	-21.1
1a	-539.38093	-539.17344	-539.21715	-539.20584	92.0	68.2
	-539.38093	-539.17344	-539.21715	-539.20606	92.0	68.7
2c	-379.20592	-379.14292	-379.17804	-379.16569	73.9	47.9
	-379.20592	-379.14292	-379.17804	-379.16738	73.9	51.5
TSac	-918.56329	-918.29178	-918.34925	-918.33754	121.0	96.3
	14.78	15.42	28.83	21.33	-45.0	-19.8

	14.78	15.42	28.83	22.53	-45.0	-23.8
1b	-271.41178	-271.27509	-271.30824	-271.29664	69.8	45.4
	-271.41178	-271.27509	-271.30824	-271.29758	69.8	47.3
2a	-622.37899	-622.24099	-622.28709	-622.27495	97.0	71.5
	-622.37899	-622.24099	-622.28709	-622.27519	97.0	72.0
TSba	-893.76719	-893.49163	-893.55043	-893.53865	123.8	99.0
	14.80	15.34	28.18	20.67	-43.0	-17.9
	14.80	15.34	28.18	21.41	-43.0	-20.4
1b	-271.41178	-271.27509	-271.30824	-271.29664	69.8	45.4
	-271.41178	-271.27509	-271.30824	-271.29749	69.8	47.2
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37545	91.9	69.0
TSbb	-718.78734	-718.59228	-718.64944	-718.63778	120.3	95.8
	15.78	16.00	28.34	20.78	-41.4	-16.0
	15.78	16.00	28.34	22.06	-41.4	-20.4
1b	-271.41178	-271.27509	-271.30824	-271.29664	69.8	45.4
	-271.41178	-271.27509	-271.30824	-271.29731	69.8	46.8
2c	-379.20592	-379.14292	-379.17804	-379.16569	73.9	47.9
	-379.20592	-379.14292	-379.17804	-379.16692	73.9	50.5
TSbc	-650.57777	-650.37739	-650.42562	-650.41327	101.5	75.5
	25.06	25.49	38.06	30.79	-42.2	-17.8
	25.06	25.49	38.06	31.98	-42.2	-21.8
1c	-194.04671	-193.94754	-193.97853	-193.96702	65.2	41.0
	-194.04671	-193.94754	-193.97853	-193.96799	65.2	43.0
2a	-622.37899	-622.24099	-622.28709	-622.27495	97.0	71.5
	-622.37899	-622.24099	-622.28709	-622.27519	97.0	72.0
TSca	-816.42604	-816.18706	-816.24316	-816.23125	118.1	93.0
	-0.21	0.92	14.09	6.73	-44.2	-19.5
	-0.21	0.92	14.09	7.49	-44.2	-22.0
1c	-194.04671	-193.94754	-193.97853	-193.96702	65.2	41.0
	-194.04671	-193.94754	-193.97853	-193.96789	65.2	42.8
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37456	91.9	67.1
TScb	-641.44410	-641.28545	-641.33949	-641.32754	113.7	88.6
	2.08	2.99	15.94	8.62	-43.4	-18.9
	2.08	2.99	15.94	9.36	-43.4	-21.3
1c	-194.04671	-193.94754	-193.97853	-193.96702	65.2	41.0
	-194.04671	-193.94754	-193.97853	-193.96769	65.2	42.4
2c	-379.20592	-379.14292	-379.17804	-379.16569	73.9	47.9
	-379.20592	-379.14292	-379.17804	-379.16682	73.9	50.3
TScc	-573.23893	-573.07500	-573.11944	-573.10738	93.5	68.2
	8.60	9.70	23.30	15.89	-45.6	-20.7
	8.60	9.70	23.30	17.03	-45.6	-24.5

Table s7 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions, without and with correction of cavities for all studied bimolecular reactions, obtained with wB97xd+IDSCRF/6-31G(d).

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
$CHCl_3$						
1a	-539.34282	-539.13605	-539.17985	-539.16816	92.2	67.6
	-539.34282	-539.13605	-539.17985	-539.16907	92.2	69.5
2a	-622.32356	-622.18625	-622.23263	-622.22086	97.6	72.8
	-622.32356	-622.18625	-622.23263	-622.22202	97.6	75.3
TSaa	-1161.66392	-1161.31829	-1161.38713	-1161.37549	144.9	120.4
	1.54	2.52	15.91	8.49	-44.9	-20.0
	1.54	2.52	15.91	9.79	-44.9	-24.4
1a	-539.34282	-539.13605	-539.17985	-539.16816	92.2	67.6
	-539.34282	-539.13605	-539.17985	-539.16838	92.2	68.0
2b	-447.35059	-447.29299	-447.33665	-447.32464	91.9	66.6
	-447.35059	-447.29299	-447.33665	-447.32606	91.9	69.6
TSab	-986.69430	-986.42888	-986.49633	-986.48439	142.0	116.8
	-0.56	0.10	12.66	5.28	-42.1	-17.4
	-0.56	0.10	12.66	6.31	-42.1	-20.8
1a	-539.34282	-539.13605	-539.17985	-539.16816	92.2	67.6
	-539.34282	-539.13605	-539.17985	-539.16838	92.2	68.0
2c	-379.17288	-379.11011	-379.14457	-379.13235	72.5	46.8
	-379.17288	-379.11011	-379.14457	-379.13384	72.5	49.9
TSac	-918.50180	-918.23105	-918.28872	-918.27686	121.4	96.4
	8.72	9.48	22.40	14.84	-43.3	-18.0
	8.72	9.48	22.40	15.91	-43.3	-21.6
1b	-271.39322	-271.25733	-271.29056	-271.27889	69.9	45.4
	-271.39322	-271.25733	-271.29056	-271.27994	69.9	47.6
2a	-622.32356	-622.18625	-622.23263	-622.22086	97.6	72.8
	-622.32356	-622.18625	-622.23263	-622.22110	97.6	73.3
TSba	-893.70511	-893.43032	-893.48886	-893.47710	123.2	98.5
	7.32	8.32	21.54	14.21	-44.3	-19.7
	7.32	8.32	21.54	15.03	-44.3	-22.5
1b	-271.39322	-271.25733	-271.29056	-271.27889	69.9	45.4
	-271.39322	-271.25733	-271.29056	-271.27978	69.9	47.2
2b	-447.35059	-447.29299	-447.33665	-447.32464	91.9	66.6
	-447.35059	-447.29299	-447.33665	-447.32579	91.9	69.0
TSbb	-718.72801	-718.53408	-718.59204	-718.58026	122.0	97.2
	9.91	10.19	22.07	14.60	-39.8	-14.8
	9.91	10.19	22.07	15.88	-39.8	-19.1
1b	-271.39322	-271.25733	-271.29056	-271.27889	69.9	45.4

