Supplementary Information for

Simplification through Complexity:The Role of Ni-Complexes in Catalysed Diyne-Cyclobutanone [4+2+2] Cycloadditions, a DFT Study

Jia-Yuan Tao, De-Cai Fang* and Gregory A. Chass*

Contents

References:

13. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr., T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, revision C.02, Gaussian, Inc., Wallingford CT, 2004.

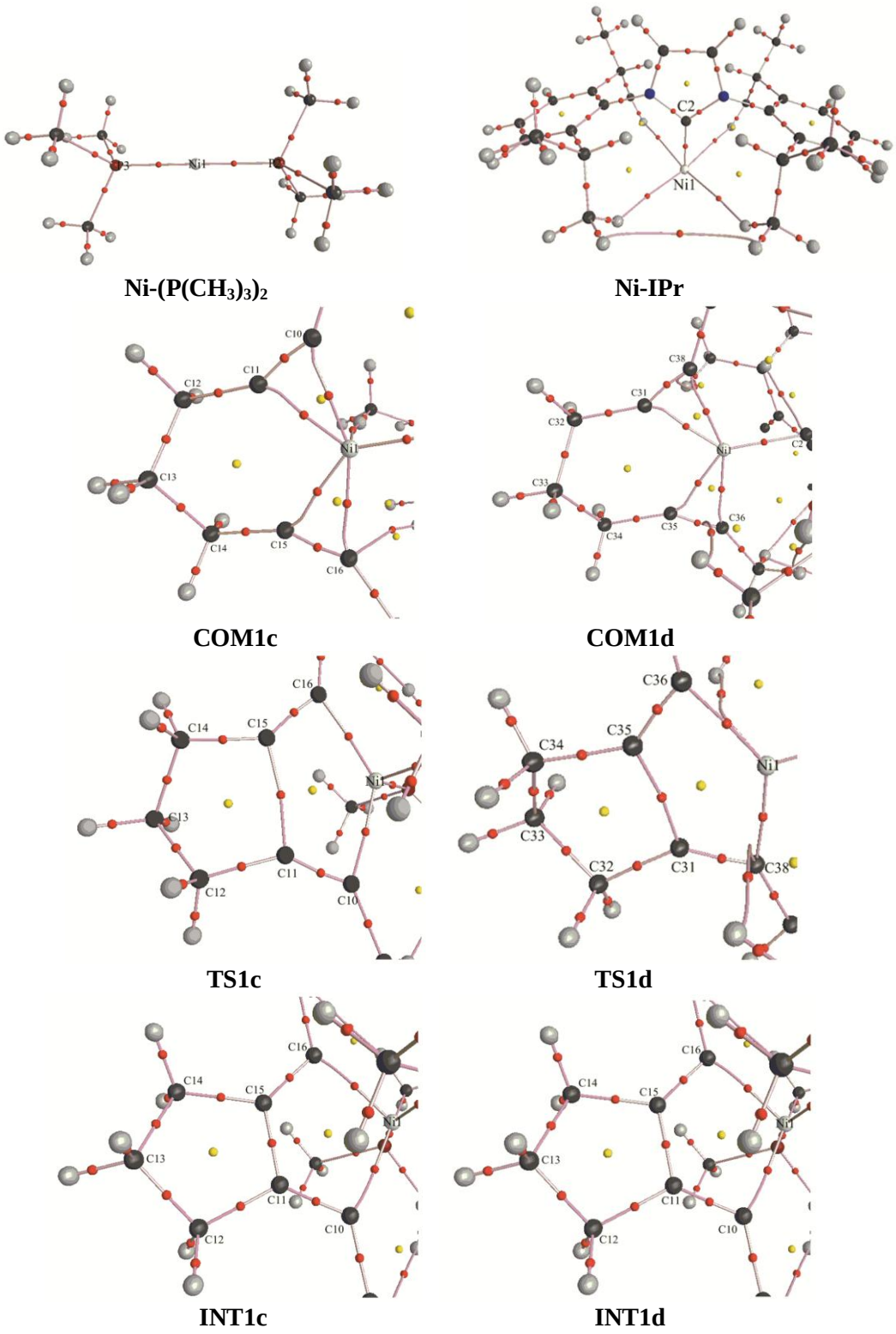


Figure S1. Topological graphs for Ni-$(P(CH_3)_3)_2$, Ni-IPr, COM1,TS1 and INT1 for reaction c & d, generated with the AIM2000 program package.Bond critical points (BCP), ring critical points (RCP) and cage critical points (CCP) are shown as red,yellow and green points, respectively. Each graph was constructed using the wavefunctions generated at the SCRF(PCM/UA0)-B3LYP/DZVP level in toluene solution.

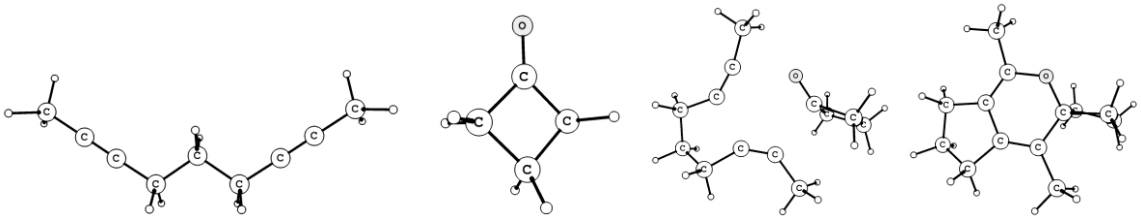


Figure S2. The optimized stationary points for reaction **a**, computed for the [2+2+2] cycloaddition reaction at SCRF(PCM)-B3LYP/DZVP level in toluene, in the absence of catalyst

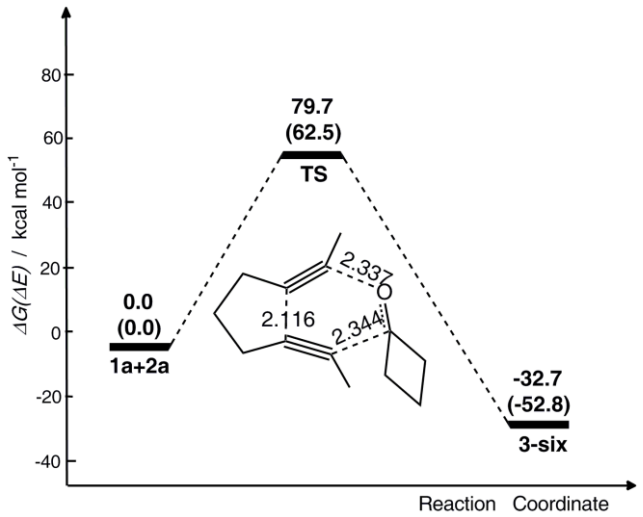


Figure S3. Reaction profiles potential energy surface for reaction **a** computed for the six-membered ring product in toluene solution, in the absence of catalyst.

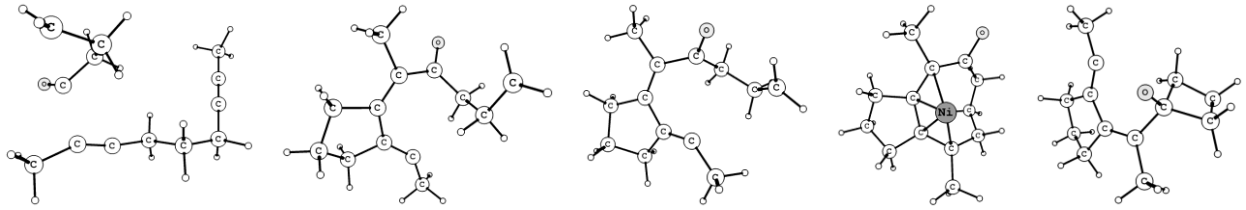


Figure S4. Some optimized stationary points for reaction **a**, computed radical reaction at SCRF(PCM)-B3LYP/DZVP level in toluene, in the absence of catalyst.

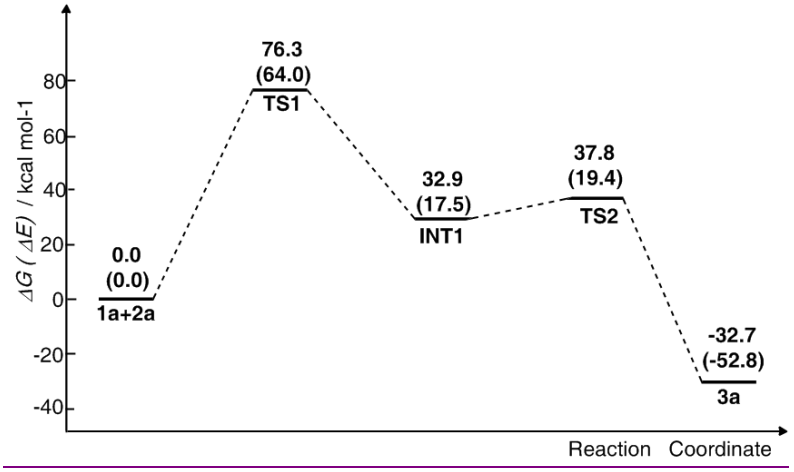


Figure S5. Reaction profile potential energy surface for the diradical diyne-cyclobutanone reaction a, at SCRF(PCM)- B3LYP/DZVP level in toluene, in the absence of catalyst.

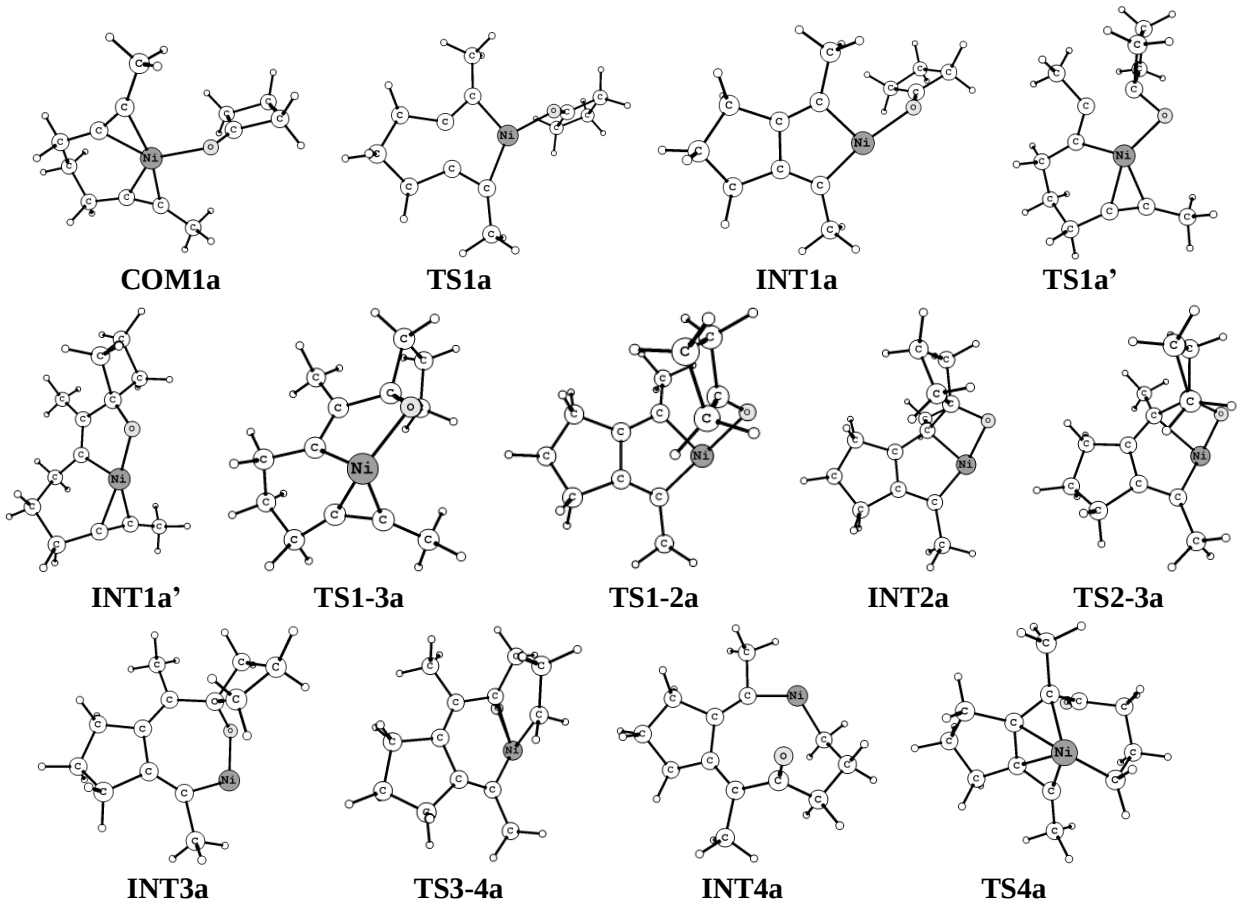
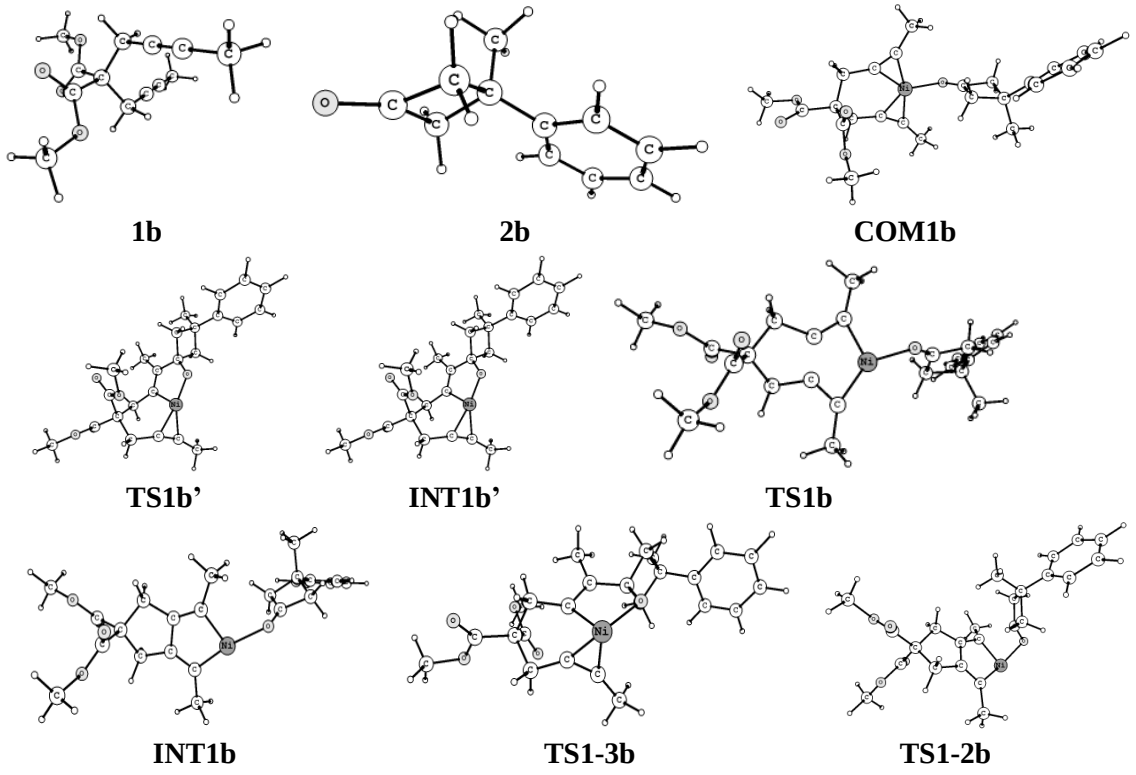


Figure S6. Some optimized stationary points for nickel catalyzed reaction **a**, computed at SCRF(PCM)-B3LYP/DZVP level in toluene.



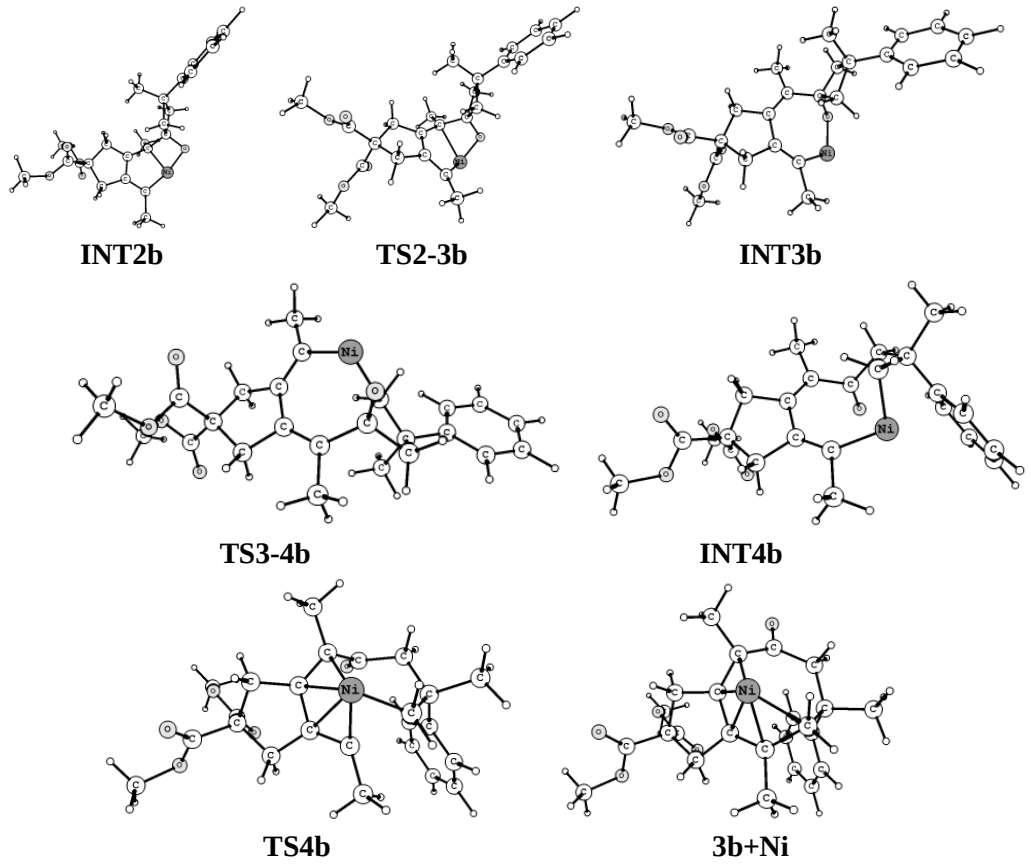


Figure S7. Some optimized stationary points for nickel catalyzed reaction **b**, computed at SCRF(PCM)-B3LYP/DZVP level in toluene.

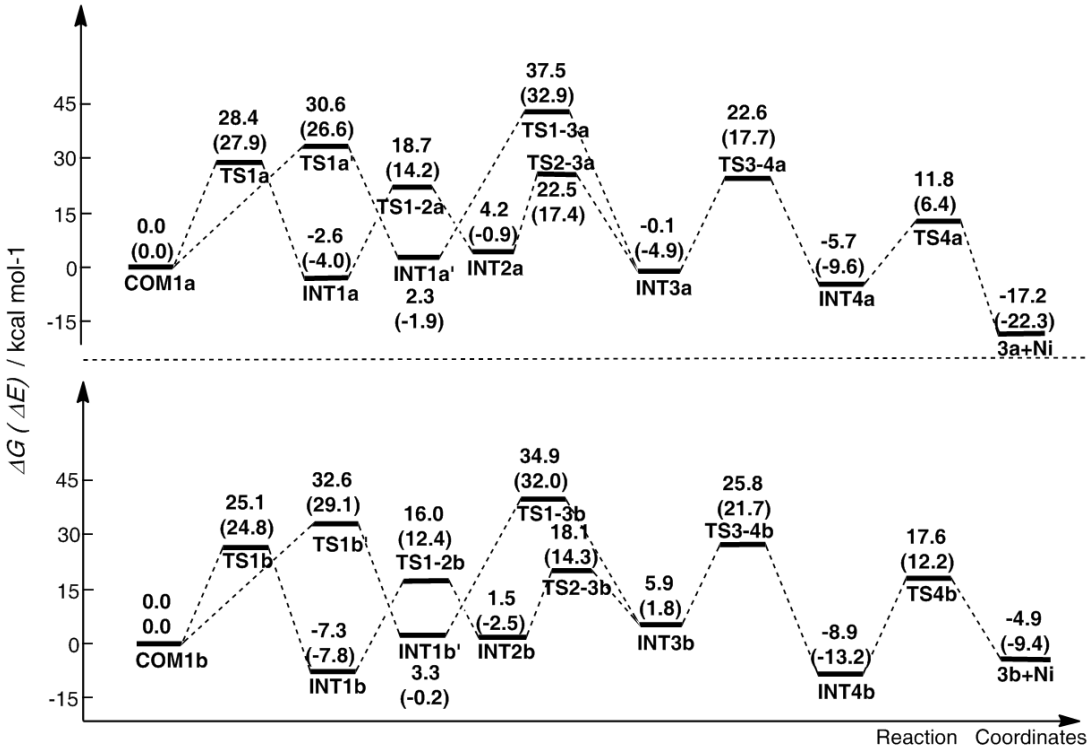


Figure S8. Reaction profiles potential energy surface for reaction **a** and **b** of Ni catalyzed [4+2+2] cycloaddition, in toluene solution.