	-271.39322	-271.25733	-271.29056	-271.27959	69.9	46.9
2c	-379.17288	-379.11011	-379.14457	-379.13235	72.5	46.8
	-379.17288	-379.11011	-379.14457	-379.13351	72.5	49.3
TSbc	-650.53676	-650.33716	-650.38601	-650.37383	102.8	77.2
	18.41	19.00	30.82	23.48	-39.7	-15.0
	18.41	19.00	30.82	24.64	-39.7	-18.9
1c	-194.03462	-193.93597	-193.96700	-193.95552	65.3	41.1
	-194.03462	-193.93597	-193.96700	-193.95658	65.3	43.4
2a	-622.32356	-622.18625	-622.23263	-622.22086	97.6	72.8
	-622.32356	-622.18625	-622.23263	-622.22110	97.6	73.3
TSca	-816.36650	-816.12816	-816.18426	-816.17261	118.1	93.6
	-5.22	-3.73	9.64	2.37	-44.8	-20.4
	-5.22	-3.73	9.64	3.18	-44.8	-23.2
1c	-194.03462	-193.93597	-193.96700	-193.95552	65.3	41.1
	-194.03462	-193.93597	-193.96700	-193.95641	65.3	43.0
2b	-447.35059	-447.29299	-447.33665	-447.32464	91.9	66.6
	-447.35059	-447.29299	-447.33665	-447.32495	91.9	67.3
TScb	-641.38862	-641.23068	-641.28494	-641.27302	114.2	89.1
	-2.14	-1.08	11.74	4.48	-43.0	-18.6
	-2.14	-1.08	11.74	5.23	-43.0	-21.2
1c	-194.03462	-193.93597	-193.96700	-193.95552	65.3	41.1
	-194.03462	-193.93597	-193.96700	-193.95621	65.3	42.6
2c	-379.17288	-379.11011	-379.14457	-379.13235	72.5	46.8
	-379.17288	-379.11011	-379.14457	-379.13345	72.5	49.1
TScc	-573.20078	-573.03736	-573.08193	-573.06994	93.8	68.6
	4.22	5.47	18.60	11.25	-44.0	-19.4
	4.22	5.47	18.60	12.38	-44.0	-23.2
THF						
1a	-539.34349	-539.13676	-539.18055	-539.16895	92.2	67.8
	-539.34349	-539.13676	-539.18055	-539.16977	92.2	69.5
2a	-622.32100	-622.18362	-622.22996	-622.21785	97.5	72.0
	-622.32100	-622.18362	-622.22996	-622.21914	97.5	74.8
TSaa	-1161.66586	-1161.32038	-1161.38995	-1161.37855	146.4	122.4
	-0.86	0.00	12.90	5.18	-43.3	-17.4
	-0.86	0.00	12.90	6.50	-43.3	-21.8
1a	-539.34349	-539.13676	-539.18055	-539.16895	92.2	67.8
	-539.34349	-539.13676	-539.18055	-539.16917	92.2	68.2
2b	-447.35177	-447.29416	-447.33783	-447.32551	91.9	66.0
	-447.35177	-447.29416	-447.33783	-447.32707	91.9	69.3
TSab	-986.69689	-986.43127	-986.49781	-986.48595	140.1	115.1
	-1.02	-0.22	12.91	5.34	-44.0	-18.6
	-1.02	-0.22	12.91	6.46	-44.0	-22.4
1a	-539.34349	-539.13676	-539.18055	-539.16895	92.2	67.8

	-539.34349	-539.13676	-539.18055	-539.16917	92.2	68.2
2c	-379.17396	-379.11122	-379.14569	-379.13343	72.6	46.8
	-379.17396	-379.11122	-379.14569	-379.13496	72.6	50.0
TSac	-918.50356	-918.23288	-918.29056	-918.27867	121.4	96.4
	8.72	9.48	22.39	14.88	-43.3	-18.1
	8.72	9.48	22.39	15.98	-43.3	-21.8
1b	-271.39342	-271.25757	-271.29080	-271.27901	69.9	45.1
	-271.39342	-271.25757	-271.29080	-271.28001	69.9	47.2
2a	-622.32100	-622.18362	-622.22996	-622.21785	97.5	72.0
	-622.32100	-622.18362	-622.22996	-622.21809	97.5	72.6
TSba	-893.70680	-893.43219	-893.49130	-893.47971	124.4	100.0
	4.78	5.65	18.49	10.76	-43.1	-17.2
	4.78	5.65	18.49	11.54	-43.1	-19.8
1b	-271.39342	-271.25757	-271.29080	-271.27901	69.9	45.1
	-271.39342	-271.25757	-271.29080	-271.27986	69.9	46.9
2b	-447.35177	-447.29416	-447.33783	-447.32551	91.9	66.0
	-447.35177	-447.29416	-447.33783	-447.32672	91.9	68.5
TSbb	-718.72995	-718.53607	-718.59482	-718.58303	123.6	98.8
	9.56	9.83	21.22	13.49	-38.2	-12.3
	9.56	9.83	21.22	14.77	-38.2	-16.6
1b	-271.39342	-271.25757	-271.29080	-271.27901	69.9	45.1
	-271.39342	-271.25757	-271.29080	-271.27915	69.9	45.4
2c	-379.17396	-379.11122	-379.14569	-379.13343	72.6	46.8
	-379.17396	-379.11122	-379.14569	-379.13457	72.6	49.1
TSbc	-650.53829	-650.33878	-650.38708	-650.37520	101.6	76.6
	18.25	18.83	31.01	23.37	-40.8	-15.2
	18.25	18.83	31.01	24.17	-40.8	-17.9
1c	-194.03484	-193.93623	-193.96725	-193.95592	65.3	41.4
	-194.03484	-193.93623	-193.96725	-193.95685	65.3	43.4
2a	-622.32100	-622.18362	-622.22996	-622.21785	97.5	72.0
	-622.32100	-622.18362	-622.22996	-622.21809	97.5	72.6
TSca	-816.36820	-816.13011	-816.18753	-816.17600	120.8	96.6
	-7.76	-6.44	6.07	-1.40	-42.0	-16.9
	-7.76	-6.44	6.07	-0.66	-42.0	-19.4
1c	-194.03484	-193.93623	-193.96725	-193.95592	65.3	41.4
	-194.03484	-193.93623	-193.96725	-193.95670	65.3	43.1
2b	-447.35177	-447.29416	-447.33783	-447.32551	91.9	66.0
	-447.35177	-447.29416	-447.33783	-447.32582	91.9	66.6
TScb	-641.39049	-641.23260	-641.28695	-641.27514	114.4	89.5
	-2.43	-1.39	11.38	3.95	-42.8	-17.9
	-2.43	-1.39	11.38	4.63	-42.8	-20.2
1c	-194.03484	-193.93623	-193.96725	-193.95592	65.3	41.4
	-194.03484	-193.93623	-193.96725	-193.95658	65.3	42.8

2c	-379.17396	-379.11122	-379.14569	-379.13343	72.6	46.8
	-379.17396	-379.11122	-379.14569	-379.13458	72.6	49.2
TScc	-573.20235	-573.03899	-573.08358	-573.07147	93.8	68.4
	4.05	5.31	18.42	11.22	-44.0	-19.8
	4.05	5.31	18.42	12.36	-44.0	-23.7
1,4-dioxane						
1a	-539.34124	-539.13439	-539.17818	-539.16669	92.2	68.0
	-539.34124	-539.13439	-539.17818	-539.16753	92.2	69.7
2a	-622.32068	-622.18328	-622.22983	-622.21791	98.0	72.9
	-622.32068	-622.18328	-622.22983	-622.21917	98.0	75.5
TSaa	-1161.65917	-1161.31331	-1161.38153	-1161.36994	143.6	119.2
	1.73	2.74	16.62	9.20	-46.6	-21.7
	1.73	2.74	16.62	10.52	-46.6	-26.1
1a	-539.34124	-539.13439	-539.17818	-539.16669	92.2	68.0
	-539.34124	-539.13439	-539.17818	-539.16691	92.2	68.4
2b	-447.34771	-447.29011	-447.33373	-447.32157	91.8	66.2
	-447.34771	-447.29011	-447.33373	-447.32311	91.8	69.4
TSab	-986.68863	-986.42311	-986.49017	-986.47827	141.1	116.1
	0.20	0.87	13.64	6.27	-42.8	-18.1
	0.20	0.87	13.64	7.37	-42.8	-21.8
1a	-539.34124	-539.13439	-539.17818	-539.16669	92.2	68.0
	-539.34124	-539.13439	-539.17818	-539.16691	92.2	68.4
2c	-379.17011	-379.10725	-379.14172	-379.12935	72.6	46.5
	-379.17011	-379.10725	-379.14172	-379.13097	72.6	49.9
TSac	-918.49740	-918.22649	-918.28415	-918.27233	121.4	96.5
	8.75	9.51	22.43	14.88	-43.4	-18.0
	8.75	9.51	22.43	16.04	-43.4	-21.9
1b	-271.39273	-271.25675	-271.28997	-271.27839	69.9	45.6
	-271.39273	-271.25675	-271.28997	-271.27938	69.9	47.6
2a	-622.32068	-622.18328	-622.22983	-622.21791	98.0	72.9
	-622.32068	-622.18328	-622.22983	-622.21815	98.0	73.4
TSba	-893.70093	-893.42582	-893.48396	-893.47239	122.4	98.0
	7.83	8.92	22.49	15.00	-45.5	-20.4
	7.83	8.92	22.49	15.78	-45.5	-23.0
1b	-271.39273	-271.25675	-271.28997	-271.27839	69.9	45.6
	-271.39273	-271.25675	-271.28997	-271.27923	69.9	47.3
2b	-447.34771	-447.29011	-447.33373	-447.32157	91.8	66.2
	-447.34771	-447.29011	-447.33373	-447.32279	91.8	68.8
TSbb	-718.72289	-718.52883	-718.58609	-718.57409	120.5	95.3
	11.01	11.31	23.60	16.23	-41.2	-16.5
	11.01	11.31	23.60	17.52	-41.2	-20.8
1b	-271.39273	-271.25675	-271.28997	-271.27839	69.9	45.6
	-271.39273	-271.25675	-271.28997	-271.27905	69.9	46.9