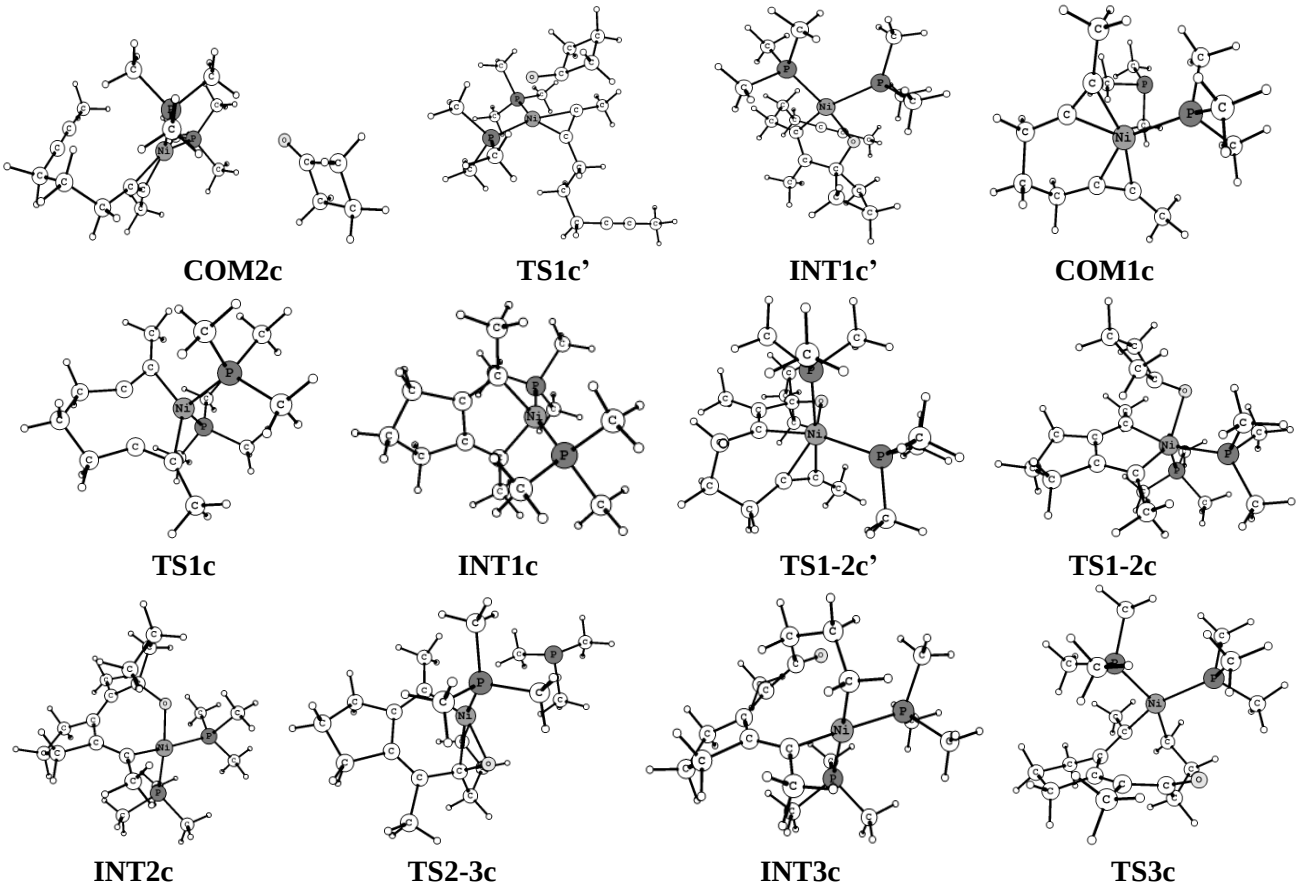


Figure S9. Some optimized stationary points for reaction **c**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

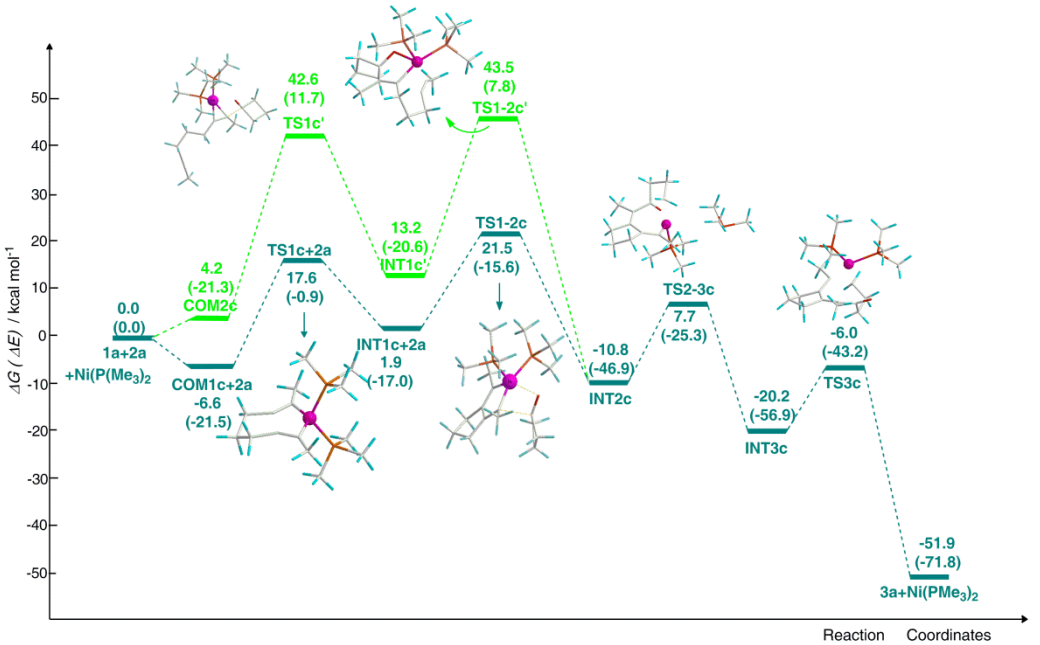


Figure S10. Reaction profiles potential energy surface for reaction **c** of Ni-$(P(CH_3)_3)_2$ catalyzed [4+2+2] cycloaddition (bottom, in teal), in toluene solution. A less stable partial-pathway initiated at COM2 is also shown (top, in green).

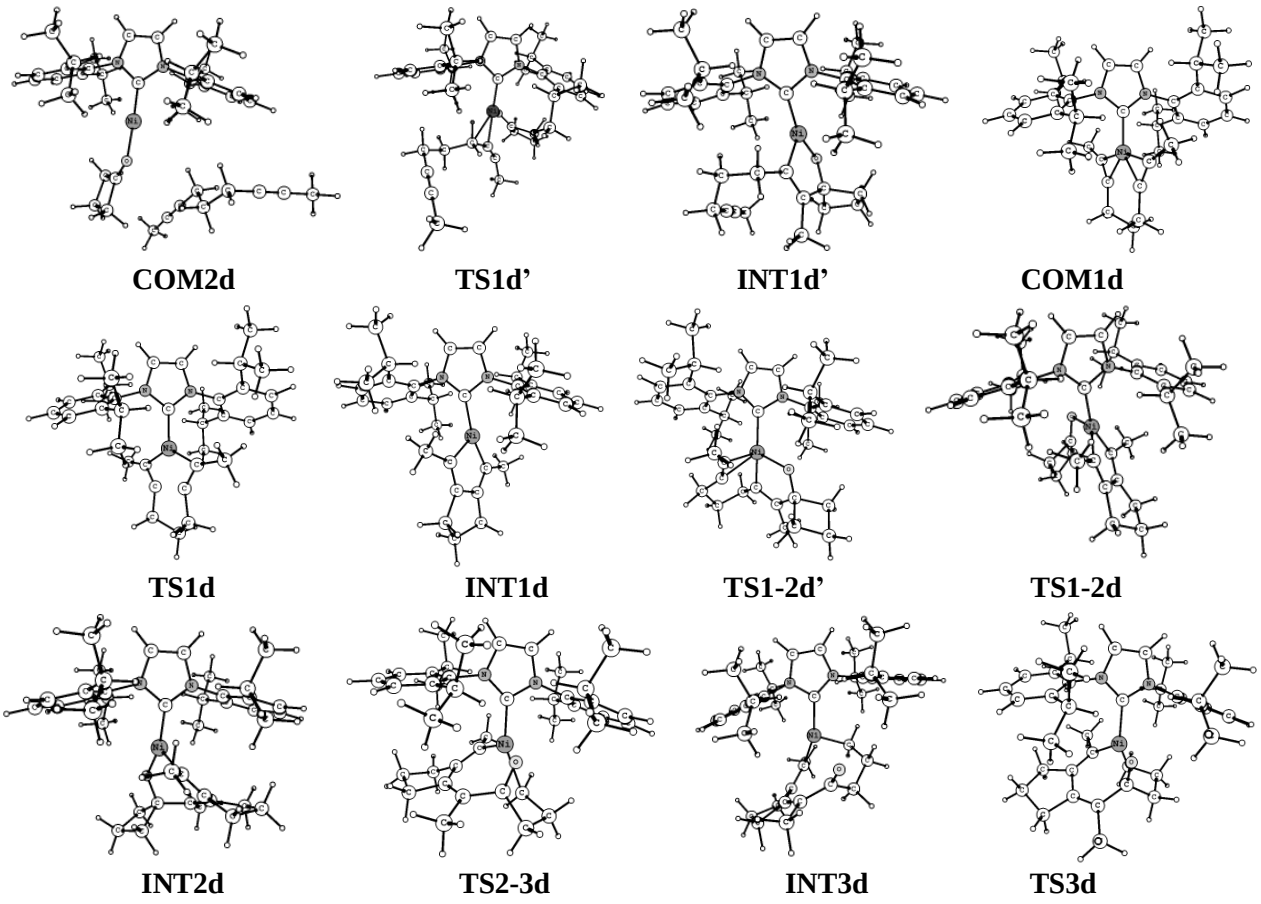


Figure S11. Some optimized stationary points for reaction **d**, at SCRF-B3LYP/DZVP level in toluene.

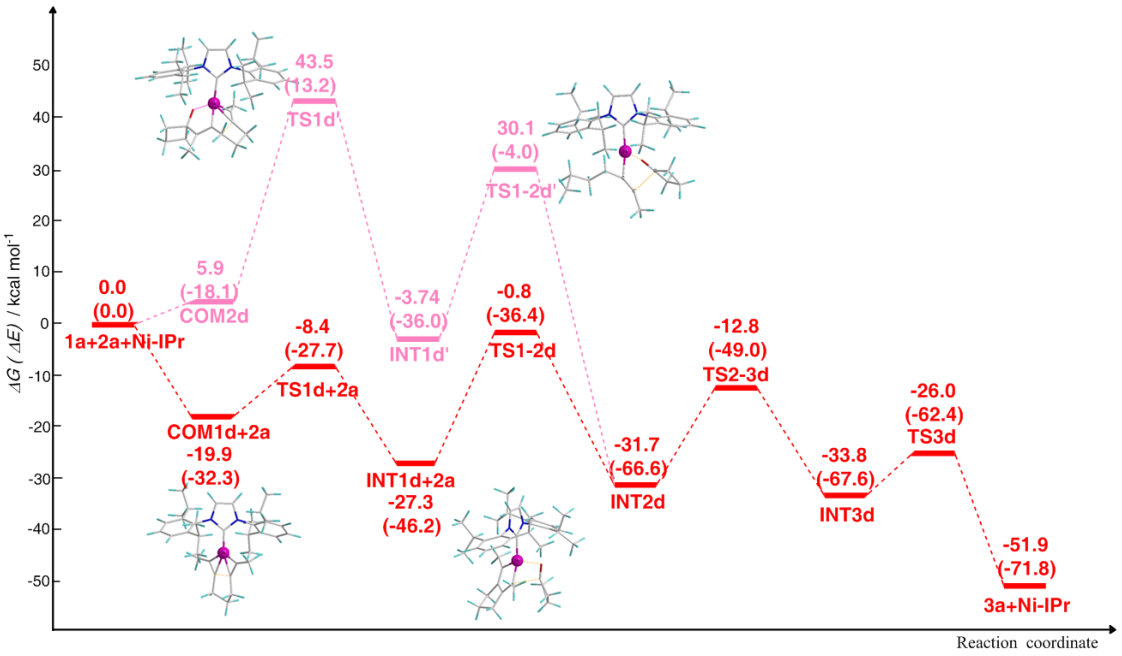


Figure S12. Reaction profiles potential energy surface for reaction **d** of IPr-Ni catalyzed [4+2+2] cycloaddition (bottom, in red), in toluene solution. A less stable partial-pathway initiated at COM2 is also shown (top, in magenta).

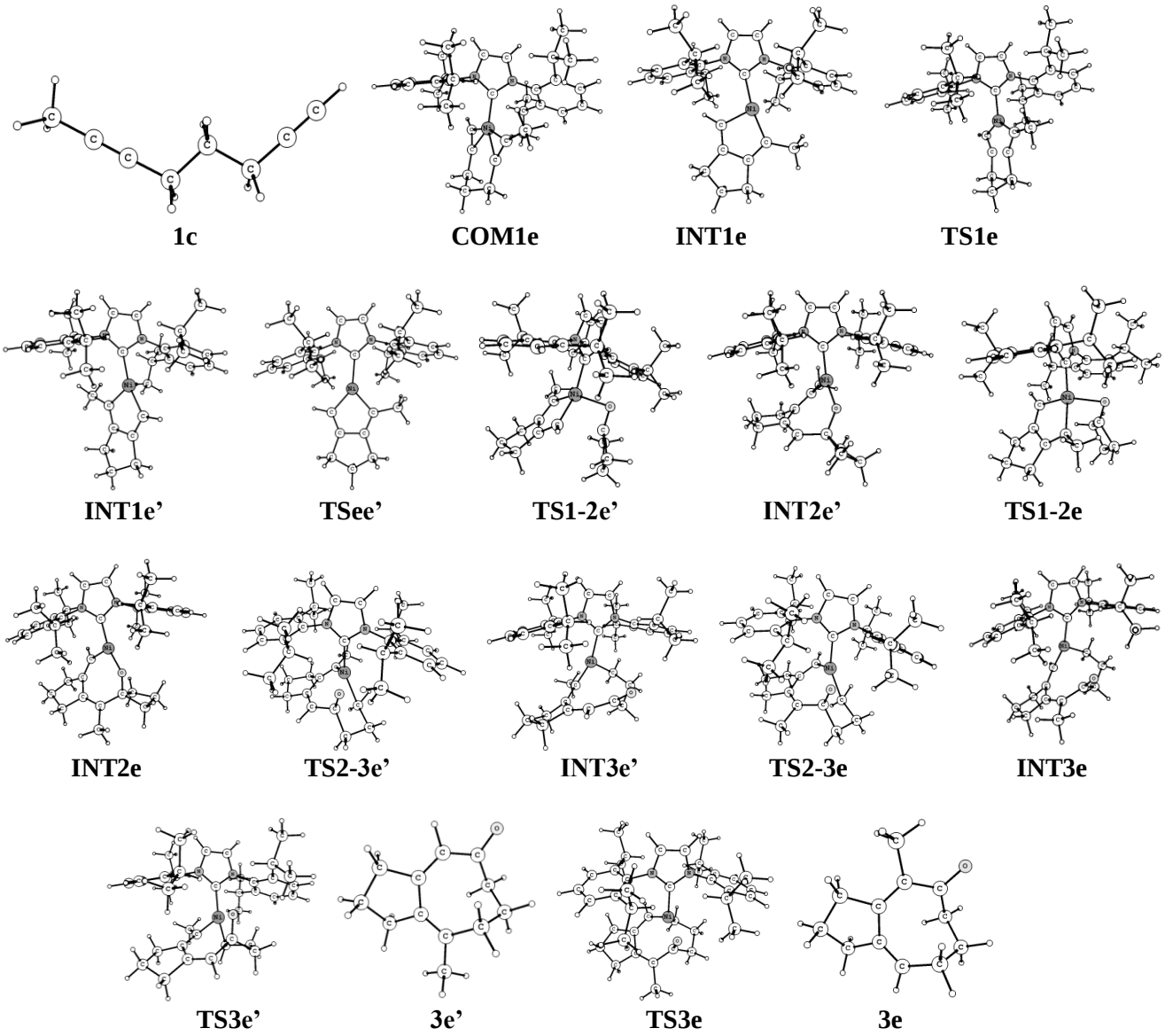


Figure S13. Some optimized stationary points for reaction **e**, at SCRF-B3LYP/DZVP level in toluene.

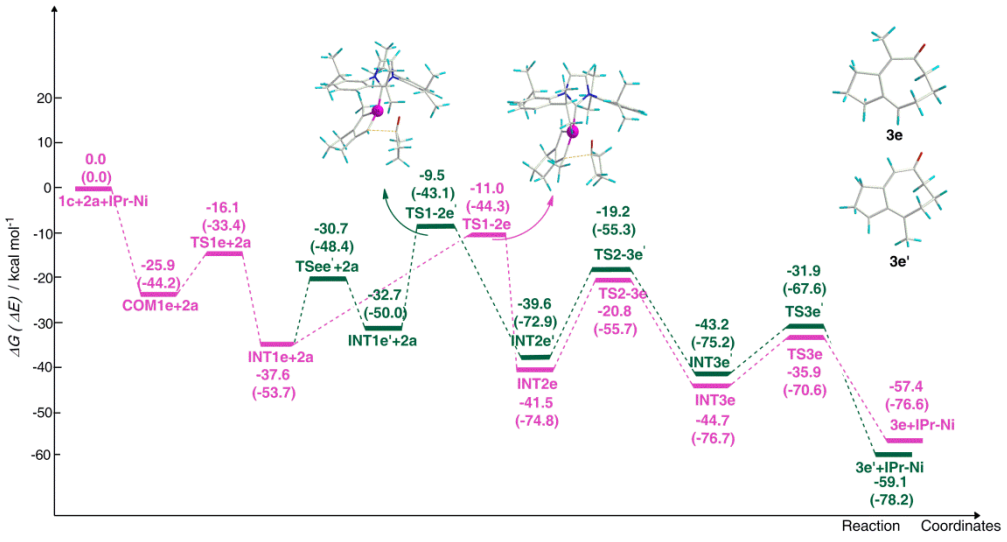


Figure S14. Reaction profiles potential energy surface for reaction **e** of Ni-IPr catalyzed [4+2+2] cycloaddition, in toluene solution.

Table S1. Some optimized Cartesian Coordinates of stationary points for reaction **a**, computed for the [2+2+2] reaction in toluene, in the absence of catalyst, with bond lengths in Å.

Species	Cartesian coordinates			Species	Cartesian coordinates		
1a	C	-0.000007	-0.260018 -0.000334	2a	C	-0.674174	0.000002 0.000187
	C	1.274847	-1.128765 0.000020		O	-1.887298	0.000001 -0.000179
	C	2.515241	-0.338318 -0.000315		C	0.384915	-1.111444 0.000125
	C	3.531242	0.328080 0.000155		C	1.484050	-0.000003 -0.000227
	C	4.763620	1.128284 0.000110		C	0.384924	1.111445 0.000121
	C	-1.274852	-1.128779 0.000104		H	0.345312	-1.751679 -0.888215
	C	-2.515254	-0.338342 0.000352		H	0.345575	-1.751227 0.888807
	C	-3.531211	0.328123 0.000011		H	2.118782	-0.000026 -0.889130
	C	-4.763620	1.128281 -0.000045		H	2.119537	0.000012 0.888133
	H	5.372083	0.913405 -0.885066		H	0.345273	1.751688 -0.888212
	H	5.371121	0.915088 0.886353		H	0.345625	1.751220 0.888810
	H	4.535359	2.199670 -0.001023				
	H	1.268837	-1.788133 -0.878249				
	H	1.268882	-1.787389 0.878845				
	H	0.000016	0.392200 0.879180				
	H	-0.000038	0.391320 -0.880501				
	H	-1.268590	-1.787716 0.878695				
	H	-1.269123	-1.787836 -0.878398				
	H	-5.371552	0.914211 -0.885781				
	H	-4.535408	2.199678 -0.000042				
	H	-5.371631	0.914220 0.885641				
TS	C	3.295257	-1.225263 0.543358	3-six	C	-1.194708	0.207645 0.145766
	C	2.234869	-1.847946 -0.355664		C	-0.941830	1.467557 -0.295456
	C	0.937042	-1.108434 -0.230724		C	-0.362246	-1.007836 -0.040445
	C	-0.301596	-1.315852 -0.208490		C	0.990895	-1.222768 -0.054499
	C	-1.187786	-2.518217 -0.234611		C	2.049270	-0.226645 0.283894
	C	3.293105	0.266978 0.204632		C	1.722722	1.078819 0.993924
	C	1.886097	0.767593 0.009499		C	1.467195	2.217261 -0.009665
	C	1.294686	1.857147 -0.098137		C	0.341641	1.849722 -0.997831
	C	0.927769	3.268936 -0.192854		C	-1.320899	-2.195416 -0.160048
	O	-1.016650	1.541748 -0.237279		O	3.235215	-0.472272 0.029384
	C	-1.720346	0.542263 -0.038198		C	-2.741798	-1.612384 -0.036225
	C	-2.461925	0.160906 1.273003		C	-2.534486	-0.273515 0.696387
	C	-3.694362	-0.229585 0.393932		C	1.512357	-2.612955 -0.378807
	C	-2.908102	0.067957 -0.923833		C	-1.911943	2.614857 -0.121385
	H	2.040418	-2.898115 -0.101368		H	2.602033	-2.612332 -0.399533
	H	2.574182	-1.821703 -1.400296		H	1.152295	-2.966315 -1.351837
	H	3.028923	-1.378740 1.595377		H	1.182574	-3.345469 0.368961
	H	4.283231	-1.666803 0.373985		H	0.852043	0.962207 1.644964
	H	3.842909	0.429128 -0.731467		H	2.384603	2.431651 -0.570185
	H	3.789106	0.863658 0.976979		H	1.210519	3.128444 0.544892
	H	-0.597272	-3.431050 -0.074637		H	0.685117	1.022690 -1.630311
	H	-1.693218	-2.621974 -1.200404		H	0.153213	2.702619 -1.661392
	H	-1.964339	-2.490904 0.535878		H	-2.741332	2.397096 0.552498
	H	0.402762	3.480163 -1.128847		H	-2.328154	2.916516 -1.092538
	H	0.276758	3.565657 0.633580		H	-1.386998	3.494393 0.272382
	H	1.843423	3.874758 -0.160301		H	-2.461379	-0.444456 1.780246
	H	-4.015979	-1.268918 0.501456		H	-3.358948	0.421210 0.529198

	H -4.559955 0.421841 0.541747 H -2.602414 1.031691 1.922637 H -2.033768 -0.650648 1.864931 H -3.299733 0.897392 -1.522420 H -2.750082 -0.788316 -1.580068		H -3.159854 -1.420387 -1.030814 H -3.428461 -2.284608 0.487363 H -1.172583 -2.746913 -1.095257 H -1.114039 -2.908540 0.649313 H 2.590604 1.324323 1.613320

Table S2. Frequencies of some stationary points for reaction **a**, computed for the [2+2+2] reaction in toluene, in the absence of catalyst.