2c	-379.17011	-379.10725	-379.14172	-379.12935	72.6	46.5
	-379.17011	-379.10725	-379.14172	-379.13059	72.6	49.1
TSbc	-650.53281	-650.33303	-650.38101	-650.36893	101.0	75.6
	18.84	19.43	31.80	24.35	-41.5	-16.5
	18.84	19.43	31.80	25.55	-41.5	-20.5
1c	-194.03406	-193.93535	-193.96637	-193.95501	65.3	41.4
	-194.03406	-193.93535	-193.96637	-193.95599	65.3	43.5
2a	-622.32068	-622.18328	-622.22983	-622.21791	98.0	72.9
	-622.32068	-622.18328	-622.22983	-622.21815	98.0	73.4
TSca	-816.36231	-816.12377	-816.17963	-816.16799	117.6	93.1
	-4.75	-3.23	10.40	3.09	-45.7	-21.2
	-4.75	-3.23	10.40	3.86	-45.7	-23.8
1c	-194.03406	-193.93535	-193.96637	-193.95501	65.3	41.4
	-194.03406	-193.93535	-193.96637	-193.95583	65.3	43.1
2b	-447.34771	-447.29011	-447.33373	-447.32157	91.8	66.2
	-447.34771	-447.29011	-447.33373	-447.32188	91.8	66.9
TScb	-641.38376	-641.22570	-641.27976	-641.26802	113.8	89.1
	-1.25	-0.15	12.76	5.37	-43.3	-18.5
	-1.25	-0.15	12.76	6.08	-43.3	-20.9
1c	-194.03406	-193.93535	-193.96637	-193.95501	65.3	41.4
	-194.03406	-193.93535	-193.96637	-193.95565	65.3	42.7
2c	-379.17011	-379.10725	-379.14172	-379.12935	72.6	46.5
	-379.17011	-379.10725	-379.14172	-379.13053	72.6	49.0
TScc	-573.19672	-573.03315	-573.07767	-573.06570	93.7	68.5
	4.67	5.93	19.09	11.71	-44.1	-19.4
	4.67	5.93	19.09	12.86	-44.1	-23.2
toluene						
1a	-539.34141	-539.13457	-539.17836	-539.16692	92.2	68.1
	-539.34141	-539.13457	-539.17836	-539.16774	92.2	69.8
2a	-622.32100	-622.18362	-622.22996	-622.21800	97.5	72.4
	-622.32100	-622.18362	-622.22996	-622.21929	97.5	75.1
TSaa	-1161.65970	-1161.31385	-1161.38205	-1161.37047	143.6	119.2
	1.70	2.72	16.48	9.07	-46.2	-21.3
	1.70	2.72	16.48	10.39	-46.2	-25.7
1a	-539.34141	-539.13457	-539.17836	-539.16692	92.2	68.1
	-539.34141	-539.13457	-539.17836	-539.16714	92.2	68.5
2b	-447.34803	-447.29044	-447.33406	-447.32191	91.8	66.2
	-447.34803	-447.29044	-447.33406	-447.32346	91.8	69.5
TSab	-986.68927	-986.42381	-986.49210	-986.48038	143.7	119.1
	0.11	0.75	12.75	5.30	-40.2	-15.3
	0.11	0.75	12.75	6.41	-40.2	-19.0
1a	-539.34141	-539.13457	-539.17836	-539.16692	92.2	68.1
	-539.34141	-539.13457	-539.17836	-539.16714	92.2	68.5

2c	-379.17043	-379.10758	-379.14205	-379.13008	72.6	47.3
	-379.17043	-379.10758	-379.14205	-379.13156	72.6	50.5
TSac	-918.49790	-918.22701	-918.28468	-918.27295	121.4	96.7
	8.75	9.50	22.42	15.09	-43.3	-18.7
	8.75	9.50	22.42	16.16	-43.3	-22.3
1b	-271.39278	-271.25682	-271.29004	-271.27850	69.9	45.6
	-271.39278	-271.25682	-271.29004	-271.27947	69.9	47.7
2a	-622.32100	-622.18362	-622.22996	-622.21800	97.5	72.4
	-622.32100	-622.18362	-622.22996	-622.21824	97.5	72.9
TSba	-893.70140	-893.42635	-893.48452	-893.47287	122.4	97.9
	7.77	8.84	22.26	14.83	-45.0	-20.1
	7.77	8.84	22.26	15.59	-45.0	-22.7
1b	-271.39278	-271.25682	-271.29004	-271.27850	69.9	45.6
	-271.39278	-271.25682	-271.29004	-271.27933	69.9	47.4
2b	-447.34803	-447.29044	-447.33406	-447.32191	91.8	66.2
	-447.34803	-447.29044	-447.33406	-447.32314	91.8	68.8
TSbb	-718.72350	-718.52944	-718.58670	-718.57500	120.5	95.9
	10.86	11.18	23.47	15.95	-41.2	-16.0
	10.86	11.18	23.47	17.24	-41.2	-20.3
1b	-271.39278	-271.25682	-271.29004	-271.27850	69.9	45.6
	-271.39278	-271.25682	-271.29004	-271.27922	69.9	47.2
2c	-379.17043	-379.10758	-379.14205	-379.13008	72.6	47.3
	-379.17043	-379.10758	-379.14205	-379.13120	72.6	49.7
TSbc	-650.53327	-650.33351	-650.38153	-650.36954	101.1	75.8
	18.79	19.38	31.73	24.50	-41.4	-17.1
	18.79	19.38	31.73	25.66	-41.4	-21.0
1c	-194.03412	-193.93542	-193.96644	-193.95515	65.3	41.5
	-194.03412	-193.93542	-193.96644	-193.95611	65.3	43.5
2a	-622.32100	-622.18362	-622.22996	-622.21800	97.5	72.4
	-622.32100	-622.18362	-622.22996	-622.21824	97.5	72.9
TSca	-816.36278	-816.12431	-816.18029	-816.16879	117.8	93.6
	-4.81	-3.31	10.11	2.74	-45.0	-20.3
	-4.81	-3.31	10.11	3.49	-45.0	-22.8
1c	-194.03412	-193.93542	-193.96644	-193.95515	65.3	41.5
	-194.03412	-193.93542	-193.96644	-193.95596	65.3	43.2
2b	-447.34803	-447.29044	-447.33406	-447.32191	91.8	66.2
	-447.34803	-447.29044	-447.33406	-447.32222	91.8	66.9
TScb	-641.38433	-641.22628	-641.28036	-641.26854	113.8	89.0
	-1.37	-0.26	12.64	5.35	-43.3	-18.8
	-1.37	-0.26	12.64	6.05	-43.3	-21.2
1c	-194.03412	-193.93542	-193.96644	-193.95515	65.3	41.5
	-194.03412	-193.93542	-193.96644	-193.95585	65.3	43.0
2c	-379.17043	-379.10758	-379.14205	-379.13008	72.6	47.3

	-379.17043	-379.10758	-379.14205	-379.13116	72.6	49.6
TScc	-573.19719	-573.03364	-573.07816	-573.06595	93.7	68.0
	4.62	5.87	19.03	12.10	-44.1	-20.9
	4.62	5.87	19.03	13.22	-44.1	-24.6
1,2-dichloroethane						
1a	-539.34384	-539.13712	-539.18091	-539.16931	92.2	67.7
	-539.34384	-539.13712	-539.18091	-539.17016	92.2	69.5
2a	-622.32534	-622.18797	-622.23412	-622.22215	97.1	71.9
	-622.32534	-622.18797	-622.23412	-622.22339	97.1	74.6
TSaa	-1161.66689	-1161.32140	-1161.39090	-1161.37929	146.3	121.8
	1.44	2.32	15.14	7.64	-43.0	-17.8
	1.44	2.32	15.14	8.95	-43.0	-22.2
1a	-539.34384	-539.13712	-539.18091	-539.16931	92.2	67.7
	-539.34384	-539.13712	-539.18091	-539.16953	92.2	68.2
2b	-447.35236	-447.29475	-447.33842	-447.32611	91.9	66.0
	-447.35236	-447.29475	-447.33842	-447.32767	91.9	69.3
TSab	-986.69814	-986.43254	-986.49915	-986.48744	140.2	115.5
	-1.22	-0.42	12.66	5.01	-43.9	-18.2
	-1.22	-0.42	12.66	6.12	-43.9	-21.9
1a	-539.34384	-539.13712	-539.18091	-539.16931	92.2	67.7
	-539.34384	-539.13712	-539.18091	-539.16953	92.2	68.2
2c	-379.17449	-379.11176	-379.14688	-379.13442	73.9	47.7
	-379.17449	-379.11176	-379.14688	-379.13603	73.9	51.1
TSac	-918.50446	-918.23381	-918.29148	-918.27942	121.4	96.0
	8.70	9.46	22.78	15.25	-44.7	-19.4
	8.70	9.46	22.78	16.41	-44.7	-23.3
1b	-271.39353	-271.25769	-271.29092	-271.27930	69.9	45.5
	-271.39353	-271.25769	-271.29092	-271.28029	69.9	47.6
2a	-622.32534	-622.18797	-622.23412	-622.22215	97.1	71.9
	-622.32534	-622.18797	-622.23412	-622.22239	97.1	72.5
TSba	-893.70766	-893.43409	-893.49037	-893.47878	118.5	94.1
	7.03	7.26	21.76	14.23	-48.6	-23.4
	7.03	7.26	21.76	15.00	-48.6	-26.0
1b	-271.39353	-271.25769	-271.29092	-271.27930	69.9	45.5
	-271.39353	-271.25769	-271.29092	-271.28011	69.9	47.2
2b	-447.35236	-447.29475	-447.33842	-447.32611	91.9	66.0
	-447.35236	-447.29475	-447.33842	-447.32736	91.9	68.6
TSbb	-718.73092	-718.53706	-718.59690	-718.58489	125.9	100.7
	9.39	9.65	20.36	12.88	-35.9	-10.8
	9.39	9.65	20.36	14.17	-35.9	-15.2
1b	-271.39353	-271.25769	-271.29092	-271.27930	69.9	45.5
	-271.39353	-271.25769	-271.29092	-271.27996	69.9	46.9
2c	-379.17449	-379.11176	-379.14688	-379.13442	73.9	47.7

	-379.17449	-379.11176	-379.14688	-379.13567	73.9	50.3
TSbc	-650.53906	-650.33959	-650.38788	-650.37583	101.6	76.3
	18.17	18.74	31.33	23.78	-42.2	-16.9
	18.17	18.74	31.33	24.97	-42.2	-20.9
1c	-194.03496	-193.93635	-193.96738	-193.95590	65.3	41.1
	-194.03496	-193.93635	-193.96738	-193.95691	65.3	43.3
2a	-622.32534	-622.18797	-622.23412	-622.22215	97.1	71.9
	-622.32534	-622.18797	-622.23412	-622.22239	97.1	72.5
TSca	-816.36906	-816.13087	-816.18724	-816.17561	118.6	94.2
	-5.50	-4.11	8.95	1.53	-43.8	-18.9
	-5.50	-4.11	8.95	2.32	-43.8	-21.6
1c	-194.03496	-193.93635	-193.96738	-193.95590	65.3	41.1
	-194.03496	-193.93635	-193.96738	-193.95672	65.3	42.9
2b	-447.35236	-447.29475	-447.33842	-447.32611	91.9	66.0
	-447.35236	-447.29475	-447.33842	-447.32642	91.9	66.6
TScb	-641.39141	-641.23356	-641.28795	-641.27614	114.5	89.6
	-2.57	-1.54	11.20	3.68	-42.7	-17.5
	-2.57	-1.54	11.20	4.39	-42.7	-19.9
1c	-194.03496	-193.93635	-193.96738	-193.95590	65.3	41.1
	-194.03496	-193.93635	-193.96738	-193.95655	65.3	42.5
2c	-379.17449	-379.11176	-379.14688	-379.13442	73.9	47.7
	-379.17449	-379.11176	-379.14688	-379.13559	73.9	50.2
TScc	-573.20313	-573.03981	-573.08441	-573.07238	93.9	68.5
	3.97	5.21	18.73	11.26	-45.3	-20.3
	3.97	5.21	18.73	12.40	-45.3	-24.1

Table s8 The energy, enthalpy, free energy(au, 298K),entropy(cal·mol^{-1}·K^{-1}) and free-energy barrier(kcal·mol^{-1}) for the reactions(without and with correction of reaction cavities), obtained with CAM-B3LYP+IDSCRF/6-311++G(d,p) and BMK+IDSCRF/6-311++G(d,p)