Species	Frequencies (cm^{-1})
1a	27 28 47 79 93 112 210 215 241 283 306 370 374 435 531 728 741 796 840 1027 1035 1048 1050 1050 1053 1080 1154 1162 1182 1269 1305 1331 1359 1401 1421 1421 1486 1487 1493 1493 1493 1493 1511 2335 2336 3024 3027 3036 3036 3065 3066 3068 3117 3117 3117 3117 3123
2a	3 398 454 619 675 741 842 927 952 970 1096 1103 1197 1221 1224 1247 1279 1433 1447 1504 1835 3056 3060 3091 3117 3122 3156
TS	**-435i** 26 40 51 86 96 136 151 160 167 213 230 237 255 267 303 349 386 402 433 461 465 481 568 673 741 751 757 824 825 881 907 929 954 964 975 1013 1022 1032 1049 1056 1066 1070 1073 1093 1118 1157 1195 1202 1209 1228 1251 1269 1279 1335 1347 1372 1406 1415 1467 1471 1478 1484 1486 1487 1499 1508 1509 1518 1637 1962 2121 3014 3023 3031 3038 3053 3070 3074 3075 3081 3091 3098 3115 3115 3120 3130 3143 3146 3159
3-six	57 84 101 118 130 146 169 205 258 289 307 338 362 372 418 447 480 531 569 590 614 635 670 768 783 819 855 864 891 916 944 973 984 1014 1030 1038 1042 1048 1067 1082 1097 1134 1149 1157 1194 1208 1224 1259 1273 1293 1308 1324 1332 1347 1355 1376 1381 1409 1419 1476 1491 1496 1497 1500 1507 1511 1516 1517 1518 1612 1676 1687 3021 3023 3029 3032 3037 3043 3055 3071 3082 3083 3086 3093 3099 3115 3132 3133 3162 3168

Table S3. Some optimized Cartesian Coordinates of stationary points for reaction **a**, computed for diradical reaction in toluene, in the absence of catalyst with bond lengths in Å.

Species	Cartesian coordinates	Species	Cartesian coordinates
TS1	C -3.38325 -1.87115 -0.13900 C -1.98442 -1.38954 -0.25997 C -0.76315 -1.59658 -0.32997 C 0.69934 -1.56541 -0.44739 C 1.4329 -1.64555 0.90682 C 2.96853 -1.59599 0.75859 C 3.47481 -0.3375 0.18421 C 3.88532 0.70343 -0.29022 C 4.39347 1.9569 -0.86433 C -2.30406 0.66881 -0.78394 O -2.92912 0.80493 -1.80271 C -1.2191 1.60658 -0.25741 C -1.28897 1.69735 1.27147 C -2.66735 2.00538 1.76109 H 1.02609 -2.3975 -1.08717 H 1.00816 -0.65012 -0.97364 H 1.10249 -0.82554 1.55290	INT1	C 1.482770 0.485385 -0.188482 C 1.043631 1.734108 -0.265812 C 0.737256 -0.792415 0.015505 C -0.550170 -1.175430 -0.233124 C -1.650630 -0.362044 -0.853934 C -1.887167 1.099231 -0.517456 C -2.030900 1.393144 0.990455 C -3.200741 0.722772 1.634573 C 1.764717 -1.833366 0.471934 C 3.059370 -1.058086 0.768950 O -2.430440 -0.928519 -1.626322 C 2.985328 0.143710 -0.181848 C -0.929580 -2.635043 -0.020575 C 1.571136 3.106799 -0.393628 H -1.979980 -2.801728 -0.258470 H -0.754168 -2.941956 1.016844 H -0.339589 -3.305234 -0.658280

	H 1.16182 -2.58029 1.41039 H 3.30397 -2.43575 0.13547 H 3.42369 -1.74552 1.74548 H -3.40089 -2.94333 0.08077 H -3.92134 -1.6933 -1.07530 H -3.91327 -1.33629 0.65441 H 3.74361 2.31233 -1.67132 H 4.44911 2.74421 -0.10481 H 5.3977 1.81799 -1.27904 H -0.56981 2.46498 1.60919 H -0.94378 0.75418 1.71081 H -3.33846 2.62923 1.17443 H -2.94156 1.81086 2.79506 H -0.24355 1.23081 -0.58380 H -1.37547 2.58325 -0.73181		H -1.042951 1.684855 -0.904404 H -2.107692 2.480720 1.128139 H -1.093200 1.109031 1.497921 H -3.635173 -0.185215 1.224219 H -3.580718 1.076305 2.589960 H 2.669647 3.129025 -0.321641 H 1.172310 3.760378 0.392024 H 1.293090 3.551389 -1.357319 H 3.294760 -0.150170 -1.194191 H 3.610796 0.985443 0.126682 H 3.058504 -0.707400 1.807494 H 3.958353 -1.664889 0.621481 H 1.410489 -2.407404 1.334056 H 1.928639 -2.560342 -0.336372 H -2.789724 1.402751 -1.056922
TS2	C 0.58125 2.99332 -0.28697 C 0.27353 1.5219 -0.10455 C 1.22626 0.56721 -0.00442 C 2.72948 0.82839 0.10361 C 3.39467 -0.56467 0.04356 C 2.31327 -1.53611 0.55580 C 1.0225 -0.90418 0.01540 C 0.00455 -1.57564 -0.50829 C -0.37847 -2.97217 -0.79648 C -1.20064 1.22234 -0.09284 O -1.92375 1.67268 -0.98145 C -1.81835 0.59288 1.16159 C -2.71294 -0.66800 1.00861 C -3.34911 -0.90674 -0.32177 H 0.09351 3.36196 -1.19607 H 1.65256 3.18776 -0.36202 H 0.18754 3.59011 0.54647 H -1.03573 0.38477 1.89511 H -2.11441 -1.54746 1.27800 H -3.49195 -0.61894 1.78988 H -3.47787 -0.11228 -1.04687 H -3.83124 -1.86400 -0.50837 H 0.41196 -3.67500 -0.48915 H -0.55533 -3.11429 -1.86949 H -1.30158 -3.25569 -0.27886 H 2.29097 -1.54019 1.65430 H 2.46293 -2.56626 0.22156 H 3.64224 -0.81361 -0.99444 H 4.31952 -0.61442 0.62700 H 3.09802 1.49049 -0.68633 H 2.94863 1.32389 1.05886 H -2.42579 1.41056 1.57248	3a	C -1.194708 0.207645 0.145766 C -0.941830 1.467557 -0.295456 C -0.362246 -1.007836 -0.040445 C 0.990895 -1.222768 -0.054499 C 2.049270 -0.226645 0.283894 C 1.722722 1.078819 0.993924 C 1.467195 2.217261 -0.009665 C 0.341641 1.849722 -0.997831 C -1.320899 -2.195416 -0.160048 C -2.741798 -1.612384 -0.036225 O 3.235215 -0.472272 0.029384 C -2.534486 -0.273515 0.696387 C 1.512357 -2.612955 -0.378807 C -1.911943 2.614857 -0.121385 H 2.602033 -2.612332 -0.399533 H 1.152295 -2.966315 -1.351837 H 1.182574 -3.345469 0.368961 H 0.852043 0.962207 1.644964 H 2.384603 2.431651 -0.570185 H 1.210519 3.128444 0.544892 H 0.685117 1.022690 -1.630311 H 0.153213 2.702619 -1.661392 H -2.741332 2.397096 0.552498 H -2.328154 2.916516 -1.092538 H -1.386998 3.494393 0.272382 H -2.461379 -0.444456 1.780246 H -3.358948 0.421210 0.529198 H -3.159854 -1.420387 -1.030814 H -3.428461 -2.284608 0.487363 H -1.172583 -2.746913 -1.095257 H -1.114039 -2.908540 0.649313 H 2.590604 1.324323 1.613320
3-step-INT1	C 1.51470 0.45493-0.05196 C 1.10108 1.67134-0.36989 C 0.74277 -0.80707-0.16179 C -0.59377 -0.99419-0.32949		

	C -1.60905 0.17279-0.30625 C -1.58688 1.13286 0.93729 C -2.89501 0.46845 1.45093 C -3.09503 -0.20856 0.07239 C 1.74158 -1.95318-0.02094 C 2.88152 -1.35348 0.82371 C 2.96210 0.11344 0.36414 C -1.15577 -2.35114-0.69101 C 1.56977 3.06411-0.42079 O -1.42710 0.68354-1.55603 H -1.91151 -2.24223-1.47534 H -1.64391 -2.83880 0.16367 H -0.38753 -3.02843-1.06984 H -0.71902 1.08885 1.59802 H -3.68972 1.14725 1.77367 H -2.70859 -0.25613 2.24941 H 2.60769 3.16175-0.06323 H 0.94149 3.71590 0.19966 H 1.52591 3.45590-1.44458 H 3.62307 0.20686-0.50690 H 3.34555 0.78467 1.13869 H 2.61054 -1.39619 1.88509 H 3.82817 -1.88924 0.70117 H 1.31017 -2.84825 0.43379 H 2.11838 -2.23994-1.01437 H -1.74185 2.16680 0.61365 H -3.37721 -1.26361 0.06164 H -3.78293 0.34467-0.57384		

Table S4. Frequencies of some stationary points for reaction **a,** computed for biradical reaction in toluene, in the absence of catalyst.

Species	Frequencies (cm^{-1})
TS1	**-469i** 15 19 22 34 41 61 72 98 127 132 139 141 196 198 216 229 265 292 320 356 372 409 443 471 498 532 537 693 752 783 812 835 862 894 958 968 1031 1046 1048 1051 1052 1060 1063 1093 1143 1153 11831192 1218 1236 1309 1315 1320 1368 1377 1393 1411 1421 1456 1468 1477 1484 1485 1488 1493 1493 1498 1503 1806 2122 2332 2964 3006 3032 3037 3045 3046 3050 3058 3075 30793115 3116 3117 3118 3132 3135 3143 3251
INT1	7 38 43 88 90 97 111 113 142 148 174 202 241 272 305 354 385 403 431 448 477 544 567 598 607 647 696 787 838 862 882 883 944 949 963 1003 1025 1032 1036 1048 1060 1061 1080 1097 1114 1148 1160 1202 1213 1248 1264 1299 1322 1333 1348 1351 1373 1404 1417 1455 1469 1470 1472 1476 1483 1495 1497 1512 1514 1618 1688 1731 2975 2990 3008 3023 3032 3033 3041 3053 3072 3092 3094 3096 3107 3112 3122 3148 3168 3256
TS2	**-86i** 38 45 89 107 116 127 131 137 164 170 213 229 247 279 320 354 373 439 483 485 516 566 600 626 657 745 790 852 856 864 886 923 932 951 1004 1025 1030 1039 1048 1060 1066 1073 1108 1134 1148 1190 1203 1210 1253 1262 1287 1315 1326 1346 1352 1389 1404 1412 1457 1466 1478 1483 1485 1494 1495 1496 1505 1514 1674 1710 1734 2957 2990 3030 3031 3033 3040 3047 3056 3077 3094 3099 3105 3112 3121 3123 3155 3156 3284
3a	39 67 113 125 145 157 166 181 210 232 247 277 298 308 339 367 403 419 454 489 518 534

	546 561 607 623 663 800 819 862 882 889 910 951 957 959 1018 1031 1045 1048 1062 1070 1078 1104 1118 1143 1160 1190 1208 1232 1256 1267 1285 1310 1318 1336 1354 1376 1387 1398 1410 1415 1419 1467 1472 1484 1494 1497 1504 1506 1509 1517 1521 1527 1611 2992 2999 3018 3021 3027 3030 3032 3050 3051 3079 3082 3097 3102 3104 3116 3120 3133 3165

Table S5. Some optimized Cartesian Coordinates of stationary points for reaction **a** in toluene, with bond lengths in Å.

Species	Cartesian coordinates			Species	Cartesian coordinates		
COM1a	C	-3.551056	-0.024103 1.081051	TS1a’	C	-1.842618	2.303314 -0.227197
	C	-3.194849	1.261065 0.312061		C	-0.926778	1.104097 -0.045989
	C	-1.751091	1.366659 -0.029316		C	0.387135	1.245359 0.084031
	C	-0.663785	1.949108 -0.299111		C	1.361364	2.371525 0.188179
	C	0.194243	3.140069 -0.527788		C	2.776243	1.911431 0.587377
	C	-3.175427	-1.298573 0.303537		C	3.287164	0.770832 -0.316228
	C	-1.730362	-1.379154 -0.039210		C	2.394239	-0.410443 -0.242185
	C	-0.634596	-1.943400 -0.314126		C	2.035778	-1.586097 0.041634
	C	0.239984	-3.120732 -0.550769		C	2.148140	-3.028328 0.353394
	Ni	-0.394827	0.004574 -0.355027		Ni	0.452186	-0.526628 -0.261920
	O	1.553477	0.021229 -0.873002		O	-1.114457	-1.577218 -0.209701
	C	2.524034	0.023180 -0.129044		C	-1.798028	-0.405423 -0.033838
	C	2.691311	0.003442 1.381169		C	-2.713757	-0.375429 1.248819
	C	4.239308	-0.037378 1.155625		C	-3.969850	-0.300144 0.331775
	C	4.025522	0.024401 -0.393764		C	-3.076757	-0.299162 -0.944463
	H	-4.628280	-0.032895 1.287607		H	-2.581574	0.466961 1.933143
	H	-3.033709	-0.023373 2.047884		H	-2.603896	-1.309004 1.805876
	H	-3.492673	2.136945 0.903881		H	-4.562351	0.610979 0.461915
	H	-3.783324	1.295693 -0.615834		H	-4.639517	-1.161260 0.411828
	H	-0.378028	4.073036 -0.446436		H	-3.183683	0.573800 -1.590873
	H	1.012525	3.186296 0.201097		H	-3.157902	-1.201485 -1.554891
	H	0.654881	3.108913 -1.521716		H	-1.349844	3.208542 0.139893
	H	-3.763855	-1.336317 -0.624262		H	-2.786340	2.193614 0.313849
	H	-3.459139	-2.182824 0.889827		H	-2.082103	2.463407 -1.284299
	H	-0.318987	-4.062189 -0.475056		H	1.415711	2.877687 -0.786521
	H	0.699683	-3.076906 -1.544663		H	1.002126	3.116093 0.911021
	H	1.059231	-3.160136 0.177492		H	3.466048	2.760755 0.526931
	H	2.296775	0.901972 1.869307		H	2.771385	1.567924 1.628067
	H	2.235352	-0.868543 1.863200		H	3.354059	1.124510 -1.352965
	H	4.778790	0.816546 1.570228		H	4.297719	0.476753 -0.006676
	H	4.712641	-0.959427 1.499399		H	1.672543	-3.255819 1.312338
	H	4.376530	-0.838286 -0.970809		H	3.201437	-3.329778 0.402380
	H	4.379517	0.936084 -0.888259		H	1.646988	-3.629526 -0.411498
INT1a’	C	2.020345	2.256651 -0.448456	TS1a	C	-4.153628	-0.460674 0.118590
	C	3.096438	1.179359 -0.769809		C	-3.105722	-1.540809 0.420115
	C	2.624674	-0.169777 -0.378672		C	-1.754465	-0.897959 0.107737
	C	2.483642	-1.181033 0.348852		C	-0.589231	-1.510053 -0.078342
	C	2.764489	-2.284639 1.295987		C	-0.157463	-2.935758 -0.095552
	C	1.111235	1.892193 0.748594		C	-3.466476	0.845581 0.530596
	C	0.110445	0.816718 0.389039		C	-2.002117	0.703090 0.087952

	C	-1.240315	0.850589	0.455888	C	-1.127704	1.676865	-0.230413
	C	-2.050067	1.931042	1.139321	C	-1.430079	3.145530	-0.206869
	Ni	0.750430	-0.731540	-0.437601	Ni	0.120042	0.176869	-0.383012
	O	-0.946369	-1.060741	-0.908692	O	1.887467	-0.171730	-0.889472
	C	-1.926530	-0.306647	-0.229665	C	2.903844	-0.032475	-0.205322
	C	-2.903317	-1.143622	0.676267	C	3.158025	0.433895	1.209754
	C	-4.117769	-0.433319	0.015739	C	4.690215	0.311091	0.912129
	C	-3.171596	0.070216	-1.108992	C	4.375717	-0.211590	-0.530336
	H	2.534029	3.204522	-0.251277	H	-4.375099	-0.442774	-0.955069
	H	1.386665	2.409570	-1.328389	H	-5.092518	-0.634901	0.655671
	H	2.199537	-2.144040	2.222916	H	-3.253336	-2.461996	-0.153011
	H	2.482836	-3.255724	0.877381	H	-3.139139	-1.809355	1.485161
	H	3.832957	-2.309731	1.539238	H	0.355429	-3.181188	-1.033925
	H	-2.638422	1.510439	1.964845	H	-1.003001	-3.627944	0.018503
	H	-1.424338	2.720661	1.560688	H	0.552404	-3.145201	0.715564
	H	-2.760780	2.399413	0.448061	H	-3.929274	1.730409	0.084065
	H	-2.836983	-2.197983	0.392755	H	-3.519369	0.964593	1.623026
	H	-2.783302	-1.055860	1.761593	H	-0.834272	3.641465	0.572271
	H	-4.952119	-1.070881	-0.292479	H	-1.129726	3.616770	-1.151992
	H	-4.514337	0.381049	0.629025	H	-2.485359	3.400414	-0.024326
	H	-3.188539	-0.586254	-1.983851	H	2.766594	1.439177	1.409593
	H	-3.271431	1.108695	-1.442528	H	2.757953	-0.243758	1.973234
	H	0.576122	2.799223	1.054166	H	5.220861	1.264945	0.929308
	H	1.733386	1.590550	1.602510	H	5.216833	-0.405044	1.545730
	H	4.014812	1.384576	-0.204637	H	4.658527	-1.251714	-0.729770
	H	3.358794	1.214447	-1.832196	H	4.726080	0.407208	-1.364159
INT1a	C	-4.233366	-1.110646	0.134893	TS1-3a	C	-1.725344	-0.059202	-0.191396
	C	-2.940474	-1.965741	0.253615		C	-0.715724	1.117445	-0.049695
	C	-1.838478	-0.939774	0.040847		C	0.630641	0.962336	-0.219361
	C	-0.550278	-0.993305	-0.348671		C	-2.187279	-0.616971	1.221703
	C	-3.847324	0.301002	0.659491		C	-3.576468	0.055219	1.044762
	C	-2.379580	0.413570	0.277201		C	-3.223440	0.368025	-0.434795
	C	-1.502201	1.413292	0.049204		C	-1.302019	2.490241	0.247547
	C	0.240001	-2.207021	-0.754338		C	1.658066	2.078019	-0.304336
	C	-1.785417	2.891010	0.158653		C	2.763903	1.831423	0.727100
	Ni	0.207010	0.746728	-0.436517		Ni	0.539454	-0.818426	-1.060724
	O	2.142182	0.394130	-0.907993		O	-1.311665	-1.037079	-1.106711
	C	3.059974	0.087170	-0.153574		C	3.140624	0.345601	0.591998
	C	4.555681	-0.060546	-0.375499		C	1.893252	-0.409933	0.236026
	C	4.675037	-0.522283	1.114529		C	1.320602	-1.582328	0.380635
	C	3.139175	-0.301641	1.312911		C	1.136075	-2.783073	1.229137
	H	-2.919453	-2.798851	-0.457700		H	-1.599221	-0.316355	2.095509
	H	-2.870270	-2.400431	1.261558		H	-2.232123	-1.708817	1.174452
	H	-4.516663	-1.035265	-0.922019		H	-3.700337	0.951471	1.661077
	H	-5.082018	-1.548715	0.672347		H	-4.447106	-0.588168	1.205262
	H	-3.969296	0.338544	1.752302		H	-3.430775	1.377010	-0.801804
	H	-4.480751	1.090370	0.239602		H	-3.662426	-0.353973	-1.127784
	H	0.678178	-2.090821	-1.754959		H	-0.578579	3.171639	0.698491
	H	-0.395395	-3.103780	-0.771623		H	-2.140919	2.404193	0.944397
	H	1.075223	-2.415529	-0.069562		H	-1.692303	2.966584	-0.660316
	H	-1.174931	3.366912	0.940977		H	2.094190	2.073828	-1.313543

	H	-1.550591	3.419961	-0.777005		H	1.200561	3.060800	-0.171902
	H	-2.838710	3.097101	0.398458		H	3.629183	2.484287	0.570729
	H	4.988660	-1.561644	1.228917		H	2.373915	2.025154	1.733265
	H	5.307360	0.114314	1.735897		H	3.874390	0.215694	-0.213768
	H	5.047287	0.887329	-0.623102		H	3.587762	-0.058629	1.507238
	H	4.818230	-0.795434	-1.144488		H	0.205681	-2.690456	1.802839
	H	2.856994	0.519585	1.982007		H	1.964850	-2.885672	1.941410
	H	2.535925	-1.175592	1.579243		H	1.064526	-3.696842	0.632471
TS1-2a	C	2.933278	2.026704	0.144758	INT2a	C	2.240565	2.672926	0.148207
	C	2.911207	0.799534	-0.809257		C	2.862163	1.344025	-0.368892
	C	1.721469	0.002032	-0.295100		C	1.784088	0.321901	-0.043308
	C	1.396472	-1.336656	-0.226702		C	1.736476	-1.114535	-0.110861
	C	2.260715	-2.421369	-0.814927		C	2.924255	-1.833369	-0.682938
	C	1.458290	2.242847	0.584418		C	0.704508	2.433250	0.199220
	C	0.848887	0.860819	0.455572		C	0.600013	0.930363	0.279195
	C	-0.298780	0.283402	0.968747		C	-0.536709	0.052234	0.673637
	C	-0.951375	0.699948	2.264951		C	-0.796899	0.063364	2.179972
	Ni	-0.355620	-1.538773	0.434295		Ni	0.026623	-1.682556	0.108404
	O	-2.271007	-1.194327	0.109821		O	-1.759500	-1.572888	-0.326728
	C	-1.998237	-0.023200	-0.351500		C	-1.792676	-0.162525	-0.210560
	C	-1.578575	0.362859	-1.782394		C	-1.899734	0.651820	-1.537093
	C	-2.213783	1.766181	-1.542902		C	-2.928900	1.590593	-0.849963
	C	-2.842655	1.259508	-0.210459		C	-3.132920	0.503228	0.241354
	H	3.537075	1.784496	1.026925		H	2.604912	2.872652	1.161491
	H	3.369088	2.919165	-0.316194		H	2.508670	3.534324	-0.470548
	H	3.855919	0.246524	-0.794559		H	3.824336	1.124098	0.106633
	H	2.746065	1.124792	-1.846540		H	3.046129	1.378892	-1.451784
	H	0.945724	2.932954	-0.102419		H	0.205911	2.794268	-0.712477
	H	1.369219	2.673459	1.587530		H	0.214959	2.942373	1.037940
	H	1.712660	-2.996878	-1.574014		H	2.738968	-2.897187	-0.858068
	H	2.549838	-3.145597	-0.040494		H	3.753849	-1.759334	0.038360
	H	3.176449	-2.040622	-1.286823		H	3.286520	-1.376193	-1.615075
	H	-1.022741	1.793206	2.351933		H	-1.167248	1.048318	2.502793
	H	-1.959187	0.285692	2.371123		H	-1.552113	-0.680549	2.449744
	H	-0.362173	0.347227	3.122358		H	0.115498	-0.149149	2.745801
	H	-0.515503	0.310012	-2.029808		H	-0.989521	1.085890	-1.963818
	H	-2.137880	-0.249098	-2.501691		H	-2.376778	0.021229	-2.293992
	H	-1.469383	2.551079	-1.389548		H	-2.465811	2.497689	-0.447587
	H	-2.926782	2.096517	-2.302406		H	-3.807004	1.880421	-1.434642
	H	-3.904036	0.996453	-0.307319		H	-3.961352	-0.168796	-0.005762
	H	-2.720410	1.875242	0.681908		H	-3.234737	0.826076	1.281662
TS2-3a	C	-2.955627	1.934411	-0.082773	INT3a	C	-3.457111	1.296139	0.020505
	C	-2.841079	0.708582	0.855471		C	-2.963873	0.114408	0.877299
	C	-1.590180	0.006473	0.332014		C	-1.555862	-0.122014	0.339576
	C	-1.344828	-1.369459	0.199397		C	-1.011423	-1.330534	0.145449
	C	-2.037513	-2.355121	1.104160		C	-1.515379	-2.722234	0.437755
	C	-1.499594	2.273884	-0.486886		C	-2.194744	2.153516	-0.214670
	C	-0.741709	0.969796	-0.274066		C	-1.007676	1.185450	-0.100633
	C	0.593131	0.724618	-0.660482		C	0.284228	1.538680	-0.312604
	C	1.147392	1.506334	-1.836822		C	0.626697	2.921339	-0.828824
	Ni	0.192540	-1.526124	-0.904153		Ni	0.477743	-1.903563	-0.633393

	O	1.845722	-1.249991	-0.349849		O	1.733842	0.221636	1.485491
	C	1.667039	0.029599	0.221701		C	1.471512	0.616997	-0.013559
	C	1.450803	0.084186	1.769197		C	2.919465	1.227142	-0.021536
	C	2.483150	1.240065	1.852698		C	3.256140	0.386322	1.238136
	C	2.983624	0.849243	0.437807		C	1.507623	-0.501244	-0.884104
	H	-3.524276	1.649179	-0.974972		H	-3.831136	0.914664	-0.936708
	H	-3.472367	2.779839	0.381841		H	-4.269015	1.858311	0.493594
	H	-3.734157	0.077447	0.833385		H	-0.852603	-3.492525	-0.031513
	H	-2.691715	1.026160	1.897523		H	-1.520188	-2.966982	1.506158
	H	-1.078745	3.059093	0.158362		H	-2.506325	-2.914412	0.008501
	H	-1.425262	2.648560	-1.514229		H	1.031281	3.567002	-0.036465
	H	-2.406698	-3.226307	0.551639		H	1.395914	2.865143	-1.607968
	H	-2.863320	-1.932400	1.692992		H	-0.237570	3.435899	-1.253136
	H	-1.299305	-2.743969	1.820826		H	3.490687	1.041032	-0.935816
	H	1.436849	2.524650	-1.541477		H	2.930665	2.297068	0.201891
	H	2.040892	1.018597	-2.236956		H	3.738948	-0.561503	0.985727
	H	0.416437	1.596356	-2.645860		H	3.836973	0.882541	2.021884
	H	0.442109	0.261151	2.148066		H	-2.114338	2.937481	0.550510
	H	1.841964	-0.838886	2.208009		H	-2.232883	2.664098	-1.182657
	H	2.004856	2.224789	1.865932		H	-3.608970	-0.767320	0.808771
	H	3.215567	1.196611	2.663787		H	-2.916251	0.405668	1.936791
	H	3.822026	0.146594	0.482709		H	1.348500	0.982820	2.172791
	H	3.230584	1.648274	-0.265008		H	1.363619	-0.760329	1.791179
TS3-4a	C	-3.366893	1.367034	-0.075403	INT4a	C	1.230513	-0.883840	0.078362
	C	-3.029696	0.054575	0.644168		C	0.022259	-1.471179	0.087461
	C	-1.595639	-0.248980	0.196300		C	1.613616	0.508961	-0.245044
	C	-1.085731	-1.492911	0.029905		C	0.943632	1.662227	-0.021913
	C	-1.796390	-2.776506	0.393274		C	2.523572	-1.698664	0.252455
	C	-2.037080	2.138021	-0.080341		C	3.666821	-0.679640	0.055192
	C	-0.932402	1.069998	-0.081198		C	3.035626	0.448333	-0.787354
	C	0.375188	1.411698	-0.249856		C	-0.193021	-2.944970	0.421506
	C	0.776837	2.852488	-0.527617		C	1.490522	3.015411	-0.456080
	Ni	0.673917	-1.490853	-0.652808		Ni	-1.739337	-1.348571	-0.233222
	C	1.578470	0.466113	-0.286409		O	-0.349843	1.729318	0.739068
	O	1.764681	-0.174997	-1.460725		C	-0.447043	1.341226	1.899303
	C	2.860155	0.959855	0.423186		C	-1.547169	2.381825	0.047890
	C	2.441121	0.448338	1.800910		C	-2.749317	1.426043	-0.021000
	C	1.518676	-0.672266	1.276865		C	-2.490152	0.207461	-0.910047
	H	-3.673190	1.149125	-1.105532		H	3.025267	0.165531	-1.850293
	H	-4.178744	1.925811	0.402047		H	3.579442	1.391992	-0.700980
	H	-3.735016	-0.746675	0.410398		H	3.976618	-0.273615	1.024705
	H	-3.057070	0.204492	1.734210		H	4.550279	-1.120179	-0.417846
	H	-1.950800	2.760062	0.821579		H	2.572860	-2.190129	1.231341
	H	-1.970061	2.816816	-0.935765		H	2.573765	-2.493490	-0.503973
	H	-1.276586	-3.281411	1.219991		H	-1.262461	-3.253387	0.374777
	H	-1.798385	-3.486308	-0.444456		H	0.321542	-3.608034	-0.284620
	H	-2.836675	-2.631034	0.709591		H	0.121624	-3.181223	1.444516
	H	-0.047476	3.444064	-0.927199		H	1.954856	2.980630	-1.445972
	H	1.130426	3.362528	0.379349		H	0.705162	3.776202	-0.488574
	H	1.592733	2.896197	-1.257689		H	2.245961	3.376181	0.254492
	H	0.605830	-0.827391	1.848983		H	-1.824636	3.272754	0.626174

	H 2.082753 -1.613186 1.179062		H -1.282174 2.708743 -0.963081
	H 1.849822 1.194331 2.340345		H -3.603181 1.997084 -0.417113
	H 3.246867 0.104603 2.457993		H -3.021734 1.120378 0.994831
	H 3.699182 0.382822 0.022357		H -3.448843 -0.340630 -1.094999
	H 3.089571 2.024279 0.326447		H -2.088918 0.493655 -1.890550
TS4a	C -1.123835 0.746677 0.334670	3a+Ni	C 1.248368 0.046121 0.285182
	C -2.568552 1.126262 0.679059		C 2.548008 0.849807 0.441988
	C -3.345718 -0.208626 0.561770		C 2.107078 2.112815 1.191076
	C -2.513565 -1.096693 -0.397737		C 0.713016 2.382350 0.615621
	C -1.086870 -0.660668 -0.092685		C 0.109684 0.986828 0.377553
	C 0.090728 -1.444577 -0.133073		C -1.279956 0.897030 0.015807
	C 1.116980 -1.243272 0.972297		C -2.222567 -0.233192 0.187410
	C 2.558402 -0.934227 0.599461		C -2.006283 -1.425620 1.125587
	C 2.746305 0.599304 0.520577		C -0.621680 -1.927859 1.534279
	Ni 0.343754 0.292466 -1.193796		Ni 0.073846 -0.027482 -1.309189
	O 0.784311 -1.295214 2.154321		O -3.353785 -0.181302 -0.333466
	C 1.868468 1.281338 -0.534918		C 0.282900 -2.361656 0.368424
	C -0.064434 1.604576 0.075527		C 1.249698 -1.296334 -0.164964
	C -0.039168 3.048020 0.491026		C 2.570110 -1.903553 -0.621271
	C 0.066982 -2.869552 -0.671538		C -2.009853 2.213023 -0.269224
	H -2.784604 -0.887977 -1.441549		H 0.797172 2.940775 -0.326264
	H -2.676997 -2.164197 -0.222575		H 0.076759 2.975133 1.279899
	H -3.390437 -0.691787 1.543906		H 2.033215 1.901229 2.264509
	H -4.374443 -0.067751 0.216019		H 2.794895 2.954092 1.060908
	H -2.648281 1.559050 1.682218		H 3.304357 0.271074 0.981783
	H -2.949804 1.875299 -0.026197		H 2.980207 1.116587 -0.531481
	H 0.328512 3.698368 -0.310419		H 2.378710 -2.747174 -1.295109
	H -1.041355 3.390681 0.774177		H 3.205215 -1.193703 -1.157048
	H 0.612601 3.209227 1.360497		H 3.148880 -2.302954 0.226233
	H 1.065771 -3.182929 -0.996525		H -2.870188 2.011956 -0.908469
	H -0.261702 -3.585220 0.096097		H -2.394149 2.671916 0.653234
	H -0.600151 -2.964496 -1.532738		H -1.376760 2.949048 -0.768663
	H 3.221892 -1.342524 1.368488		H -2.560090 -1.145943 2.033872
	H 2.810105 -1.382310 -0.369206		H -2.578024 -2.248408 0.682180
	H 3.803130 0.804292 0.297126		H -0.790430 -2.797574 2.181153
	H 2.546575 1.031362 1.508348		H -0.101205 -1.188635 2.151063
	H 2.094656 2.343519 -0.627276		H 0.912603 -3.194804 0.712064
	H 2.110600 0.838684 -1.555290		H -0.329699 -2.791272 -0.439660

Table S6. Frequencies of some stationary points for reaction **a**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

Species	Frequencies (cm^{-1})
1a	27 28 47 79 93 112 210 215 241 283 306 370 374 435 531 728 741 796 840 1027 1035 1048 1050 1050 1053 1080 1154 1162 1182 1269 1305 1331 1359 1401 1421 1421 1486 1487 1493 1493 1493 1493 1511 2335 2336 3024 3027 3036 3036 3065 3066 3068 3117 3117 3117 3117 3123
2a	3 398 454 619 675 741 842 927 952 970 1096 1103 1197 1221 1224 1247 1279 1433 1447 1504 1835 3056 3060 3091 3117 3122 3156

COM1a	14 35 39 52 58 67 85 87 114 123 131 199 216 229 231 287 311 312 377 394 402 411 419 491 503 525 558 636 693 725 739 748 854 863 873 922 956 968 970 1024 1038 1045 1045 1049 1061 1094 1125 1128 1138 1168 1199 1215 1220 1225 1251 1284 1285 1356 1358 1384 1408 1409 1432 1446 1476 1484 1492 1492 1498 1498 1499 1502 1788 2032 2052 3014 3015 3016 3017 3042 3056 3060 3061 3065 3089 3090 3095 3098 3100 3100 3116 3121 3161
TS1a’	**-139i** 42 59 75 78 86 112 141 198 208 220 243 265 284 306 322 336 384 387 434 455 470 515 529 571 605 650 717 736 768 785 841 847 878 892 951 963 974 984 1026 1032 1036 1048 1057 1061 1071 1087 1121 1129 1169 1187 1204 1217 1225 1233 1261 1277 1281 1345 1354 1382 1409 1411 1472 1478 1479 1485 1486 1492 1503 1505 1510 1519 1688 2051 3013 3034 3035 3041 3051 3063 3066 3076 3086 3091 3110 3117 3119 3119 3130 3136 3147 3157
INT1a’	44 66 83 86 109 129 145 157 186 219 232 259 279 293 309 365 372 385 411 430 467 512 531 559 593 660 693 723 729 787 834 846 870 878 917 936 974 993 1003 1006 1032 1034 1050 1056 1064 1073 1123 1135 1159 1180 1199 1214 1225 1237 1264 1270 1272 1331 1337 1347 1374 1409 1417 1477 1479 1482 1484 1490 1493 1500 1502 1506 1520 1662 2089 3023 3030 3037 3038 3052 3055 3058 3071 3081 3092 3095 3113 3113 3123 3126 3130 3137 3141
TS1a	**-226i** 9 23 35 54 73 86 98 115 118 155 164 217 234 248 266 289 359 408 424 455 481 537 557 586 627 651 689 704 744 842 852 860 921 922 932 964 971 987 1008 1014 1029 1035 1055 1060 1092 1125 1142 1159 1162 1194 1205 1214 12191256 1260 1292 1309 1319 1348 1404 1407 1431 1445 1482 1483 1488 1492 1493 1495 1502 1511 1582 1715 1728 2985 3005 3011 3024 3048 3049 3054 3056 3071 3077 3086 3093 3098 3103 3107 3111 3115 3165
INT1a	22 29 37 52 79 102 130 140 146 160 177 183 215 226 256 303 325 335 406 418 466 495 526 597 603 614 661 694 742 760 852 858 861 904 925 932 957 972 992 1008 1025 1026 1041 1054 1098 1109 1131 1145 1150 1193 1204 1220 1223 1237 1255 1286 1291 1308 1317 1337 1398 1401 1425 1439 1482 1484 1485 1490 1495 1498 1503 1510 1684 1688 1776 2983 2991 3009 3014 3042 3044 3052 3057 3062 3064 3074 3082 3083 3099 3102 3119 3127 3167
TS1-3a	**-374i** 33 73 92 99 107 127 137 179 200 219 230 280 318 323 343 388 411 416 475 492 526 577 595 609 640 670 699 777 783 820 854 882 892 914 948 969 973 976 1001 1022 1041 1043 1057 1067 1070 1116 1125 1137 1159 1194 1205 1211 1235 1259 1266 1268 1274 1330 1337 1363 1397 1411 1472 1474 1483 1485 1489 1491 1500 1508 1514 1530 1571 1783 3024 3024 3037 3038 3051 3053 3063 3077 3090 3101 3109 3112 3114 3123 3128 3131 3143 3149
TS1-2a	**-317i** 55 64 105 106 110 125 156 177 193 202 207 230 236 274 313 326 358 416 456 483 488 536 608 620 640 667 731 735 756 848 866 870 906 932 939 973 993 997 998 1001 1026 1045 1053 1072 1090 1107 1140 1162 1188 1201 1211 1234 1235 1250 1271 1299 1307 1340 1363 1397 1399 1426 1460 1472 1478 1481 1486 1489 1495 1502 1511 1512 1551 1579 2999 3006 3013 3018 3049 3052 3053 3066 3070 3081 3085 3089 3094 3111 3113 3125 3141 3152
INT2a	51 89 94 108 114 126 170 204 213 223 238 259 281 298 332 366 388 437 483 513 534 598 616 637 650 701 716 775 789 829 852 891 897 912 928 939 962 971 1003 1012 1031 1039 1045 1068 1086 1104 1135 1153 1160 1188 1191 1208 1231 1239 1258 1266 1281 1289 1303 1332 1343 1376 1400 1408 1470 1475 1481 1492 1493 1496 1497 1505 1514 1518 1578 2995 3005 3018 3027 3058 3059 3060 3061 3068 3078 3087 3094 3112 3119 3123 3125 3134 3137
TS2-3a	**-405i** 70 75 82 95 117 126 159 190 223 235 244 258 284 304 335 361 423 440 466 527 559 611 628 660 696 699 759 786 836 857 883 899 924 936 943 970 977 1007 1015 1026 1043 1046 1062 1078 1093 1132 1147 1160 1192 1196 1213 1239 1244 1261 1271 1283 1305

	1314 1328 1345 1395 1399 1415 1465 1478 1482 1485 1492 1495 1502 1510 1513 1514 1518 3003 3013 3020 3021 3056 3064 3070 3071 3077 3077 3098 3100 3105 3118 3121 3136 3141 3147
INT3a	47 72 98 113 131 133 162 172 183 239 250 254 281 297 318 336 370 396 423 504 528 585 614 631 655 693 747 779 800 860 871 876 928 934 942 951 968 972 997 1011 1030 1041 1061 1069 1072 1093 1137 1144 1154 1196 1202 1217 1238 1250 1258 1268 1270 1301 1320 1332 1349 1413 1420 1444 1470 1482 1489 1496 1500 1503 1506 1513 1516 1660 1715 2826 3016 3018 3028 3041 3050 3056 3065 3075 3083 3086 3097 3108 3111 3119 3132 3142 3145
TS3-4a	**-335i** 54 73 99 111 119 143 161 179 183 224 245 281 300 302 319 357 394 406 458 486 527 546 599 611 615 691 722 755 788 861 871 889 948 953 964 979 996 1006 1017 1029 1038 1041 1063 1085 1096 1117 1147 1161 1171 1210 1216 1236 1240 1267 1285 1305 1312 1321 1334 1355 1408 1420 1450 1485 1489 1493 1494 1494 1503 1512 1518 1519 1605 1655 3003 3004 3009 3021 3024 3048 3059 3066 3072 3087 3091 3093 3106 3116 3117 3136 3155 3175
INT4a	43 59 82 95 107 125 128 171 180 220 232 240 252 266 284 310 327 370 405 436 479 537 559 581 609 643 679 733 750 807 850 875 894 897 929 938 955 964 997 1024 1029 1044 1059 1067 1068 1100 1131 1143 1156 1194 1213 1249 1251 1256 1281 1319 1330 1346 1361 1379 1408 1419 1429 1449 1486 1487 1494 1496 1502 1507 1512 1518 1667 1694 1734 2828 2880 3004 3020 3025 3028 3042 3042 3054 3064 3075 3087 3101 3106 3107 3112 3122 3134
TS4a	**-419i** 73 86 104 118 145 164 178 186 194 221 240 253 285 313 324 352 394 402 456 479 543 551 561 592 635 673 732 764 795 848 879 884 894 920 941 943 1014 1027 1038 1043 1049 1054 1065 1091 1115 1148 1151 1165 1197 1210 1237 1244 1267 1281 1312 1323 1347 1348 1367 1412 1416 1418 1458 1484 1487 1489 1493 1496 1497 1503 1512 1513 1531 1715 2624 3011 3015 3019 3028 3040 3050 3059 3080 3083 3087 3091 3104 3109 3118 3120 3129 3138
3a	39 67 113 125 145 157 166 181 210 232 247 277 298 308 339 367 403 419 454 489 518 534 546 561 607 623 663 800 819 862 882 889 910 951 957 959 1018 1031 1045 1048 1062 1070 1078 1104 1118 1143 1160 1190 1208 1232 1256 1267 1285 1310 1318 1336 1354 1376 1387 1398 1410 1415 1419 1467 1472 1484 1494 1497 1504 1506 1509 1517 1521 1527 1611 2992 2999 3018 3021 3027 3030 3032 3050 3051 3079 3082 3097 3102 3104 3116 3120 3133 3165

Table S7. Some optimized Cartesian Coordinates of stationary points for reaction **b**.