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
CAM THF						
1a	-539.34293	-539.13723	-539.18092	-539.16880	91.9	66.4
	-539.34293	-539.13723	-539.18092	-539.16963	91.9	68.2
2a	-622.41649	-622.27992	-622.32670	-622.31410	98.5	71.9
	-622.41649	-622.27992	-622.32670	-622.31538	98.5	74.6
TSaa	-1161.73940	-1161.39627	-1161.46644	-1161.45440	147.7	122.3
	12.56	13.10	25.84	17.88	-42.7	-16.0
	12.56	13.10	25.84	19.21	-42.7	-20.5
BMK THF						
1a	-539.27122	-539.06691	-539.11071	-539.09868	92.2	66.9
	-539.27122	-539.06691	-539.11071	-539.09949	92.2	68.6
2a	-622.33581	-622.19960	-622.24557	-622.23295	96.8	70.2

	-622.33581	-622.19960	-622.24557	-622.23427	96.8	73.0
TSaa	-1161.59217	-1161.25032	-1161.31789	-1161.30563	142.2	116.4
	9.32	10.16	24.09	16.32	-46.8	-20.7
	9.32	10.16	24.09	17.65	-46.8	-25.1
CAM toluene						
1d	-578.63753	-578.40201	-578.45144	-578.44017	104.0	80.3
	-578.63753	-578.40201	-578.45144	-578.44028	104.0	80.6
2a	-622.41189	-622.27524	-622.32196	-622.30954	98.3	72.2
	-622.41189	-622.27524	-622.32196	-622.31112	98.3	75.5
TSda	-1201.03629	-1200.66320	-1200.73527	-1200.72371	151.7	127.4
	8.24	8.82	23.93	16.32	-50.7	-25.2
	8.24	8.82	23.93	17.38	-50.7	-28.7
BMK toluene						
1a	-578.55968	-578.32541	-578.37388	-578.36231	102.0	77.7
	-578.55968	-578.32541	-578.37388	-578.36242	102.0	77.9
2a	-622.33143	-622.19492	-622.24040	-622.22785	95.7	69.3
	-622.33143	-622.19492	-622.24040	-622.22937	95.7	72.5
TSaa	-1200.88342	-1200.51098	-1200.58140	-1200.56958	148.2	123.3
	4.83	5.87	20.63	12.91	-49.5	-23.6
	4.83	5.87	20.63	13.94	-49.5	-27.1

Table s9 The energy, enthalpy, free energy(au, 298K) and entropy(cal·mol^{-1}·K^{-1}) for the reactions in Scheme 2, obtained with CAM-B3LYP+IDSCRF/6-31G(d) and wB97x+IDSCRF/6-31G(d)

species	E	H	G(gas)	G(sol)	S(gas)	S(sol)
CAM toluene						
1a	-539.20918	-539.00191	-539.04550	-539.03396	91.7	67.5
	-539.20918	-539.00191	-539.04550	-539.03477	91.7	69.2
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13706	96.9	74.2
TSaa	-1161.43110	-1161.08530	-1161.15433	-1161.14243	145.3	120.2
	10.99	11.57	24.49	17.12	-43.3	-18.7
	10.99	11.57	24.49	18.45	-43.3	-23.1
1d	-578.49606	-578.25871	-578.30796	-578.29670	103.7	80.0
	-578.49606	-578.25871	-578.30796	-578.29681	103.7	80.2
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13722	96.9	74.5
TSda	-1200.72528	-1200.34944	-1200.42110	-1200.40992	150.8	127.3
	6.41	6.96	21.78	14.14	-49.7	-24.1
	6.41	6.96	21.78	15.13	-49.7	-27.4
1e	-617.78176	-617.51416	-617.56715	-617.55645	111.5	89.0
	-617.78176	-617.51416	-617.56715	-617.55646	111.5	89.0
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4

	-622.23943	-622.10182	-622.14785	-622.13751	96.9	75.1
TSea	-1240.01687	-1239.61094	-1239.68518	-1239.67410	156.2	132.9
	2.71	3.16	18.71	11.36	-52.2	-27.5
	2.71	3.16	18.71	12.47	-52.2	-31.2
1f	-768.15534	-767.87653	-767.93293	-767.92224	118.7	96.2
	-768.15534	-767.87653	-767.93293	-767.92249	118.7	96.7
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13757	96.9	75.2
TSfa	-1390.39133	-1389.97364	-1390.05287	-1390.04206	166.8	144.0
	2.16	2.96	17.51	10.00	-48.8	-23.6
	2.16	2.96	17.51	11.29	-48.8	-28.0
1g	-696.35820	-696.02951	-696.08644	-696.07583	119.8	97.5
	-696.35820	-696.02951	-696.08644	-696.07610	119.8	98.0
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13766	96.9	75.4
TSga	-1318.59011	-1318.12283	-1318.20208	-1318.19151	166.8	144.5
	4.72	5.33	20.21	12.60	-49.9	-24.4
	4.72	5.33	20.21	13.96	-49.9	-28.9
1h	-770.12564	-769.83171	-769.88852	-769.87717	119.6	95.7
	-770.12564	-769.83171	-769.88852	-769.87732	119.6	96.0
2a	-622.23943	-622.10182	-622.14785	-622.13576	96.9	71.4
	-622.23943	-622.10182	-622.14785	-622.13732	96.9	74.7
TSha	-1392.34919	-1391.91642	-1391.99601	-1391.98477	167.5	143.8
	9.96	10.74	25.33	17.67	-48.9	-23.3
	9.96	10.74	25.33	18.75	-48.9	-26.9
wB97x	toluene					
1a	-539.37859	-539.17098	-539.21470	-539.20317	92.0	67.8
	-539.37859	-539.17098	-539.21470	-539.20403	92.0	69.6
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27172	96.3	74.0
TSaa	-1161.73888	-1161.39209	-1161.46008	-1161.44837	143.1	118.5
	9.12	9.71	23.18	15.87	-45.2	-20.7
	9.12	9.71	23.18	17.18	-45.2	-25.1
1d	-578.68187	-578.44396	-578.49278	-578.48165	102.7	79.3
	-578.68187	-578.44396	-578.49278	-578.48176	102.7	79.5
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27191	96.3	74.4
TSda	-1201.04939	-1200.67237	-1200.74422	-1200.73280	151.2	127.2
	4.59	5.13	19.38	12.14	-47.8	-23.5
	4.59	5.13	19.38	13.10	-47.8	-26.7
1e	-617.98385	-617.71571	-617.76854	-617.75784	111.2	88.7
	-617.98385	-617.71571	-617.76854	-617.75785	111.2	88.7
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4