Species	Cartesian coordinates	Species	Cartesian coordinates
1b	C 0.000071 -0.334287 0.000172 C 0.268634 0.536704 1.261720 C 1.455175 1.394666 1.128915 C 2.438289 2.099491 1.024007 C 3.626184 2.954521 0.904798 C -0.268178 0.537783 -1.260684 C -1.454944 1.395437 -1.127840 C -2.438281 2.100033 -1.023425 C -3.626598 2.954581 -0.904895 C -1.208951 -1.275510 0.182317 O -1.547539 -2.074866 -0.671694 O -1.842296 -1.115733 1.353708 C -2.992504 -1.969484 1.568709 C 1.208844 -1.275707 -0.182698 O 1.546905 -2.076220 0.670443 O 1.842596 -1.114799 -1.353720 C 2.992662 -1.968613 -1.569295 H 4.385419 2.677270 1.643929 H 3.368725 4.007409 1.062225 H 4.075133 2.863448 -0.090158 H 0.390117 -0.123780 2.124621 H -0.614678 1.154187 1.448215 H -0.389284 -0.122056 -2.124149 H 0.615127 1.155516 -1.446390 H -3.374698 4.004143 -1.090939 H -4.059128 2.885659 0.099070 H -4.396855 2.658326 -1.625010 H -2.690161 -3.018671 1.546715 H -3.372331 -1.697381 2.553155 H -3.744919 -1.787692 0.798342 H 3.372781 -1.695634 -2.553381 H 3.744924 -1.787735 -0.798560 H 2.690077 -3.017751 -1.548386	2b	C 2.673986 0.001063 -0.590686 O 3.822162 0.001863 -0.983891 C 1.689575 -1.104645 -0.211109 C 0.799493 -0.000952 0.472865 C 1.689543 1.105276 -0.206963 C -0.677456 -0.000245 0.118481 C -1.385983 1.205513 -0.014630 C -2.758976 1.208817 -0.286052 C -3.452079 0.000926 -0.425856 C -2.759474 -1.207556 -0.288703 C -1.386469 -1.205416 -0.017311 C 0.986610 -0.003827 2.002137 H 1.234367 -1.541141 -1.108079 H 2.083484 -1.910819 0.416508 H 1.234355 1.545131 -1.102313 H 2.083467 1.909108 0.423641 H -0.864823 2.155464 0.093333 H -3.286434 2.155560 -0.389678 H -4.519118 0.001383 -0.640481 H -3.287329 -2.153850 -0.394380 H -0.865675 -2.155812 0.088543 H 0.523756 0.881393 2.451393 H 2.050109 -0.004217 2.271528 H 0.523941 -0.890828 2.448056
COM1b	C -3.667516 0.368155 -0.184125 C -3.096510 0.097718 -1.605829 C -1.689210 -0.378333 -1.614509 C -0.570034 -0.611615 -2.150020 C 0.409804 -0.583342 -3.265115 C -3.506462 -0.892090 0.717623 C -2.092104 -1.294756 0.905575 C -1.100007 -1.768078 1.526271 C -0.418504 -2.362090 2.703778 Ni -0.575303 -1.266048 -0.299467 O 1.311159 -1.961118 -0.238091 C -5.153741 0.728682 -0.318724 O -5.628080 1.830158 -0.105543 O -5.887270 -0.327969 -0.726820 C -7.301397 -0.081275 -0.910443 C -2.985962 1.607244 0.427756	TS1b’	C 0.353316 -2.608756 -1.342093 C 0.183468 -1.161516 -0.923303 C -1.014367 -0.610097 -0.767666 C -2.432767 -1.060399 -0.822960 C -3.425730 -0.043050 -0.203796 C -3.225590 1.367975 -0.833623 C -1.829795 1.850536 -0.709700 C -0.907116 2.630357 -0.348182 C -0.248073 3.859887 0.140209 Ni -0.124636 0.951294 -0.887177 O 1.755630 1.026050 -0.792571 C 1.714220 -0.335897 -0.651492 C 2.285920 -0.840357 0.714531 C 3.605731 -1.273869 -0.016247 C 2.907000 -1.016112 -1.402393 C -3.285053 0.039997 1.329131

	O -2.397380 2.458795 -0.209294 O -3.149125 1.653825 1.764526 C -2.608327 2.819981 2.420418 C 2.335222 -1.337959 0.009257 C 2.622860 0.099267 0.387817 C 4.089714 -0.350077 0.752388 C 3.787687 -1.762696 0.119224 C 5.219761 0.442241 0.116893 C 6.406056 -0.195741 -0.282752 C 7.472727 0.535674 -0.816544 C 7.372901 1.924598 -0.957132 C 6.199268 2.572991 -0.556022 C 5.134874 1.837284 -0.022354 C 4.286340 -0.445305 2.276504 H -3.172638 1.015511 -2.198655 H -3.733626 -0.657704 -2.078995 H -0.020121 -0.129555 -4.166816 H 1.301695 -0.005435 -2.995151 H 0.748418 -1.594022 -3.519528 H -4.056769 -1.708369 0.238116 H -3.973292 -0.707967 1.690757 H -1.112741 -2.514571 3.539699 H 0.031346 -3.329073 2.451973 H 0.393040 -1.714541 3.056977 H 2.551865 0.763605 -0.481190 H 1.995752 0.507587 1.187170 H 3.980371 -2.647714 0.734953 H 4.235492 -1.915929 -0.869719 H -7.456377 0.689447 -1.668922 H -7.719852 -1.033073 -1.237253 H -7.755372 0.237099 0.030747 H -3.085050 3.724736 2.035609 H -2.832324 2.688699 3.479249 H -1.529312 2.879838 2.259959 H 6.503925 -1.275408 -0.178473 H 4.231910 2.361546 0.286890 H 8.380557 0.019742 -1.124437 H 6.109615 3.652875 -0.659875 H 8.199739 2.494884 -1.376209 H 5.235827 -0.935906 2.515626 H 4.297874 0.552092 2.728600 H 3.479470 -1.021434 2.746141		O -3.215209 1.066808 1.972621 O -3.273707 -1.193353 1.877524 C -3.188071 -1.240318 3.321227 C -4.861582 -0.493177 -0.539615 O -5.158937 -1.191922 -1.489793 O -5.756345 0.027316 0.318607 C -7.146539 -0.294894 0.066629 C 4.829570 -0.410539 0.274380 C 5.781102 -0.142037 -0.723830 C 6.952233 0.568702 -0.438097 C 7.202757 1.023120 0.861544 C 6.269266 0.754733 1.869048 C 5.099704 0.044515 1.576005 C 3.987217 -2.748761 0.217214 H 1.757458 -1.685750 1.165216 H 2.361990 -0.028729 1.440362 H 2.705122 -1.937703 -1.949813 H 3.393958 -0.300317 -2.066744 H -0.597849 -3.142376 -1.258440 H 1.085990 -3.132238 -0.721279 H 0.685492 -2.683198 -2.383278 H -2.725957 -1.195201 -1.870314 H -2.555480 -2.028835 -0.328619 H -3.507631 1.307059 -1.891360 H -3.894830 2.079900 -0.341474 H 0.296447 3.658516 1.067656 H -0.991454 4.643059 0.330950 H 0.476137 4.230545 -0.591603 H -7.704370 0.203457 0.858731 H -7.448246 0.079925 -0.913845 H -7.295053 -1.376076 0.108514 H -3.197651 -2.299635 3.577076 H -2.262601 -0.769676 3.660240 H -4.043471 -0.727218 3.766703 H 4.810513 -3.047127 -0.441921 H 4.313334 -2.906824 1.251597 H 3.141796 -3.419326 0.025105 H 5.611709 -0.489253 -1.741354 H 4.391603 -0.155819 2.377739 H 7.669196 0.767986 -1.233038 H 6.449975 1.099920 2.885879 H 8.111294 1.579234 1.085636
INT1b’	C 3.281704 -0.123103 -0.065871 C 3.489815 1.195449 0.760563 C 2.333433 2.108910 0.628401 C 1.685280 3.096636 0.210419 C 1.335135 4.451190 -0.272434 C 2.350897 0.104037 -1.297734 C 0.903675 0.280247 -0.901498 C -0.166132 -0.460901 -1.272990 C -0.148101 -1.540826 -2.330669	TS1b	C -4.036206 -0.492802 0.231425 C -3.093677 -1.265187 -0.729029 C -1.725241 -0.596421 -0.607099 C -1.838641 0.505247 0.556298 C -3.079352 0.049159 1.318359 C -0.602663 -0.909024 -1.240961 C -1.020880 1.543389 0.829395 C -0.238350 -1.916302 -2.275707 C -1.212097 2.512409 1.957495

	Ni 0.481676 1.561852 0.385321		Ni 0.152080 0.566081 -0.390356
	O -1.107258 0.760068 0.522174		O 1.777275 0.773646 -1.312857
	C 4.673097 -0.567306 -0.547310		C -4.730804 0.663336 -0.507025
	O 5.066927 -0.519580 -1.696167		O -4.669770 0.881516 -1.701342
	O 5.428813 -0.973822 0.491547		O -5.431512 1.430397 0.356056
	C 6.770401 -1.415719 0.170497		C -6.139695 2.547638 -0.225588
	C 2.687847 -1.287189 0.748143		C -5.085906 -1.446686 0.805431
	O 2.621279 -2.420782 0.307526		O -4.961182 -2.085033 1.834437
	O 2.230981 -0.920613 1.954891		O -6.159938 -1.544414 -0.005546
	C 1.557059 -1.951607 2.715810		C -7.201725 -2.452110 0.422664
	C -1.437075 -0.132221 -0.529761		C 2.912483 0.650806 -0.847676
	C -2.660234 0.364205 -1.381507		C 3.449047 0.363933 0.530170
	C -3.542632 -0.824338 -0.869959		C 4.864962 0.821605 0.004799
	C -2.325887 -1.316405 -0.014671		C 4.278261 0.856754 -1.460472
	C -4.795890 -0.441608 -0.093844		C 6.015824 -0.139811 0.245372
	C -5.598611 0.637634 -0.500691		C 6.124093 -0.844265 1.455624
	C -6.788608 0.948964 0.167097		C 7.213236 -1.687479 1.702645
	C -7.206100 0.180420 1.259850		C 8.218956 -1.838321 0.741265
	C -6.421869 -0.903251 1.671608		C 8.126536 -1.135911 -0.465709
	C -5.233076 -1.208929 0.999273		C 7.035688 -0.293765 -0.708265
	C -3.937715 -1.810210 -1.986618		C 5.220313 2.234604 0.502192
	H 0.974663 4.407347 -1.304879		H -3.469592 -1.241131 -1.754264
	H 0.548003 4.903746 0.338331		H -3.021806 -2.312564 -0.413291
	H 2.217034 5.101242 -0.238700		H 0.174624 -1.431528 -3.168880
	H -0.861971 -1.309374 -3.130978		H -1.098555 -2.524084 -2.587846
	H 0.831499 -1.659498 -2.796482		H 0.534795 -2.599577 -1.901561
	H -0.435724 -2.512907 -1.913670		H -3.527863 0.852240 1.904391
	H -2.980210 1.354750 -1.051178		H -2.845940 -0.777199 2.000343
	H -2.505016 0.379230 -2.465842		H -0.457274 2.338608 2.737070
	H -2.461727 -1.231770 1.065625		H -1.046804 3.540024 1.609567
	H -1.978236 -2.326496 -0.254562		H -2.200451 2.477214 2.440622
	H 2.459913 -0.764006 -1.951804		H 2.984050 0.941344 1.337912
	H 2.732630 0.970231 -1.849474		H 3.379881 -0.702378 0.777372
	H 4.367843 1.723835 0.369161		H 4.575134 0.000883 -2.078597
	H 3.694218 0.952428 1.804324		H 4.406548 1.776077 -2.042047
	H 7.339132 -0.600658 -0.282803		H -6.871518 2.193732 -0.955849
	H 7.211635 -1.711514 1.121891		H -6.637513 3.041654 0.608930
	H 6.730771 -2.263397 -0.516892		H -5.438023 3.228321 -0.713159
	H 2.244104 -2.773790 2.927805		H -7.973045 -2.388176 -0.344619
	H 1.236075 -1.466020 3.636796		H -6.812244 -3.470343 0.493423
	H 0.696313 -2.322938 2.156621		H -7.596350 -2.143742 1.393538
	H -5.293867 1.248041 -1.349287		H 5.354524 -0.737757 2.218513
	H -4.640278 -2.058294 1.334625		H 6.984863 0.247038 -1.652104
	H -7.389088 1.794121 -0.166028		H 7.274371 -2.227644 2.645780
	H -6.734533 -1.511402 2.519068		H 8.903213 -1.244044 -1.220818
	H -8.129058 0.423119 1.783461		H 9.064894 -2.496569 0.929986
	H -3.064493 -2.126566 -2.567297		H 5.439025 2.223333 1.575087
	H -4.406316 -2.707891 -1.566513		H 6.104249 2.616651 -0.019242
	H -4.654672 -1.350063 -2.676692		H 4.394622 2.935697 0.330139
INT1b	C 4.056223 0.591880 0.214674	TS1-3b	C -1.535566 0.128053 -0.750073
	C 2.857866 1.064083 -0.680691		C -0.071868 0.591255 -0.971708

	C	1.737267	0.116749	-0.290293		C	0.998703	-0.245433	-0.831253
	C	2.064367	-0.541489	0.984735		C	-2.162241	0.587255	0.622605
	C	3.390371	-0.011613	1.495603		C	-3.375069	1.242947	-0.118509
	C	0.584501	-0.265577	-0.870238		C	-2.670258	0.936696	-1.483467
	C	1.169562	-1.468151	1.384217		C	0.120845	2.036575	-1.402441
	C	0.053517	0.138727	-2.216800		C	2.419067	0.061605	-1.264989
	C	-3.074763	-1.093165	-0.662168		C	3.386506	-0.143095	-0.081234
	Ni	-0.314869	-1.547747	0.204700		Ni	-0.020481	-1.929649	-0.750387
	O	-2.076717	-1.804445	-0.745560		O	-1.730335	-1.243650	-0.989901
	C	1.269003	-2.332394	2.615719		C	-0.190246	-2.557269	2.261890
	C	4.878161	-0.477915	-0.521914		C	3.234445	0.986146	0.952302
	O	4.687630	-0.873620	-1.655330		O	2.924394	0.840886	2.117987
	O	5.871555	-0.945527	0.269940		O	3.488321	2.185683	0.387326
	C	6.729486	-1.945839	-0.321064		C	3.416785	3.329793	1.270624
	C	4.965484	1.779747	0.537734		C	4.842957	-0.215195	-0.553213
	O	4.933054	2.436858	1.562138		O	5.192802	-0.466437	-1.690735
	O	5.787099	2.062096	-0.497485		O	5.697082	-0.021520	0.470409
	C	6.664648	3.197022	-0.320979		C	2.973376	-1.499580	0.545185
	C	-4.476893	-1.243725	-1.209401		C	1.490544	-1.641782	0.390463
	C	-4.711665	0.275472	-0.856525		C	0.446825	-2.170179	0.982432
	C	-3.346502	0.270254	-0.067167		C	7.107176	-0.111524	0.151327
	C	-5.955679	0.595702	-0.046372		C	-4.725790	0.573673	0.106797
	C	-7.171994	-0.056747	-0.306339		C	-5.119555	0.167932	1.393726
	C	-8.332157	0.275977	0.401908		C	-6.389613	-0.369407	1.629546
	C	-8.295986	1.273517	1.382862		C	-7.302150	-0.510158	0.577386
	C	-7.091674	1.936301	1.645533		C	-6.928484	-0.102148	-0.707799
	C	-5.933947	1.600434	0.934899		C	-5.656075	0.434818	-0.936091
	C	-4.633045	1.162982	-2.112195		C	-3.525845	2.750057	0.167916
	H	3.124220	1.039642	-1.739319		H	-1.561804	1.308010	1.189122
	H	2.602714	2.099083	-0.416159		H	-2.391615	-0.271063	1.257313
	H	3.247917	0.805898	2.212076		H	-2.368579	1.837163	-2.024016
	H	4.031212	-0.755257	1.975071		H	-3.212868	0.276828	-2.162587
	H	-0.160294	-0.736576	-2.844620		H	1.133555	2.402748	-1.229350
	H	0.778363	0.764208	-2.756244		H	-0.558130	2.686975	-0.841568
	H	-0.882448	0.712200	-2.148070		H	-0.114254	2.175430	-2.464762
	H	0.450193	-2.131004	3.322510		H	2.715825	-0.638055	-2.054581
	H	1.202417	-3.401288	2.365089		H	2.521872	1.061905	-1.684204
	H	2.212084	-2.178958	3.159980		H	3.471810	-2.313230	0.005109
	H	-5.062531	-1.938004	-0.594666		H	3.264448	-1.553150	1.597050
	H	-4.549583	-1.550425	-2.258081		H	-0.772155	-1.713450	2.653223
	H	-3.464199	0.197260	1.021133		H	0.574544	-2.809064	3.007758
	H	-2.607654	1.047197	-0.285943		H	-0.868424	-3.406254	2.143235
	H	7.219049	-1.547857	-1.213351		H	7.627068	0.071008	1.091283
	H	7.465946	-2.186702	0.445855		H	7.343849	-1.105473	-0.234714
	H	6.150702	-2.832749	-0.590030		H	7.373739	0.643465	-0.591605
	H	7.243296	3.261416	-1.242443		H	2.414066	3.419810	1.694004
	H	6.081930	4.108537	-0.168101		H	4.145915	3.228131	2.077788
	H	7.322308	3.037921	0.536884		H	3.650855	4.192110	0.646722
	H	-7.221487	-0.832899	-1.068534		H	-4.269199	3.202467	-0.498973
	H	-5.007382	2.129959	1.151455		H	-3.853651	2.921766	1.199846
	H	-9.263526	-0.245126	0.187562		H	-2.577322	3.281150	0.024833
	H	-7.051570	2.714813	2.405263		H	-5.389730	0.747608	-1.943757

	H	-9.196539	1.531298	1.936910	H	-4.428268	0.272986	2.228353
	H	-5.509805	1.008457	-2.749597	H	-7.627434	-0.203566	-1.536651
	H	-4.598809	2.221715	-1.835271	H	-6.666028	-0.680115	2.636000
	H	-3.738065	0.937839	-2.705020	H	-8.289553	-0.931874	0.756755
TS1-2b	C	-2.927626	0.781803	0.167210	INT2b	C	-2.870056	-0.684390	-0.181019
	C	-2.371739	0.046244	1.430975		C	-2.973959	0.617233	-1.045418
	C	-1.388768	-0.947759	0.838885		C	-1.771440	1.426838	-0.599060
	C	-0.972112	-0.508944	-0.458769		C	-0.914680	0.688343	0.168133
	C	-1.780051	0.696040	-0.894211		C	-1.392033	-0.730465	0.331740
	C	-0.976154	-2.220085	1.170920		C	-1.340875	2.765469	-0.904376
	C	-0.028502	-1.273778	-1.120987		C	0.261934	1.394114	0.755910
	C	-1.426893	-2.925232	2.422050		C	-2.118201	3.544157	-1.924167
	C	0.024027	-1.402673	-2.625644		C	0.061706	1.719667	2.237026
	Ni	0.381555	-2.775456	-0.016748		Ni	0.338816	3.005379	-0.271714
	O	2.193525	-2.515499	-0.681188		O	2.073971	2.458227	-0.089225
	C	2.743985	-0.207152	-1.501449		C	2.742815	0.507939	1.342607
	C	-4.176230	0.050917	-0.354174		C	-3.832862	-0.610648	1.016931
	O	-4.260818	-0.545498	-1.409963		O	-4.536476	0.337536	1.304435
	O	-5.185246	0.137731	0.538686		O	-3.772564	-1.747162	1.740743
	C	-6.421653	-0.511942	0.162973		C	-4.631823	-1.807938	2.904251
	C	-3.285408	2.244022	0.449971		C	-3.216530	-1.911825	-1.031281
	O	-2.951425	2.875114	1.434606		O	-2.409078	-2.690906	-1.500551
	O	-3.982708	2.773831	-0.576865		O	-4.544191	-1.982809	-1.246983
	C	-4.353370	4.166543	-0.444587		C	1.732821	1.142552	0.335833
	C	2.040842	-1.230926	-0.592828		C	2.084787	0.017870	-0.684843
	C	2.295471	-0.386426	0.664998		C	2.915379	-0.734444	0.407757
	C	2.990111	0.697943	-0.238155		C	-4.998455	-3.077425	-2.079596
	C	4.448725	0.988890	0.085184		C	4.339254	-1.115841	0.034841
	C	4.895370	1.061736	1.415493		C	5.374088	-1.060595	0.983835
	C	6.220758	1.395618	1.716285		C	6.674477	-1.464589	0.660932
	C	7.129729	1.668871	0.687902		C	6.966865	-1.937245	-0.623854
	C	6.696802	1.609674	-0.641704		C	5.944903	-2.002592	-1.578135
	C	5.370321	1.275608	-0.936277		C	4.646356	-1.597334	-1.248815
	C	2.201206	2.018693	-0.295990		C	2.188662	-1.976255	0.959091
	H	-3.171881	-0.400386	2.025448		H	-3.928125	1.119820	-0.871384
	H	-1.873575	0.786998	2.066790		H	-2.913916	0.383254	-2.115992
	H	-1.161122	1.602354	-0.854169		H	-0.814300	-1.422499	-0.292635
	H	-2.180535	0.615312	-1.906966		H	-1.315421	-1.102100	1.358230
	H	-0.571302	-3.149067	3.074480		H	-1.631082	4.480278	-2.211488
	H	-1.878048	-3.896412	2.176078		H	-3.096542	3.802701	-1.488223
	H	-2.151108	-2.349582	3.013933		H	-2.330726	2.959990	-2.831212
	H	-0.002816	-0.420531	-3.118377		H	0.061013	0.799192	2.840724
	H	0.927297	-1.921739	-2.959883		H	0.870106	2.356736	2.607159
	H	-0.840394	-1.970372	-2.994381		H	-0.889688	2.231369	2.410735
	H	1.414417	-0.051999	1.218575		H	1.259175	-0.541308	-1.137545
	H	2.965168	-0.919426	1.347826		H	2.705414	0.437884	-1.480785
	H	3.644990	-0.652293	-1.936546		H	3.635164	1.137313	1.400060
	H	2.156416	0.251071	-2.299322		H	2.387285	0.297372	2.356240
	H	-7.107365	-0.328870	0.990103		H	-5.677212	-1.698495	2.607104
	H	-6.809862	-0.080533	-0.762677		H	-4.455901	-2.790415	3.341516
	H	-6.259947	-1.583674	0.026366		H	-4.367778	-1.018040	3.611111

	H	-3.460545	4.790494	-0.361173		H	-4.555450	-3.003430	-3.075249
	H	-4.906166	4.405446	-1.352820		H	-4.725644	-4.033233	-1.626883
	H	-4.981222	4.307484	0.438155		H	-6.081512	-2.969576	-2.130742
	H	2.612970	2.684946	-1.062565		H	1.166733	-1.734654	1.271212
	H	1.148401	1.834339	-0.533378		H	2.133445	-2.768106	0.203202
	H	2.247258	2.541995	0.665583		H	2.716866	-2.379386	1.830906
	H	4.204509	0.858037	2.231548		H	5.166324	-0.693448	1.987554
	H	5.053730	1.240382	-1.977199		H	3.864904	-1.654933	-2.004578
	H	6.543057	1.440406	2.755297		H	7.460564	-1.406826	1.412265
	H	7.392420	1.822218	-1.451876		H	6.158843	-2.366957	-2.581720
	H	8.162057	1.924612	0.919481		H	7.978523	-2.247799	-0.878864
TS2-3b	C	-2.901527	0.756731	0.162049	INT3b	C	-3.214499	-0.557745	-0.259898
	C	-2.212133	0.145729	1.418403		C	-2.324339	0.150133	-1.314389
	C	-1.183514	-0.804404	0.819328		C	-1.133997	0.628638	-0.500811
	C	-0.833119	-0.354618	-0.474729		C	-0.903963	-0.339615	0.593600
	C	-1.812951	0.703862	-0.953445		C	-2.202785	-1.132448	0.777810
	C	-0.780655	-2.063689	1.291379		C	0.222009	-0.551543	1.316948
	C	1.689756	-1.062883	-0.697692		C	0.194354	-1.464422	2.523769
	C	0.245094	-0.867253	-1.230846		C	-0.535638	1.817265	-0.643947
	C	-0.854086	-2.384342	2.760202		C	-0.736768	2.970438	-1.591292
	Ni	0.171463	-2.873160	-0.143184		Ni	0.721204	2.664669	0.274827
	O	1.834625	-2.465417	-0.562576		O	1.465742	1.526021	1.369791
	C	2.837209	-0.392638	-1.518765		C	2.148314	-0.124596	-0.420090
	C	-4.112423	-0.103174	-0.241059		C	-4.038909	-1.689772	-0.879903
	O	-4.203912	-0.765945	-1.256089		O	-3.809242	-2.222343	-1.947273
	O	-5.072346	-0.044467	0.704571		O	-5.037169	-2.073381	-0.052713
	C	-6.270418	-0.812520	0.442053		C	-5.852475	-3.171414	-0.518410
	C	-3.364210	2.198455	0.393442		C	-4.162423	0.449759	0.412599
	O	-3.031962	2.904392	1.326267		O	-4.176503	0.740990	1.589880
	O	-4.156027	2.613066	-0.616458		O	-5.001335	0.997776	-0.500666
	C	-4.634770	3.976842	-0.533586		C	1.550303	0.162106	1.004144
	C	0.121493	-0.859042	-2.742327		C	2.846519	-0.478604	1.608661
	C	2.139891	-0.221104	0.536157		C	3.246921	-1.038511	0.208127
	C	3.029520	0.668540	-0.390648		C	-5.966903	1.933539	0.024791
	C	4.452676	0.932821	0.069472		C	4.678574	-0.795607	-0.239490
	C	5.513204	0.984179	-0.850612		C	5.746009	-0.881522	0.669046
	C	6.816437	1.281406	-0.435633		C	7.069497	-0.710736	0.248702
	C	7.084576	1.537670	0.914078		C	7.353237	-0.450647	-1.096324
	C	6.036713	1.493816	1.841326		C	6.300158	-0.365591	-2.013948
	C	4.735891	1.195315	1.420326		C	4.979172	-0.537493	-1.587249
	C	2.345930	2.005792	-0.740009		C	2.912053	-2.535356	0.051647
	H	-2.928274	-0.338151	2.085091		H	-1.775691	3.320674	-1.619309
	H	-1.733459	0.952664	1.985418		H	-0.150267	3.864327	-1.255565
	H	-1.311193	1.676749	-1.048565		H	-0.382840	2.768519	-2.608489
	H	-2.259887	0.475555	-1.924128		H	0.629832	-0.953271	3.390898
	H	-1.211238	-3.403953	2.939962		H	-0.818770	-1.763847	2.797214
	H	-1.463829	-1.684961	3.349177		H	0.778713	-2.380827	2.373029
	H	0.164247	-2.341947	3.174341		H	3.506657	0.326220	1.940596
	H	0.338029	0.135239	-3.157955		H	2.739440	-1.206088	2.416317
	H	0.836028	-1.556599	-3.189058		H	2.565721	0.795312	-0.838012
	H	-0.883445	-1.140767	-3.069224		H	1.482378	-0.587480	-1.153624

	H	1.369075	0.286293	1.121079		H	-2.033963	-2.198706	0.587503
	H	2.735878	-0.856799	1.196628		H	-2.621117	-1.036850	1.781701
	H	3.673573	-1.095222	-1.581321		H	-2.854051	0.943841	-1.845275
	H	2.611435	-0.016833	-2.520041		H	-2.016195	-0.596801	-2.054835
	H	-6.919982	-0.636087	1.299120		H	-6.594803	-3.332169	0.263263
	H	-6.744641	-0.467674	-0.479672		H	-6.335644	-2.911087	-1.463018
	H	-6.027551	-1.873861	0.353952		H	-5.241134	-4.065767	-0.659559
	H	-3.793788	4.673978	-0.533553		H	-6.558185	2.253884	-0.833338
	H	-5.252904	4.119527	-1.419565		H	-6.600717	1.446520	0.769636
	H	-5.224436	4.114543	0.375520		H	-5.461384	2.785933	0.485048
	H	1.314142	1.850506	-1.075636		H	5.542199	-1.080693	1.719080
	H	2.319305	2.669649	0.131639		H	4.171313	-0.467728	-2.313054
	H	2.887049	2.522667	-1.541064		H	7.879016	-0.778242	0.972347
	H	5.323776	0.787711	-1.904712		H	6.507531	-0.163123	-3.062590
	H	3.933202	1.164204	2.155278		H	8.380901	-0.314008	-1.424792
	H	7.623002	1.310521	-1.166553		H	3.563608	-3.150947	0.682906
	H	6.232539	1.689676	2.894382		H	1.872615	-2.742494	0.327016
	H	8.097850	1.765881	1.239719		H	3.052663	-2.855866	-0.986981
TS3-4b	C	3.219347	0.545757	-0.100727	INT4b	C	0.796861	-0.704800	-0.104823
	C	2.336996	0.316535	-1.351402		C	-0.336868	-1.445007	-0.062637
	C	1.095906	-0.399153	-0.815346		C	-2.177298	-0.052328	-1.759363
	C	0.371162	-1.306301	-1.512642		C	-3.184887	0.974997	-1.200859
	C	0.598624	-1.665085	-2.961057		C	-2.389623	2.182415	-0.625424
	C	2.189180	0.762237	1.033200		C	-1.198942	1.794573	0.271114
	C	0.912575	0.032781	0.605314		C	0.168915	1.791531	-0.364884
	C	-0.143137	-0.067208	1.458175		C	0.997284	0.723491	-0.456800
	C	-0.047153	0.445297	2.887390		C	2.420257	0.835784	-0.986313
	Ni	-1.002664	-2.074166	-0.472270		Ni	-2.130926	-1.019316	-0.138094
	O	-1.467872	-2.095969	1.363855		O	-1.344870	1.653074	1.482320
	C	-2.205620	-0.216182	-0.530364		C	0.548228	3.175848	-0.881134
	C	4.122239	1.766814	-0.301900		C	4.432469	-0.733957	-0.925146
	O	3.874884	2.894945	0.082254		O	4.600191	-0.649918	-2.128013
	O	5.215642	1.449342	-1.025048		O	5.288593	-1.366045	-0.096072
	C	6.124806	2.536179	-1.317469		C	6.459712	-1.949382	-0.713143
	C	4.097886	-0.688725	0.166366		C	3.668896	0.380218	1.179002
	O	4.183827	-1.668621	-0.547099		O	3.356883	-0.027575	2.279978
	O	4.780122	-0.547240	1.324689		O	4.481688	1.442464	0.980628
	C	-1.480354	-0.757236	1.192189		C	3.211004	-0.210428	-0.166123
	C	-2.757915	-0.052888	1.695251		C	2.181705	-1.351001	0.053021
	C	-3.088926	0.687108	0.387066		C	-0.256518	-2.938948	0.243437
	C	5.661883	-1.637965	1.675736		C	4.998563	2.072453	2.174864
	C	-4.564313	0.729508	0.000318		C	-3.954132	0.186742	-0.103443
	C	-5.571784	0.740845	0.978525		C	-4.388134	-1.136657	-0.395071
	C	-6.922994	0.835003	0.623556		C	-5.087641	-1.901744	0.564318
	C	-7.293999	0.922163	-0.722402		C	-5.368750	-1.369887	1.817277
	C	-6.299630	0.920379	-1.708176		C	-4.969631	-0.052607	2.111195
	C	-4.951338	0.828683	-1.347756		C	-4.277887	0.708551	1.174620
	C	-2.538116	2.130946	0.396090		C	-4.172912	1.498069	-2.270534
	H	2.873772	-0.245645	-2.114739		H	2.457945	0.533708	-2.040177
	H	2.057528	1.291412	-1.775054		H	2.864212	1.828308	-0.917172
	H	2.006628	1.837339	1.136542		H	2.328586	-1.812326	1.032636

	H 2.584809 0.417154 1.990143		H 2.322769 -2.133478 -0.703538
	H -0.248249 -1.328573 -3.575860		H -1.223513 -3.359185 0.554471
	H 0.662081 -2.752385 -3.096527		H 0.048910 -3.505549 -0.648302
	H 1.506217 -1.224049 -3.390761		H 0.457909 -3.167387 1.045000
	H 0.980481 0.461454 3.253922		H 0.387092 3.274712 -1.962991
	H -0.441572 1.465765 2.988495		H -0.039982 3.960230 -0.393117
	H -0.622499 -0.190922 3.568321		H 1.599720 3.403034 -0.688893
	H -1.587288 0.335862 -1.236336		H -3.047481 2.850210 -0.060050
	H -2.834888 -0.948389 -1.060453		H -2.019024 2.748670 -1.485280
	H -3.486793 -0.836581 1.918068		H -2.604720 -0.716339 -2.520282
	H -2.636327 0.575444 2.582120		H -1.245663 0.373590 -2.129307
	H 6.502692 2.972629 -0.390033		H 7.018065 -2.407146 0.103186
	H 6.935873 2.087221 -1.890418		H 6.165502 -2.702018 -1.448284
	H 5.618641 3.306163 -1.904214		H 7.055429 -1.174906 -1.201792
	H 6.123227 -1.345623 2.619013		H 5.580847 1.355863 2.759024
	H 5.092291 -2.562436 1.796087		H 5.632378 2.886228 1.822321
	H 6.420659 -1.775301 0.901648		H 4.178814 2.458774 2.785036
	H -2.663667 2.600694 -0.585586		H -4.297764 -1.542589 -1.399268
	H -3.076672 2.739023 1.131583		H -3.961006 1.707343 1.450149
	H -1.472594 2.148680 0.645737		H -5.416794 -2.906153 0.304202
	H -5.307203 0.675678 2.031898		H -5.195097 0.377217 3.085437
	H -4.193680 0.835405 -2.129663		H -5.904061 -1.958823 2.559457
	H -7.685513 0.838091 1.400745		H -4.868557 2.230857 -1.843180
	H -6.574057 0.991077 -2.759456		H -3.628571 1.976907 -3.092313
	H -8.344078 0.990873 -1.000496		H -4.763927 0.677562 -2.689972
TS4b	C -0.442906 0.017822 -0.738862	3b+Ni	C -0.044341 -0.429242 -0.851665
	C -1.702544 0.816847 -1.077381		C -1.389490 0.134015 -1.311068
	C -2.832050 0.156833 -0.225246		C -2.366023 -0.115913 -0.135963
	C -2.300276 -1.262300 0.136908		C -1.748296 -1.317254 0.613959
	C -0.791440 -1.081507 0.167286		C -0.240445 -1.226819 0.353423
	C 0.138842 -1.827983 0.928979		C 0.678177 -1.980790 1.191424
	C 1.279194 -1.078239 1.615861		C 1.879545 -1.361360 1.843370
	C 2.724728 -1.439021 1.292806		C 3.141587 -0.849539 1.133728
	C 3.368046 -0.829116 0.006168		C 3.211407 -0.048510 -0.183382
	Ni 0.706110 -1.793644 -1.026211		Ni 0.903281 -2.284681 -0.824632
	O 1.006674 -0.261051 2.489361		O 1.969185 -1.418674 3.076164
	C -0.328325 -3.020908 1.756155		C 1.054613 -0.466707 -1.738349
	C -3.094198 0.985817 1.047334		C 0.875807 0.088294 -3.144262
	O -2.567407 2.044233 1.324865		O -1.918831 2.191919 0.577972
	O -4.007009 0.374911 1.832481		O -3.236397 0.859449 1.847733
	C -4.357138 1.069392 3.052552		C 0.013826 -2.981010 2.143872
	C -4.126346 0.085368 -1.043812		C -2.457650 1.122233 0.775286
	O -4.516244 -0.892195 -1.654860		O -4.263292 -1.538775 -0.745785
	O -4.759818 1.274837 -1.054567		O -4.381028 0.692137 -1.100125
	C -5.975478 1.344118 -1.836921		C -3.411491 1.945838 2.785722
	C 2.485282 -1.106307 -1.238303		C -3.769879 -0.429577 -0.668578
	C 0.756077 0.028591 -1.435781		C -5.702815 0.521310 -1.664778
	C 1.139032 1.097847 -2.416792		C 2.488716 -0.799352 -1.359292
	C 3.694223 0.675018 0.120288		C 2.705740 1.396358 -0.047085
	C 4.380818 1.311088 -0.934297		C 2.821407 2.284285 -1.134394
	C 4.737543 2.659811 -0.869781		C 2.408043 3.614487 -1.036660

	C 4.417452 3.419859 0.262030		C 1.864691 4.096601 0.160329
	C 3.738418 2.806093 1.316561		C 1.741285 3.229389 1.247388
	C 3.382469 1.451685 1.247193		C 2.158207 1.896230 1.144065
	C 4.716106 -1.589164 -0.180830		C 4.723397 -0.010601 -0.546759
	H -2.620573 -1.957648 -0.646009		H -2.173276 -2.239901 0.206572
	H -2.710874 -1.618840 1.083365		H -1.986413 -1.299962 1.678713
	H -1.605411 1.873665 -0.819102		H -1.321356 1.198955 -1.545266
	H -1.932918 0.749699 -2.146441		H -1.747027 -0.383901 -2.207737
	H 1.627860 0.680410 -3.303645		H 1.633595 -0.320725 -3.820002
	H 0.252932 1.652129 -2.750402		H -0.102097 -0.150765 -3.570062
	H 1.831389 1.825107 -1.977340		H 0.981100 1.181780 -3.159026
	H 0.504786 -3.700687 1.969025		H 0.763117 -3.683312 2.520114
	H -0.740254 -2.700912 2.723753		H -0.440084 -2.505703 3.022707
	H -1.092934 -3.599697 1.230706		H -0.755546 -3.563196 1.629198
	H 3.344209 -1.188286 2.159338		H 3.702044 -0.314502 1.904709
	H 2.751383 -2.528979 1.167692		H 3.700419 -1.781001 0.960837
	H 2.933638 -0.705080 -2.146204		H 3.089226 -0.670913 -2.265483
	H 2.458880 -2.236667 -1.401309		H 2.658182 -1.919453 -1.142667
	H -4.774514 2.052134 2.821003		H -3.877999 2.801458 2.291719
	H -5.101462 0.439830 3.539972		H -4.060117 1.551342 3.567664
	H -3.475687 1.186806 3.686923		H -2.446778 2.245491 3.201328
	H -6.707367 0.625244 -1.461725		H -6.381308 0.103609 -0.917367
	H -6.338829 2.364122 -1.714432		H -6.021620 1.520960 -1.959121
	H -5.761696 1.134387 -2.887464		H -5.661115 -0.141612 -2.532045
	H 2.842133 1.020453 2.081600		H 2.049466 1.254978 2.012566
	H 4.648972 0.753395 -1.828901		H 3.245297 1.942499 -2.076416
	H 3.475217 3.379643 2.203840		H 1.315926 3.586227 2.183427
	H 5.267168 3.116569 -1.704359		H 2.512467 4.275688 -1.895456
	H 4.693135 4.471443 0.317759		H 1.539897 5.132289 0.240610
	H 5.237561 -1.266657 -1.086101		H 4.906340 0.574384 -1.452500
	H 5.381254 -1.406359 0.670756		H 5.307298 0.437915 0.263360
	H 4.546173 -2.668938 -0.259304		H 5.105280 -1.024214 -0.720334

Table S8. Frequencies of some stationary points for reaction **b**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

Species	Frequencies (cm^{-1})
1b	26 30 33 33 39 52 58 72 105 139 147 156 160 175 189 210 226 260 261 295 302 320 330 370 374 378 420 425 524 616 658 748 770 800 802 828 864 922 960 998 1048 1048 1050 1050 1075 1088 1136 1161 1167 1175 1175 1210 1210 1256 1267 1274 1312 1359 1364 1420 1420 1473 1475 1476 1481 1491 1492 1492 1492 1498 1498 1504 1504 1764 1780 2339 2339 3038 3038 3074 3074 3076 3077 3119 3119 3119 3119 3130 3131 3173 3173 3198 3198
2b	47 61 131 146 266 286 299 312 396 410 412 427 525 549 626 660 697 710 729 773 850 858 884 902 922 957 980 995 1011 1018 1045 1097 1105 1110 1124 1168 1172 1196 1209 1214 1257 1321 1328 1358 1419 1434 1455 1471 1504 1509 1526 1627 1651 1837 3029 3051 3056 3111 3122 3123 3125 3160 3164 3173 3179 3189
COM1b	10 12 19 27 33 39 42 53 60 65 74 85 97 106 111 119 123 137 141 154 156 167 183 195 213 225 236 256 267 277 289 293 305 311 317 328 341 346 373 388 396 406 411 416 422 435 443 476 520 549 550 556 626 629 662 677 708 710 731 738 773 781 821 823 836 850 851 890 892 902 909 924 954 968 981 996 998 1010 1019 1038 1045 1045 1045 1051 1064 1092 1099 1109 1110 1124 1128 1136 1137 1172 1174 1174 1178 1195 1208 1208 1211 1229 1229 1254 1259 1270 1314 1321 1329 1344 1359 1365 1409 1410 1419 1432 1451 1469 1471 1472 1475 1483 1492 1493 1497 1498 1498 1498 1505 1505 1506 1510 1527 1627 1652 1766 1788 1790 2033 2053 3019 3020 3030 3051 3052 3055 3061 3069 3071 3094 3094 3103 3103 3105 3109 3111 3120 3124 3127 3159 3163 3165 3168 3172 3179 3190 3190 3195
TS1b’	**-135i** 16 24 28 32 38 46 58 65 71 85 91 100 113 128 143 149 152 157 180 184 198 224 233 238 243 254 258 264 278 298 306 325 327 337 352 366 395 401 413 413 435 443 466 474 489 503 537 552 554 598 619 627 664 685 709 720 727 774 785 802 821 825 830 847 851 894 899 904 915 919 925 960 967 977 990 991 1010 1020 1036 1038 1046 1048 1056 1062 1076 1084 1089 1118 1123 1126 1141 1143 1164 1171 1173 1174 1175 1200 1203 1210 1221 1226 1238 1255 1277 1285 1312 1316 1326 1335 1359 1360 1408 1410 1414 1469 1469 1473 1474 1475 1478 1482 1488 1490 1498 1499 1502 1503 1503 1506 1509 1515 1526 1626 1650 1692 1774 1797 2053 3028 3037 3040 3050 3054 3072 3073 3074 3098 3111 3113 3113 3117 3120 3122 3132 3132 3152 3157 3163 3165 3170 3172 3174 3179 3188 3196 3201
INT1b’	18 19 27 40 42 51 58 65 72 81 91 99 117 122 131 137 148 154 168 180 202 211 222 229 238 251 263 275 286 301 313 322 335 340 351 363 382 399 406 410 414 441 456 472 493 513 542 548 555 599 617 628 663 678 709 711 730 735 774 792 806 826 831 847 848 852 892 899 919 929 934 936 966 978 981 990 995 1010 1011 1033 1043 1046 1050 1057 1077 1081 1082 1111 1114 1114 1131 1137 1156 1170 1173 1174 1177 1197 1209 1210 1222 1233 1237 1246 1271 1281 1303 1310 1326 1328 1341 1359 1365 1409 1412 1419 1469 1470 1471 1473 1474 1480 1482 1488 1491 1498 1498 1499 1503 1504 1504 1510 1513 1525 1626 1650 1659 1770 1786 2092 3029 3033 3038 3048 3058 3058 3067 3073 3076 3096 3110 3119 3123 3128 3131 3139 3140 3142 3152 3156 3161 3171 3171 3176 3177 3187 3198 3201
TS1b	**-185i** 7 9 20 23 27 38 47 55 61 74 86 93 100 106 118 125 136 148 152 162 171 177 192 204 210 246 260 262 280 292 300 308 315 326 339 340 369 411 413 419 422 431 450 458 480 519 549 560 571 627 627 641 666 704 710 715 723 742 772 773 804 830 850 854 886 896 899 917 924 939 955 956 973 981 997 997 1011 1016 1023 1030 1038 1046 1053 1071 1095 1100 1108 1120 1127 1129 1143 1155 1173 1174 1175 1185 1189 1196 1206 1207 1211 1228 1240 1260 1277 1288 1319 1321 1329 1335 1359 1405 1408 1419 1431 1451