	-622.37483	-622.23658	-622.28232	-622.27213	96.3	74.8
TSea	-1240.35781	-1239.95058	-1240.02404	-1240.01315	154.6	131.7
	0.55	1.07	16.83	9.53	-52.9	-28.4
	0.55	1.07	16.83	10.56	-52.9	-31.9
1f	-768.36311	-768.08377	-768.14009	-768.12953	118.5	96.3
	-768.36311	-768.08377	-768.14009	-768.12978	118.5	96.8
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27224	96.3	75.1
TSfa	-1390.73821	-1390.31921	-1390.39640	-1390.38568	162.5	139.9
	-0.17	0.72	16.32	9.00	-52.4	-27.8
	-0.17	0.72	16.32	10.25	-52.4	-32.0
1g	-696.59273	-696.26306	-696.31979	-696.30922	119.4	97.1
	-696.59273	-696.26306	-696.31979	-696.30949	119.4	97.7
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27229	96.3	75.2
TSga	-1318.96404	-1318.49544	-1318.57478	-1318.56373	167.0	143.7
	2.21	2.64	17.15	10.03	-48.7	-24.8
	2.21	2.64	17.15	11.33	-48.7	-29.2
1h	-770.37138	-770.07681	-770.13329	-770.12184	118.9	94.8
	-770.37138	-770.07681	-770.13329	-770.12199	118.9	95.1
2a	-622.37483	-622.23658	-622.28232	-622.27049	96.3	71.4
	-622.37483	-622.23658	-622.28232	-622.27193	96.3	74.4
TSha	-1392.73305	-1392.29929	-1392.37846	-1392.36685	166.6	142.2
	8.26	8.85	23.31	15.99	-48.5	-24.0
	8.26	8.85	23.31	16.99	-48.5	-27.3
CAM 1,2-dichloroethane						
1a	-539.21126	-539.00410	-539.04768	-539.03611	91.7	67.4
	-539.21126	-539.00410	-539.04768	-539.03633	91.7	67.8
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27815	91.9	69.4
TSab	-986.49711	-986.23144	-986.29894	-986.28716	142.1	117.3
	10.79	11.19	23.59	16.03	-41.6	-16.2
	10.79	11.19	23.59	17.14	-41.6	-19.9
1d	-578.49803	-578.26078	-578.30999	-578.29895	103.6	80.3
	-578.49803	-578.26078	-578.30999	-578.29906	103.6	80.6
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27843	91.9	70.0
TSdb	-1025.79135	-1025.49557	-1025.56490	-1025.55348	145.9	121.9
	6.11	6.52	21.30	13.85	-49.6	-24.6
	6.11	6.52	21.30	15.07	-49.6	-28.7
1e	-617.78360	-617.51611	-617.56906	-617.55846	111.4	89.1
	-617.78360	-617.51611	-617.56906	-617.55847	111.4	89.2
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1

	-447.30305	-447.24518	-447.28886	-447.27870	91.9	70.5
TSeb	-1065.08024	-1064.75431	-1064.82559	-1064.81450	150.0	126.7
	4.02	4.38	20.29	12.90	-53.3	-28.6
	4.02	4.38	20.29	14.23	-53.3	-33.0
1f	-768.15783	-767.87917	-767.93566	-767.92516	118.9	96.8
	-768.15783	-767.87917	-767.93566	-767.92541	118.9	97.3
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27882	91.9	70.8
TSfb	-1215.44943	-1215.11171	-1215.18897	-1215.17820	162.6	139.9
	7.18	7.93	22.31	14.78	-48.2	-22.9
	7.18	7.93	22.31	16.33	-48.2	-28.1
1h	-770.12797	-769.83419	-769.89138	-769.88004	120.4	96.5
	-770.12797	-769.83419	-769.89138	-769.88019	120.4	96.8
2b	-447.30305	-447.24518	-447.28886	-447.27660	91.9	66.1
	-447.30305	-447.24518	-447.28886	-447.27846	91.9	70.0
TShb	-1217.41443	-1217.06176	-1217.13939	-1217.12760	163.4	138.6
	10.41	11.05	25.63	18.22	-48.9	-24.1
	10.41	11.05	25.63	19.49	-48.9	-28.3
wB97x 1,2-dichloroethane						
1a	-539.38093	-539.17344	-539.21715	-539.20584	92.0	68.2
	-539.38093	-539.17344	-539.21715	-539.20606	92.0	68.7
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37583	91.9	69.8
TSab	-986.77250	-986.50623	-986.57375	-986.56196	142.1	117.3
	5.74	6.21	18.67	11.38	-41.8	-17.3
	5.74	6.21	18.67	12.51	-41.8	-21.1
1d	-578.68400	-578.44633	-578.49545	-578.48442	103.4	80.2
	-578.68400	-578.44633	-578.49545	-578.48453	103.4	80.4
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37602	91.9	70.2
TSdb	-1026.08393	-1025.78731	-1025.85643	-1025.84509	145.5	121.6
	0.49	1.07	15.93	8.52	-49.8	-25.0
	0.49	1.07	15.93	9.70	-49.8	-29.0
1e	-617.98596	-617.71784	-617.77021	-617.75956	110.2	87.8
	-617.98596	-617.71784	-617.77021	-617.75957	110.2	87.8
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37625	91.9	70.7
TSeb	-1065.38998	-1065.06337	-1065.13464	-1065.12352	150.0	126.6
	-2.08	-1.79	13.76	6.46	-52.2	-27.7
	-2.08	-1.79	13.76	7.72	-52.2	-31.9
1f	-768.36570	-768.08646	-768.14314	-768.13256	119.3	97.0
	-768.36570	-768.08646	-768.14314	-768.13281	119.3	97.5
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4