	1472 1474 1475 1476 1482 1483 1493 1494 1498 1498 1501 1505 1505 1506 1509 1527 1579 1628 1652 1726 1740 1766 1790 2987 3008 3032 3046 3051 3051 3056 3060 3069 3071 3076 3083 3090 3111 3115 3117 3129 3129 3149 3161 3165 3166 3167 3174 3180 3190 3192 3195
INT1b	5 13 17 26 34 42 46 58 60 70 86 98 104 117 122 130 147 148 151 160 164 190 195 200 207 217 242 267 276 290 298 301 311 313 323 330 349 370 410 414 416 424 429 434 471 499 539 547 549 592 626 641 662 664 693 710 719 738 760 773 792 798 827 849 853 880 895 899 921 924 939 957 958 980 984 997 1011 1016 1019 1026 1028 1041 1045 1067 1084 1099 1106 1111 1113 1125 1132 1155 1172 1174 1174 1178 1181 1196 1200 1210 1211 1223 1234 1262 1266 1280 1297 1313 1322 1329 1331 1359 1400 1402 1422 1427 1447 1471 1473 1474 1475 1479 1482 1494 1496 1498 1498 1502 1505 1505 1506 1511 1527 1627 1652 1689 1691 1766 1776 1790 2985 2994 3031 3033 3046 3051 3053 3055 3056 3064 3068 3069 3078 3116 3122 3123 3128 3130 3131 3161 3163 3164 3165 3174 3180 3190 3191 3193
TS1-3b	**-369i** 3 22 27 30 40 51 61 70 84 87 92 101 114 120 140 147 151 164 186 195 200 208 221 238 239 257 265 278 294 306 328 331 345 360 376 398 407 413 425 433 446 467 483 506 522 551 560 598 607 626 627 633 665 700 710 713 756 774 806 817 828 835 843 849 850 899 908 918 924 934 947 960 977 979 990 995 997 1005 1010 1037 1045 1049 1061 1078 1084 1093 1101 1122 1125 1130 1143 1146 1170 1174 1174 1176 1195 1198 1205 1212 1214 1234 1239 1249 1281 1286 1305 1319 1327 1328 1351 1359 1397 1413 1417 1466 1470 1471 1472 1474 1475 1481 1487 1490 1498 1498 1500 1504 1506 1506 1509 1524 1529 1573 1626 1650 1773 1790 1794 3024 3024 3039 3052 3054 3065 3072 3073 3084 3100 3105 3109 3111 3129 3136 3139 3149 3153 3157 3163 3164 3170 3171 3174 3180 3188 3197 3199
TS1-2b	**-325i** 13 27 31 34 38 55 62 71 72 83 94 100 111 117 143 149 157 163 171 179 195 204 211 220 238 247 258 260 289 303 306 319 325 331 351 361 381 401 414 424 433 441 470 491 503 542 550 553 606 627 641 651 665 711 716 735 761 774 793 797 804 828 846 851 874 880 912 923 926 945 951 960 980 984 994 1001 1007 1011 1029 1045 1050 1061 1065 1082 1089 1095 1104 1108 1113 1131 1171 1171 1173 1174 1178 1181 1182 1200 1201 1211 1220 1225 1261 1277 1281 1306 1317 1319 1327 1358 1374 1397 1402 1409 1415 1456 1465 1471 1471 1474 1475 1481 1485 1489 1498 1498 1504 1504 1506 1506 1508 1511 1525 1541 1582 1626 1651 1771 1793 3000 3009 3033 3036 3059 3066 3068 3070 3071 3071 3074 3082 3118 3120 3123 3129 3130 3134 3144 3160 3165 3167 3168 3175 3181 3189 3195 3196
INT2b	18 23 28 35 39 58 59 69 78 82 88 106 113 132 146 148 160 175 183 192 203 217 222 235 253 259 268 280 291 302 312 329 339 356 361 374 404 413 420 431 434 472 494 510 541 553 557 610 618 627 655 677 700 711 719 727 766 774 794 800 822 829 849 854 860 871 896 922 932 940 945 953 964 970 979 984 992 1010 1032 1038 1044 1049 1063 1071 1078 1091 1105 1107 1114 1119 1127 1167 1170 1174 1175 1180 1182 1195 1203 1211 1224 1226 1227 1234 1258 1282 1297 1301 1308 1321 1327 1343 1358 1376 1401 1407 1410 1469 1470 1473 1474 1476 1482 1486 1491 1496 1497 1498 1499 1504 1505 1506 1508 1509 1525 1590 1625 1651 1772 1795 2996 3004 3030 3043 3053 3059 3059 3064 3072 3073 3096 3107 3112 3116 3122 3125 3131 3132 3139 3158 3163 3169 3171 3174 3179 3187 3198 3199
TS2-3b	**-403i** 13 26 32 34 41 53 58 70 76 78 85 95 99 131 143 146 160 170 176 201 205 210 227 233 252 261 265 273 297 305 312 320 344 356 359 364 408 411 428 436 455 467 490 514 552 558 570 617 627 653 668 688 706 710 737 756 774 778 802 823 829 849 861 873 879 906 922 935 936 945 954 963 979 981 986 992 1010 1021 1034 1044 1056 1060 1072 1077 1086 1095 1103 1114 1127 1129 1168 1170 1175 1175 1183 1185 1195 1206 1211 1225 1228 1231 1239 1279 1287 1292 1306 1325 1327 1329 1338 1357 1393 1404 1413 1422 1463 1470 1472 1474 1474 1476 1481 1493 1498 1498 1504 1504 1505 1506 1507 1508

	1513 1515 1525 1626 1651 1771 1793 3001 3019 3026 3029 3058 3067 3068 3071 3072 3075 3101 3102 3112 3115 3118 3137 3138 3139 3142 3158 3163 3169 3170 3172 3178 3188 3196 3198
INT3b	17 29 30 33 39 53 58 78 80 88 94 101 117 135 146 149 150 161 184 191 206 210 226 237 251 259 261 276 282 290 307 325 332 342 357 369 383 395 412 428 446 467 481 513 518 554 574 604 628 630 651 668 691 709 710 752 773 775 803 808 826 834 849 870 874 886 914 921 938 947 952 960 966 972 977 988 996 1014 1022 1040 1048 1053 1065 1075 1082 1085 1093 1108 1115 1129 1134 1168 1175 1176 1176 1187 1187 1200 1211 1212 1220 1230 1232 1243 1272 1285 1300 1303 1320 1327 1329 1345 1359 1414 1414 1423 1442 1473 1474 1475 1476 1483 1494 1501 1501 1503 1506 1508 1509 1511 1512 1514 1516 1527 1628 1654 1662 1722 1789 1809 2814 3029 3032 3044 3053 3063 3068 3070 3072 3084 3090 3112 3113 3122 3129 3136 3138 3147 3151 3165 3167 3172 3177 3187 3191 3194 3195 3206
TS3-4b	**-296i** 14 27 29 32 45 58 61 77 82 86 96 103 117 139 145 148 155 165 169 176 194 198 216 237 245 266 278 286 300 306 316 320 330 343 354 367 376 412 421 424 440 451 492 500 529 552 565 576 618 627 631 652 690 710 714 730 750 763 775 781 810 829 850 853 892 896 924 932 937 955 966 968 981 984 991 996 1010 1019 1037 1040 1045 1066 1075 1079 1090 1103 1109 1115 1136 1145 1164 1171 1174 1174 1178 1195 1196 1199 1208 1214 1215 1233 1243 1278 1284 1298 1304 1325 1326 1329 1345 1359 1409 1412 1420 1446 1471 1474 1475 1480 1487 1493 1493 1498 1498 1499 1503 1504 1506 1510 1513 1518 1525 1605 1626 1650 1659 1769 1792 2996 3007 3022 3026 3035 3066 3070 3070 3071 3071 3091 30963120 3129 3130 3135 3120 3129 3130 3135 3148 3158 3159 3165 3166 3168 3169 3175 3182 3189 3193 3196
INT4b	18 20 32 50 55 64 68 77 86 91 93 97 110 121 127 139 153 159 166 177 193 199 210 223 226 239 245 261 279 285 298 304 320 329 350 357 361 398 421 426 444 455 474 492 508 539 559 562 601 618 623 642 656 701 711 715 745 753 768 776 798 810 829 845 850 860 891 912 919 941 959 965 970 972 982 993 995 1002 1007 1031 1032 1045 1055 1063 1067 1076 1090 1098 1106 1116 1136 1150 1170 1174 1174 1177 1191 1197 1210 1211 1212 1226 1233 1264 1284 1293 1305 1320 1324 1343 1349 1365 1402 1405 1419 1461 1474 1475 1477 1486 1492 1496 1497 1499 1500 1504 1504 1505 1505 1506 1510 1516 1521 1602 1618 1638 1679 1723 1768 1793 2993 3023 3027 3037 3052 3055 3056 3066 3069 3071 3077 3097 3110 3117 3120 3125 3132 3157 3164 3166 3166 3167 3175 3186 3192 3192 3195 3235
TS4b	**-367i** 16 30 34 40 50 58 82 85 90 103 109 137 142 148 153 163 168 175 189 194 199 209 227 228 248 261 267 283 291 299 307 323 333 352 360 387 406 412 416 420 428 463 474 504 536 563 570 576 590 625 629 644 683 708 714 720 747 772 779 791 803 826 833 858 876 881 924 935 943 947 963 978 988 988 1000 1012 1013 1035 1042 1050 1055 1059 1074 1080 1086 1101 1110 1116 1125 1148 1165 1174 1174 1174 1187 1191 1208 1211 1218 1222 1228 1240 1272 1294 1296 1312 1316 1332 1339 1348 1371 1408 1409 1417 1420 1460 1471 1474 1476 1480 1486 1490 1496 1498 1498 1502 1505 1506 1506 1508 1511 1513 1530 1532 1627 1652 1726 1770 1794 2581 3015 3023 3034 3042 3058 3067 3071 3072 3090 3098 3107 3110 3117 3128 3130 3136 3140 3146 3159 3168 3168 3169 3179 3187 3195 3197 3234
3b	10 25 31 34 48 53 60 73 82 84 96 109 130 137 145 155 161 181 189 193 209 215 240 246 259 272 272 281 306 312 321 336 341 349 355 382 386 401 414 422 429 456 497 500 515 549 564 582 606 620 628 643 678 706 712 721 741 773 780 810 820 834 852 862 874 892 911 927 943 967 971 979 983 990 994 1006 1011 1029 1045 1050 1054 1057 1076 1084 1096 1102 1108 1126 1149 1174 1174 1175 1176 1181 1192 1209 1211 1213 1216 1233 1240 1262 1278 1298 1307 1319 1329 1335 1343 1355 1366 1386 1404 1420 1421 1424 1472 1473 1475 1476 1478 1483 1497 1498 1498 1499 1504 1505 1508 1509 1513 1513 1516 1523 1531 1629 1654 1658 1773 1799 2408 3021 3023 3029 3036 3056 3070 3071

	3071 3074 3100 3109 3112 3118 3128 3133 3135 3136 3143 3160 3167 3168 3170 3179 3188 3195 3197 3217

Table S9. Some optimized Cartesian Coordinates of stationary points for reaction **c.**

Species	Cartesian coordinates			Species	Cartesian coordinates		
COM2c	C	-1.523181	0.605340 -1.749948	TS1c'	C	-0.965710	0.438597 -0.372786
	C	-1.654707	-0.642002 -1.453534		C	-2.384519	0.038741 -0.605476
	C	-2.210201	-1.935007 -1.965679		C	-2.819433	-1.256510 0.096904
	C	-3.315548	-2.608045 -1.126220		C	-4.276773	-1.665295 -0.208852
	C	-4.684285	-1.887484 -1.114539		C	-5.287974	-0.707702 0.271656
	C	-4.763018	-0.696812 -0.253361		C	-6.121890	0.080103 0.672707
	C	-4.838747	0.270523 0.476753		C	-7.130225	1.034638 1.153786
	C	-4.844143	1.459255 1.337555		C	-0.331719	1.556609 -0.052006
	C	5.082259	-0.277767 -0.152879		C	-0.902624	2.703430 0.755519
	Ni	-0.587014	0.240052 -0.141860		Ni	0.668084	-0.260743 0.130650
	O	4.286291	0.308538 0.549919		O	1.779365	0.989186 -1.634202
	C	5.832173	-1.611255 -0.018408		C	0.642091	3.169897 -2.056350
	C	6.482663	-1.332228 -1.412352		C	1.460560	4.214760 -1.241443
	C	5.722113	0.030071 -1.513895		C	2.024900	3.098487 -0.312831
	C	-1.911680	1.656832 -2.736402		P	2.157756	-0.385592 1.801628
	P	0.329894	2.177560 0.324328		C	3.913755	0.088871 1.455214
	C	1.547406	2.742873 -0.957195		C	2.381145	-2.016185 2.654889
	C	1.323089	2.523313 1.857047		C	1.767854	0.703762 3.249131
	C	-0.834864	3.623233 0.378615		P	0.993854	-1.980166 -1.159710
	P	-0.048859	-1.271325 1.354017		C	0.596653	-3.706170 -0.611679
	C	-1.400246	-1.686870 2.558640		C	2.757231	-2.143040 -1.682670
	C	1.362732	-1.031718 2.537998		C	0.141859	-1.887745 -2.793248
	C	0.382308	-2.956504 0.704869		C	1.212246	2.024496 -1.132643
	H	1.089520	2.694415 -1.948744		H	3.935683	1.097134 1.034441
	H	1.892344	3.766861 -0.768903		H	4.530732	0.058558 2.360642
	H	2.410772	2.071080 -0.942922		H	4.338182	-0.588461 0.708864
	H	1.677933	3.560861 1.880195		H	3.052174	-1.935390 3.517816
	H	0.711282	2.344161 2.747174		H	1.410455	-2.389556 2.995075
	H	2.188496	1.856001 1.891204		H	2.800444	-2.748205 1.957977
	H	-1.416517	3.662730 -0.545721		H	2.506077	0.596404 4.052587
	H	-1.534174	3.494842 1.211079		H	1.747569	1.748834 2.926902
	H	-0.302967	4.573392 0.508786		H	0.777183	0.451672 3.639154
	H	-1.124774	-2.520462 3.216014		H	0.836966	-4.439004 -1.390867
	H	-1.612253	-0.807444 3.175034		H	1.166859	-3.951030 0.289151
	H	-2.315664	-1.937960 2.017234		H	-0.466290	-3.787878 -0.367045
	H	1.162709	-0.165725 3.175499		H	3.374486	-2.448816 -0.832379
	H	1.504954	-1.910567 3.178820		H	2.875360	-2.882030 -2.483525
	H	2.287776	-0.836094 1.987360		H	3.093104	-1.161533 -2.026049
	H	0.598423	-3.665207 1.513365		H	-0.941816	-1.937784 -2.655138
	H	-0.443976	-3.343890 0.103671		H	0.391919	-0.922836 -3.241808
	H	1.261212	-2.879257 0.057005		H	0.452317	-2.699808 -3.461122
	H	5.174116	-2.484809 0.044323		H	-0.441495	3.318995 -2.068091
	H	6.519951	-1.635759 0.834596		H	0.987073	3.017713 -3.084619
	H	6.205712	-2.053614 -2.184471		H	0.846584	4.957623 -0.722492
	H	7.570637	-1.238821 -1.389238		H	2.220795	4.745228 -1.823277

	H 4.997248 0.121044 -2.330320		H 1.792195 3.217458 0.748940
	H 6.347740 0.929751 -1.505191		H 3.100039 2.922376 -0.423936
	H -2.600935 -1.786841 -2.985550		H -3.053352 0.859595 -0.306961
	H -1.391843 -2.661420 -2.061395		H -2.528445 -0.076423 -1.691613
	H -2.972644 -2.748184 -0.095575		H -2.690154 -1.145129 1.179162
	H -3.483301 -3.610221 -1.542660		H -2.160834 -2.075014 -0.213050
	H -5.449750 -2.601477 -0.782886		H -4.476650 -2.644657 0.244423
	H -4.954111 -1.610169 -2.142703		H -4.399091 -1.798265 -1.292478
	H -5.180139 1.218378 2.352467		H -8.077864 0.529781 1.371001
	H -3.834052 1.879452 1.404890		H -6.795937 1.529931 2.071932
	H -5.508151 2.235608 0.940834		H -7.326462 1.810628 0.405843
	H -2.650551 2.344075 -2.304991		H -0.892974 3.648267 0.200470
	H -1.057637 2.267534 -3.053805		H -1.940305 2.508047 1.056033
	H -2.361593 1.219984 -3.639301		H -0.324518 2.868825 1.671751
INT1c’	C 2.928982 -1.878521 -1.040854	COM1c	C -1.531843 -0.198434 -1.837749
	C 0.719071 1.172015 -0.763672		C -1.672031 -1.325714 -1.278358
	C 1.766466 0.507869 -1.312844		C -1.983567 -2.779650 -1.290654
	C 0.728724 2.671931 -0.540540		C -2.502940 -3.302857 0.057623
	C 0.843743 3.123223 0.935635		C -1.511359 -2.998954 1.192064
	C 2.256763 3.037869 1.562256		C -1.200388 -1.551438 1.324719
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	C 2.255603 1.959628 -1.434051		C 0.070850 3.357470 -0.661402
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	C 1.518729 1.812991 -0.043564		C 1.207782 1.831071 0.534404
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	H	-1.063787	-4.434690	0.442710	H	-1.271930	-0.118620	3.128379
INT3c	C	-4.531351	0.623031	-0.541262	TS3c	C	-4.390244	0.770924	-0.192961
	C	-3.626836	0.032629	-1.643725		C	-3.569525	0.347834	-1.425422
	C	-2.288998	-0.193712	-0.930408		C	-2.236244	-0.142514	-0.840023
	C	-2.601612	-0.498701	0.471667		C	-2.487636	-0.604216	0.497694
	C	-4.022227	-0.015751	0.769755		C	-3.883648	-0.148293	0.930633
	C	-1.055813	0.077862	-1.455109		C	-0.994209	0.083912	-1.498994
	C	0.880335	-1.662860	-1.676633		C	0.138725	-1.282442	-2.038576
	C	0.611695	-2.952581	-0.887547		C	0.265152	-2.666025	-1.400525
	C	-0.690273	-2.896456	-0.082385		C	-0.828112	-2.984021	-0.374544
	Ni	0.653236	0.013630	-0.595134		Ni	0.676102	0.217334	-0.637527
	O	0.324358	-2.012703	1.896082		O	0.336115	-2.560824	1.657682
	C	-0.625722	-1.926568	1.100094		C	-0.644334	-2.231673	0.945194
	C	-1.827568	-1.110878	1.417667		C	-1.686948	-1.326340	1.381603
	C	-2.205386	-1.095275	2.889327		C	-1.952791	-1.301039	2.879764
	C	-0.980393	0.563409	-2.901103		C	-1.066621	0.929978	-2.780481
	P	2.853988	-0.165977	0.023300		P	2.837694	-0.321058	-0.017957

	C 3.625385 -1.831396 0.252724 C 3.569024 0.652863 1.529411 C 3.927665 0.535717 -1.316220 P 0.250677 2.012344 0.413097 C 1.405186 3.374374 -0.100812 C -1.354260 2.880351 0.121282 C 0.323159 2.101482 2.263311 H -4.396880 1.710395 -0.505514 H -5.596811 0.434499 -0.711944 H -3.556224 0.690701 -2.513915 H -4.040141 -0.924485 -1.998353 H -4.642443 -0.875140 1.059955 H -4.063206 0.682747 1.614316 H 1.894190 -1.697740 -2.105313 H 0.211199 -1.640247 -2.542668 H 0.559457 -3.813709 -1.573415 H 1.419683 -3.171099 -0.186244 H -0.879859 -3.878108 0.379067 H -1.540952 -2.671766 -0.726707 H -2.721188 -0.175105 3.180981 H -2.869706 -1.933127 3.146830 H -1.305218 -1.196483 3.501291 H 0.051404 0.620254 -3.259290 H -1.539425 -0.073848 -3.599177 H -1.407383 1.573377 -2.991802 H 4.695609 -1.721107 0.459725 H 3.146113 -2.339871 1.092941 H 3.503914 -2.444036 -0.642194 H 3.118435 0.213089 2.424411 H 4.652798 0.499050 1.575603 H 3.376965 1.727742 1.539322 H 4.992159 0.423702 -1.080680 H 3.716504 0.017095 -2.255824 H 3.707856 1.596951 -1.463325 H 1.170881 4.311464 0.416769 H 2.445649 3.114964 0.105183 H 1.306909 3.536441 -1.178945 H -1.350187 3.864069 0.604266 H -1.524317 3.009099 -0.950373 H -2.175034 2.287047 0.525313 H 0.150094 3.123925 2.618415 H -0.446772 1.443924 2.675436 H 1.288433 1.754577 2.634787		C 3.592835 -1.971007 -0.403181 C 3.188322 -0.244851 1.797696 C 4.149769 0.781549 -0.732763 P 0.365049 2.103947 0.466863 C 1.755763 3.330183 0.572790 C -0.988017 3.231645 -0.095052 C -0.069394 1.906852 2.252971 H -4.168131 1.817045 0.051852 H -5.472208 0.697562 -0.348917 H -3.476999 1.165190 -2.145096 H -4.081790 -0.472337 -1.955602 H -4.527332 -1.034194 1.039550 H -3.881510 0.343606 1.909615 H 1.081627 -0.965246 -2.513248 H -0.541309 -1.366929 -2.889111 H 0.228979 -3.419098 -2.200728 H 1.226393 -2.784900 -0.902616 H -0.754480 -4.046118 -0.109162 H -1.817988 -2.812372 -0.803449 H -2.136814 -0.293833 3.273040 H -2.828691 -1.908208 3.152077 H -1.088686 -1.712852 3.407027 H -0.076475 1.060552 -3.228472 H -1.721328 0.493205 -3.546366 H -1.456322 1.927890 -2.560757 H 4.659063 -1.972926 -0.148826 H 3.091092 -2.747076 0.180219 H 3.486152 -2.208648 -1.466103 H 2.502387 -0.930181 2.304474 H 4.222269 -0.533376 2.019126 H 3.019182 0.763689 2.184602 H 5.140609 0.537578 -0.332818 H 4.172242 0.654787 -1.820136 H 3.934148 1.831482 -0.524203 H 1.438331 4.232312 1.108198 H 2.611299 2.901695 1.101230 H 2.080511 3.615886 -0.432392 H -1.129856 4.056110 0.612641 H -0.742059 3.650896 -1.075018 H -1.919829 2.668733 -0.181899 H -0.141966 2.880728 2.751122 H -1.027287 1.389384 2.328155 H 0.678801 1.295131 2.762747
3a	C -1.194708 0.207645 0.145766 C -0.941830 1.467557 -0.295456 C -0.362246 -1.007836 -0.040445 C 0.990895 -1.222768 -0.054499 C 2.049270 -0.226645 0.283894 C 1.722722 1.078819 0.993924 C 1.467195 2.217261 -0.009665 C 0.341641 1.849722 -0.997831	$Ni\text{-}(P(CH_3)_3)_2$	Ni 0.000005 0.005732 0.003267 P 2.137609 0.000846 0.000594 P -2.137612 -0.000299 0.000851 C 2.987844 -0.796478 1.447001 H 2.680122 -1.843835 1.519494 H 4.079928 -0.750548 1.354588 H 2.687076 -0.292739 2.370403 C 2.979293 -0.862136 -1.413174