	-447.40071	-447.34268	-447.38636	-447.37636	91.9	70.9
TSfb	-1215.76431	-1215.42600	-1215.50324	-1215.49244	162.6	139.8
	1.32	1.97	16.48	9.02	-48.6	-23.6
	1.32	1.97	16.48	10.49	-48.6	-28.6
1h	-770.37386	-770.07964	-770.13645	-770.12503	119.6	95.5
	-770.37386	-770.07964	-770.13645	-770.12518	119.6	95.9
2b	-447.40071	-447.34268	-447.38636	-447.37425	91.9	66.4
	-447.40071	-447.34268	-447.38636	-447.37602	91.9	70.2
TShb	-1217.77137	-1217.41762	-1217.49358	-1217.48203	159.9	135.6
	2.01	2.95	18.34	10.82	-51.6	-26.4
	2.01	2.95	18.34	12.03	-51.6	-30.4
CAM 1,4-dioxane						
1a	-539.20904	-539.00175	-539.04534	-539.03369	91.7	67.2
	-539.20904	-539.00175	-539.04534	-539.03391	91.7	67.7
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10075	72.5	49.9
TSac	-918.32085	-918.04967	-918.10715	-918.09507	121.0	95.6
	17.64	18.27	31.17	23.76	-43.3	-18.4
	17.64	18.27	31.17	24.85	-43.3	-22.1
1d	-578.49592	-578.25856	-578.30782	-578.29664	103.7	80.1
	-578.49592	-578.25856	-578.30782	-578.29675	103.7	80.4
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10104	72.5	50.5
TSdc	-957.61314	-957.31194	-957.37193	-957.36027	126.2	101.7
	14.24	14.84	29.73	22.35	-49.9	-25.2
	14.24	14.84	29.73	23.54	-49.9	-29.2
1e	-617.78163	-617.51403	-617.56702	-617.55629	111.5	89.0
	-617.78163	-617.51403	-617.56702	-617.55630	111.5	89.0
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10133	72.5	51.2
TSec	-996.90390	-996.57259	-996.63499	-996.62373	131.3	107.6
	11.08	11.59	27.30	19.96	-52.7	-28.1
	11.08	11.59	27.30	21.28	-52.7	-32.5
1f	-768.15515	-767.87635	-767.93279	-767.92222	118.8	96.5
	-768.15515	-767.87635	-767.93279	-767.92247	118.8	97.1
2c	-379.13992	-379.07703	-379.11148	-379.09925	72.5	46.8
	-379.13992	-379.07703	-379.11148	-379.10148	72.5	51.5
TSfc	-1147.26631	-1146.92338	-1146.99022	-1146.97929	140.7	117.7
	18.05	18.83	33.92	26.47	-50.6	-25.6
	18.05	18.83	33.92	28.02	-50.6	-30.8
CAM toluene						
1h	-770.12564	-769.83171	-769.88852	-769.87717	119.6	95.7
	-770.12564	-769.83171	-769.88852	-769.87732	119.6	96.0

2c	-379.14023	-379.07736	-379.11180	-379.09963	72.5	46.9
	-379.14023	-379.07736	-379.11180	-379.10148	72.5	50.8
TShc	-1149.23502	-1148.87697	-1148.94543	-1148.93365	144.1	119.3
	19.36	20.14	34.44	27.08	-48.0	-23.3
	19.36	20.14	34.44	28.33	-48.0	-27.5
wB97x 1,4-dioxane						
1a	-539.37842	-539.17081	-539.21452	-539.20276	92.0	67.3
	-539.37842	-539.17081	-539.21452	-539.20298	92.0	67.7
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16205	72.5	49.7
TSac	-918.55643	-918.28466	-918.34212	-918.33031	120.9	96.1
	14.78	15.44	28.44	20.69	-43.6	-17.6
	14.78	15.44	28.44	21.79	-43.6	-21.3
1d	-578.68162	-578.44383	-578.49304	-578.48180	103.6	79.9
	-578.68162	-578.44383	-578.49304	-578.48191	103.6	80.1
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16236	72.5	50.3
TSdc	-957.86570	-957.56375	-957.62377	-957.61019	126.3	97.7
	10.98	11.63	26.47	20.16	-49.8	-28.6
	10.98	11.63	26.47	21.39	-49.8	-32.7
1e	-617.98371	-617.71556	-617.76848	-617.75773	111.4	88.8
	-617.98371	-617.71556	-617.76848	-617.75774	111.4	88.8
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16268	72.5	51.0
TSec	-997.17312	-996.84108	-996.90318	-996.89212	130.7	107.4
	7.63	8.11	23.98	16.40	-53.2	-27.8
	7.63	8.11	23.98	17.76	-53.2	-32.3
1f	-768.36279	-768.08342	-768.14007	-768.12946	119.2	96.9
	-768.36279	-768.08342	-768.14007	-768.12971	119.2	97.4
2c	-379.20157	-379.13845	-379.17292	-379.16052	72.5	46.5
	-379.20157	-379.13845	-379.17292	-379.16283	72.5	51.3
TSfc	-1147.53655	-1147.19260	-1147.25988	-1147.24893	141.6	118.5
	17.45	18.37	33.33	25.76	-50.2	-24.8
	17.45	18.37	33.33	27.36	-50.2	-30.2
wB97x toluene						
1h	-770.37138	-770.07681	-770.13329	-770.12184	118.9	94.8
	-770.37138	-770.07681	-770.13329	-770.12199	118.9	95.1
2c	-379.20189	-379.13878	-379.17325	-379.16103	72.5	46.8
	-379.20189	-379.13878	-379.17325	-379.16286	72.5	50.7
TShc	-1149.54786	-1149.18902	-1149.25749	-1149.24580	144.1	119.5
	15.95	16.67	30.78	23.26	-47.3	-22.1
	15.95	16.67	30.78	24.50	-47.3	-26.3

The estimation of activation free-energy barrier from rate constant is based on the conventional transition state theory, which is coded into our ‘‘srate’’ program.

$$\mathrm{k} = \frac{kT}{h} e^{-\frac{\Delta G^{\neq}}{RT}}$$