	C -1.320899 -2.195416 -0.160048 C -2.741798 -1.612384 -0.036225 C -2.534486 -0.273515 0.696387 C 1.512357 -2.612955 -0.378807 C -1.911943 2.614857 -0.121385 O 3.235215 -0.472272 0.029384 H 2.602033 -2.612332 -0.399533 H 1.152295 -2.966315 -1.351837 H 1.182574 -3.345469 0.368961 H 0.852043 0.962207 1.644964 H 2.384603 2.431651 -0.570185 H 1.210519 3.128444 0.544892 H 0.685117 1.022690 -1.630311 H 0.153213 2.702619 -1.661392 H -2.741332 2.397096 0.552498 H -2.328154 2.916516 -1.092538 H -1.386998 3.494393 0.272382 H -2.461379 -0.444456 1.780246 H -3.358948 0.421210 0.529198 H -3.159854 -1.420387 -1.030814 H -3.428461 -2.284608 0.487363 H -1.172583 -2.746913 -1.095257 H -1.114039 -2.908540 0.649313 H 2.590604 1.324323 1.613320		H 4.071891 -0.814765 -1.327359 H 2.668543 -1.910766 -1.437718 H 2.675192 -0.399393 -2.356721 C 2.995733 1.647895 -0.038555 H 2.694886 2.195889 -0.936354 H 2.693445 2.237268 0.832150 H 4.087352 1.539676 -0.035401 C -2.985547 1.081143 -1.249486 H -2.676232 0.788311 -2.257269 H -4.077633 1.010828 -1.176407 H -2.684358 2.121569 -1.094696 C -2.981302 -1.625171 -0.315333 H -2.675888 -2.349226 0.445985 H -4.073786 -1.527859 -0.298176 H -2.672912 -2.012805 -1.290660 C -2.996092 0.536834 1.557809 H -4.087681 0.500401 1.455312 H -2.694028 -0.112486 2.384747 H -2.695593 1.559239 1.805355

Table S10. Frequencies of some stationary points for reaction **c**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

Species	Frequencies (cm^{-1})
COM2c	9 11 17 20 25 28 30 33 37 39 44 46 54 66 76 87 96 105 131 139 147 151 166 177 178 190 193 202 205 212 225 238 239 251 259 263 267 276 288 297 334 344 358 361 365 400 450 453 493 516 578 622 650 656 676 690 698 702 705 709 743 785 796 804 842 857 859 863 865 869 883 927 950 954 957 961 963 967 969 970 985 1027 1038 1048 1054 1064 1071 1097 1103 1138 1160 1186 1199 1222 1223 1249 1249 1279 1287 1328 1329 1331 1333 1350 1355 1361 1375 1384 1405 1418 1435 1448 1469 1473 1476 1480 1480 1481 1484 1485 1486 1489 1491 1494 1494 1495 1497 1499 1500 1504 1505 1511 1838 1892 2339 2985 3002 3022 3030 3031 3032 3033 3034 3034 3034 3035 3047 3056 3060 3065 3073 3084 3091 3101 3108 3109 3118 3121 3123 3124 3125 3125 3127 3129 3148 3150 3151 3151 3153 3154 3156
TS1c’	**-348i** 17 26 27 32 33 46 48 59 62 65 70 77 91 111 131 140 143 150 151 163 163 177 183 189 191 197 208 214 228 234 236 241 249 251 255 259 264 272 290 318 336 364 373 391 422 449 457 486 548 608 654 661 690 693 711 712 715 723 752 762 790 801 808 809 839 861 863 865 877 894 944 962 964 966 967 969 972 973 977 990 1022 1035 1043 1046 1051 1054 1068 1073 1113 1154 1181 1190 1208 1231 1239 1241 1261 1298 1325 1327 1332 1334 1336 1351 1357 1366 1392 1404 1421 1426 1466 1469 1471 1473 1477 1477 1480 1481 1483 1484 1485 1485 1489 1491 1493 1494 1496 1499 1500 1505 1506 1513 1685 2333 2995 3017 3025 3035 3036 3036 3036 3036 3037 3038 3042 3056 3056 3060 3069 3073 3088 3102 3107 3112 3116 3116 3126 3127 3129 3130 3130 3133 3134 3138 3142 3146 3149 3159 3160 3161
INT1c’	24 28 36 46 48 55 61 72 76 80 102 109 120 128 144 152 159 163 170 179 184 188

	199 203 209 213 218 220 236 253 256 262 273 275 290 300 310 323 331 358 362 370 375 394 431 495 509 537 587 592 654 658 676 696 710 712 713 722 726 764 809 811 828 853 864 865 868 871 873 928942 948 956 964 966 969 970 975 977 979 991 1029 1038 1047 1053 1059 1070 1072 1132 1159 1162 1188 1191 1232 1239 1256 1260 1267 1286 1321 1328 1335 1337 1338 1349 1359 1363 1377 1385 1411 1418 1465 1467 1470 1477 1478 1479 1479 1481 1483 1486 1486 1490 1493 1493 1497 1498 1501 1505 1506 1508 1510 1518 1644 2338 3015 3018 3022 3030 3034 3037 3038 3039 3043 3044 3045 3045 3054 3057 3065 3066 3078 3092 3105 3108 3119 3120 3122 3126 3128 3132 3133 3134 3135 3137 3148 3161 3169 3170 3172 3174
COM1c	9 14 24 25 33 42 50 54 60 102 114 140 143 153 156 163 175 180 186 194 205 215 219 234 238 246 248 254 268 270 285 300 314 324 349 381 401 402 412 508 543 573 640 657 696 699 707 710 744 774 802 802 849 854 864 865 871 882 962 964 967 968 971 982 9871024 1037 1042 1049 1056 1062 1125 1126 1164 1221 1283 1331 1334 1336 1337 1354 1356 1357 1360 1384 1409 1411 1470 1473 1474 1475 1479 1480 1481 1482 1485 1486 1488 1491 1494 1499 1501 1501 1502 1506 1511 2004 2014 3012 3014 3018 3022 3023 3024 3024 3038 3039 3040 3043 3060 3064 3094 3099 3100 3105 3111 3111 3115 3116 3124 3126 3129 3131 3131 3134 3153 3157 3161
TS1c	**-209i** 23 30 38 52 68 75 86 94 113 123 128 139 142 151 156 162 176 180 190 203 208 212 219 220 222 253 255 261 267 279 303 321 328 342 369 385 420 465 526 585 595 644 650 700 702 703 704 765 795 798 830 852 852 855 859 892 907 951 958 959 959 961 962 980 1014 1035 1037 1054 1063 1065 1107 1112 1150 1201 1272 1325 1326 1327 1331 1334 1338 1347 1350 1364 1407 1409 1472 1472 1477 1478 1478 1478 1479 1485 1486 1486 1487 1491 1491 1495 1498 1499 1501 1502 1505 1803 1885 2999 3001 3001 3003 3028 3028 3029 3029 3029 3030 3043 3063 3067 3071 3076 3086 3090 3103 3120 3121 3121 3122 3123 3123 3139 3140 3140 3140 3140 3142
INT1c	26 39 52 58 66 76 85 101 110 113 126 136 141 150 164 167 170 177 182 190 199 206214 229 240 243 251 256 258 262 268 318 338 345 374 445 473 520 595 602 630 655 657 707 710 718 718 721 801 801 856 856 861 864 864 869 928 940 962 963 963 964 968 9831009 1014 1023 1033 1056 1058 1074 1126 1149 1177 1195 1254 1312 1317 1328 1329 1329 1330 1345 1349 1351 1408 1411 1464 1465 1474 1475 1476 1477 1478 1479 1482 1485 1489 1489 1491 1491 1493 1497 1497 1498 1514 1550 1632 2983 2985 2998 2999 3034 3035 3035 3037 3037 3045 3045 3046 3048 3055 3056 3079 3080 3095 3127 3128 3129 3130 3142 3142 3149 3149 3151 3151 3160 3161
TS1-2c’	**-303i** 5 46 51 66 78 84 95 103 106 111 123 130 139 140 146 152 161 170 174 185 185 193 200 208 221 235 240 246 255 263 265 276 283 285 291 301 328 340 354 373 386 394 422 468 481 518 535 572 601 647 652 675 696 698 708 712 715 773 779 802 808 818 835 855 861 864 874877 881 908 938 950 961 962 965 968 969 972 978 985 1013 1020 1034 1041 1050 1056 1073 1105 1123 1148 1168 1187 1205 1207 1231 1251 1261 1264 1278 1320 1329 1332 1334 1337 1337 1350 1359 1366 1409 1412 1466 1468 1470 1476 1476 1478 1479 1481 1482 1484 1485 1487 1491 1493 1495 1502 15031508 1509 1510 1513 1529 1610 1946 3021 3022 3026 3028 3039 3039 3039 3040 3041 3042 3044 3045 3048 3055 3075 3084 3089 3093 3095 3102 3107 3116 3124 3126 3130 3130 3132 3134 3136 3143 3154 3161 3161 3166 3171 3178
TS1-2c	**-273i** 38 52 60 68 76 85 95 105 114 127 129 136 140 145 152 166 169 174 176 180 195 207 213 216 225 232 238 240 256 261 265 270 273 281 290 302 310 321 326 344 352 401 443 461 477 546 608 613 643 647 655 661 700 707 711 717 731 747 753 804 810 854 855 862 862 862 868 874 912 938 944 962 965 968 969 972 979 984 993 1002 1007 1012 1028 1051 1059 1064 1071 1093 11401149 1183 1203 1216

	12351240 1248 1269 1302 1308 1326 1331 13321334 1339 1352 1355 1372 1403 1404 1452 1465 1470 1471 1476 1478 1480 1482 1482 14843009 3032 3034 3041 3042 3042 3044 3045 3045 3051 3056 3059 3071 3074 3076 3083 3101 3105 3123 3124 3126 3132 3135 3137 3138 3139 3145 3148 3152 3163 3164 3165 3167
INT2c	23 37 49 53 67 74 95 106 108 113 118 132 141 148 149 156 169 169 176 180 187 196 203 216 218 221 230 242 250 256 261 268 276 278 285 304 315 326 334 352 369 433 442 509 531 574 606 628 649 651 657 688 709 710 715 724 727 774 783 805 808 835 856 857 860 868 871 888 915 934 948 958 963 964 968 970 973 975 988 989 1008 1014 1030 1045 1058 1063 1070 1093 1140 1145 1150 1194 1201 1220 1238 1243 1244 1270 1271 1299 1306 1319 1323 1327 1333 1336 1337 1348 1359 1406 1414 1466 1469 1470 1475 1477 1480 1480 1482 1483 1485 1487 1488 1491 1494 1496 1499 1503 1504 1504 1506 1511 1517 1657 1695 2994 3009 3009 3023 3035 3039 3039 3042 3044 3047 3050 3050 3055 3056 3065 3066 3069 3071 3093 3103 3107 3120 3125 3126 3128 3130 3135 3138 3139 3147 3147 3156 3160 3170 3171 3172
TS2-3c	**-243i** 11 19 29 34 40 44 55 56 70 83 96 104 126 135 145 157 162 178 183 191 195 207 209 218 222 228 230 243 247 251 254 256 270 295 298 304 315 322 334 377 425 429 446 488 522 561 616 617 639 641 666 693 699 701 728 730 731 766 788 798 815 852 854 857 873 876 878 913 935 939 959 964 966 976 979 982 986 989 9971010 1020 1023 1040 1047 1062 1083 1098 1135 1142 1153 1172 1198 1211 1237 1248 1259 1270 1303 1315 1317 1329 1332 1333 1335 1336 1347 1355 1359 1409 1418 1447 1469 1474 1477 1479 1481 1482 1483 1484 1486 1488 1489 1491 1491 1494 1498 1500 1502 1506 1508 1513 1516 1603 1652 2985 3003 3005 3015 3019 3024 3025 3027 3041 3042 3043 3044 3053 3062 3063 3074 3090 3096 3099 3107 3116 3117 3117 3118 3126 3128 3129 3131 3134 3138 3139 3142 3153 3158 3162 3163
INT3c	19 38 59 71 78 81 85 106 114 119 132 142 146 149 159 162 170 178 183 186 194 199217 226 231 240 243 249 263 269 277 279 280 288 293 304 320 339 347 361 364 390 419 464 512 519 552 593 624 645 652 656 694 704 707 713 713 731 768 805 810 817 852 861 865 870 877 879 886 912 936 953 961 965 968 970 974 976 989 994 1021 1028 1035 1054 1061 1074 1082 1104 1120 1152 1167 1204 1224 1253 1256 1281 1298 1316 1329 1331 1336 1337 1338 1345 1357 1363 1368 1391 1395 1406 1471 1472 1476 1477 1479 1482 1483 1484 1485 1488 1490 1492 1497 1499 1501 1503 1506 1509 1512 1514 1514 1524 1554 1637 1656 2986 2998 3000 3001 30133016 3024 3039 3040 3045 3047 3047 3048 3049 3062 3069 3079 3093 3099 3109 3115 3123 3130 3133 3134 3138 3141 3142 3144 3145 3149 3154 3162 3170 3176 3182
TS3c	**-322i** 22 38 51 66 79 86 97 110 117 127 129 142 144 150 164 166 171 183 196 202 209 218 223 234 249 254 255 259 265 271 278 282 293 300 312 324 329 338 354 358 387 410 443 467 526 554 579 616 635 650 658 681 704 709 714 718 735 750 808 811 824 858 860 865 866 872 879901 914 948 960 965 968 968 970 974 984 989 1024 1026 1034 1043 1059 1065 1082 1094 1119 1149 1153 1188 1212 1243 1252 1265 1299 1319 1324 1326 1332 1335 1336 1338 1346 1354 1360 1371 1376 1403 1412 1432 1459 1470 1472 1477 1480 1483 1485 1485 1486 1487 1487 1491 1494 1501 1503 1506 1507 1513 1514 1517 1519 1526 1548 1600 2977 2999 3005 3011 3018 3023 3035 3036 3039 3039 3040 3043 3044 3049 3065 3078 3094 3096 3100 3106 3121 3127 3129 3129 3130 3131 3135 3135 3144 3149 3152 3153 3161 3162 3172 3177
Ni-$(P(CH_3)_3)_2$	4 36 44 113 115 165 166 174 187 189 199 200 206 207 246 247 256 257 258 351 361 642 655 698 698 698 699 794 795 853 855 858 860 957 957 958 958 960 9841326 1326 1327 1327 1349 1349 1467 1467 1476 1476 1476 1477 1482 1482 1483 1483 1497 1498 3030 3030 3030 3031 3032 3032 3125 3125 3126 3126 3127 3127 3145 3145 3145 3145 3146 3146

Table S11. Some optimized Cartesian Coordinates of stationary points for reaction **d**

Species	Cartesian coordinates			Species	Cartesian coordinates		
COM2d	C	4.007501	3.141475 0.368682	TS1d'	C	0.468053	2.603983 -0.897889
	C	4.004746	4.334657 0.600339		C	-0.212306	3.539531 -1.398303
	C	4.020087	5.774720 0.893658		C	-0.385136	4.978990 -1.706693
	C	4.046291	1.697193 0.090011		C	1.735240	2.033312 -0.374895
	C	4.341804	1.369300 -1.387725		C	2.890163	2.137552 -1.388346
	C	4.523891	-0.143767 -1.635975		C	4.264566	1.712780 -0.827927
	C	5.728982	-0.706168 -1.002694		C	4.741810	2.551712 0.284460
	C	6.732182	-1.152180 -0.481662		C	5.125608	3.251921 1.200735
	C	7.944583	-1.692430 0.148974		C	5.586973	4.097462 2.310373
	Ni	-0.501407	0.493568 -0.503500		Ni	-0.101612	0.687799 -0.521586
	O	0.348335	1.891328 -1.386643		O	-1.492702	1.047102 -1.879746
	C	0.448637	3.111022 -1.239968		C	-2.219357	2.060111 -1.788009
	C	1.003693	4.201288 -2.145072		C	-3.193312	2.648976 -2.815103
	C	0.469726	5.244408 -1.107569		C	-3.811486	3.509053 -1.668232
	C	0.017659	4.085353 -0.158005		C	-2.958628	2.729051 -0.619373
	C	-1.405062	-0.908461 0.215209		C	-0.277268	-1.040105 0.302783
	N	-2.773143	-1.035118 0.411395		N	-1.325716	-1.536304 1.053062
	C	-3.114106	-2.286551 0.922951		C	-1.145095	-2.878622 1.385938
	C	-1.954769	-2.979811 1.066640		C	0.034138	-3.260104 0.835165
	N	-0.927548	-2.139857 0.638331		N	0.554037	-2.138897 0.189354
	C	0.462956	-2.515875 0.636380		C	1.829634	-2.148717 -0.482770
	C	1.004667	-3.120764 -0.517529		C	1.866170	-2.217047 -1.892732
	C	2.356982	-3.492075 -0.487213		C	3.126135	-2.277228 -2.507348
	C	3.139580	-3.271367 0.646549		C	4.300138	-2.282938 -1.754468
	C	2.579926	-2.673273 1.775795		C	4.237069	-2.217423 -0.362315
	C	1.232690	-2.283758 1.796189		C	3.004341	-2.142393 0.303307
	C	0.184931	-3.335847 -1.786520		C	0.606716	-2.262438 -2.753595
	C	0.195400	-4.806438 -2.248374		C	0.478961	-3.619144 -3.478290
	C	0.657697	-2.389710 -2.909450		C	0.547929	-1.088217 -3.750147
	C	0.661024	-1.587054 3.028175		C	2.975452	-2.068501 1.829561
	C	1.217548	-0.153340 3.149647		C	3.776787	-0.867801 2.371580
	C	0.892755	-2.391977 4.322071		C	3.469946	-3.384774 2.465983
	C	-3.730701	0.006662 0.142917		C	-2.499464	-0.793294 1.438969
	C	-4.079417	0.893568 1.184157		C	-2.416361	0.110924 2.519861
	C	-5.027899	1.888752 0.906489		C	-3.587309	0.784976 2.897473
	C	-5.611579	1.995232 -0.356735		C	-4.795764	0.557478 2.239247
	C	-5.253371	1.103703 -1.368192		C	-4.853630	-0.349266 1.180408
	C	-4.308828	0.091527 -1.141264		C	-3.709808	-1.040156 0.753860
	C	-3.430043	0.825691 2.563643		C	-1.120485	0.369460 3.283285
	C	-4.467415	0.758465 3.701545		C	-1.263896	0.040103 4.783222
	C	-2.450894	2.000864 2.762014		C	-0.625840	1.814561 3.072255
	C	-3.921258	-0.851384 -2.276554		C	-3.815358	-2.021303 -0.412617
	C	-3.157689	-0.096042 -3.383639		C	-4.288942	-1.329356 -1.706757

	C	-5.139037	-1.605891	-2.846085		C	-4.722681	-3.218615	-0.060994
	H	-1.770820	-3.981126	1.432257		H	0.541199	-4.214903	0.842687
	H	-4.136653	-2.566853	1.137466		H	-1.862893	-3.434363	1.973449
	H	2.809409	-3.951174	-1.363471		H	3.190676	-2.328588	-3.592045
	H	3.203307	-2.498745	2.649891		H	5.160461	-2.218632	0.212988
	H	4.189355	-3.555028	0.644658		H	5.266497	-2.336438	-2.253125
	H	-5.313035	2.592770	1.685429		H	-3.555940	1.495826	3.720583
	H	-5.712304	1.199653	-2.349987		H	-5.802216	-0.516535	0.674725
	H	-6.346251	2.774568	-0.552927		H	-5.693810	1.088204	2.550949
	H	-2.838984	-0.091893	2.612381		H	-0.351946	-0.292603	2.878786
	H	-5.158560	-0.080559	3.564038		H	-1.593391	-0.993654	4.935949
	H	-3.962071	0.625968	4.665207		H	-0.300951	0.166492	5.291670
	H	-5.064070	1.674851	3.768974		H	-1.986749	0.697612	5.278623
	H	-2.973366	2.964518	2.728361		H	-1.338016	2.545242	3.473249
	H	-1.950711	1.922711	3.734815		H	0.332196	1.966463	3.583449
	H	-1.685098	1.992711	1.978816		H	-0.483600	2.024974	2.006871
	H	-3.236020	-1.600161	-1.872880		H	-2.818058	-2.417551	-0.615608
	H	-2.261108	0.380533	-2.972484		H	-3.599722	-0.530989	-1.994170
	H	-2.846053	-0.789882	-4.173602		H	-4.329081	-2.056255	-2.526757
	H	-3.782436	0.678459	-3.844253		H	-5.292365	-0.902721	-1.595489
	H	-5.670809	-2.156266	-2.061939		H	-4.373682	-3.737250	0.838777
	H	-5.855768	-0.926892	-3.321735		H	-5.755919	-2.900977	0.118797
	H	-4.815619	-2.327131	-3.605725		H	-4.734977	-3.941282	-0.884940
	H	-0.419631	-1.498300	2.893958		H	1.938631	-1.924987	2.142604
	H	0.984456	0.425220	2.248915		H	3.416744	0.078150	1.956504
	H	0.772663	0.357711	4.012017		H	3.680502	-0.815491	3.462279
	H	2.305419	-0.158356	3.285759		H	4.844196	-0.949478	2.139885
	H	0.494030	-3.409064	4.237666		H	2.883988	-4.243742	2.121662
	H	1.956408	-2.469732	4.572952		H	4.519887	-3.578228	2.218763
	H	0.393225	-1.901696	5.165720		H	3.387528	-3.335550	3.557852
	H	-0.852180	-3.073869	-1.564765		H	-0.258526	-2.158639	-2.096506
	H	-0.155294	-5.477202	-1.456062		H	0.484379	-4.454412	-2.768936
	H	-0.462482	-4.934308	-3.115884		H	-0.460291	-3.659890	-4.041939
	H	1.197399	-5.135402	-2.545512		H	1.299049	-3.778541	-4.187725
	H	0.590800	-1.345524	-2.584068		H	0.568017	-0.128505	-3.225722
	H	1.695271	-2.598627	-3.196310		H	1.379048	-1.120037	-4.464515
	H	0.031464	-2.512907	-3.801330		H	-0.386311	-1.128708	-4.320904
	H	3.089122	1.242661	0.375528		H	1.632358	0.934292	-0.080669
	H	4.815170	1.236796	0.722659		H	2.003092	2.504240	0.577820
	H	0.606549	3.984324	0.761063		H	-2.390632	3.296793	0.118151
	H	-1.045171	4.034373	0.101677		H	-3.545404	1.965001	-0.090123
	H	2.095074	4.168882	-2.239608		H	-2.729762	3.191685	-3.645454
	H	0.565329	4.232083	-3.149341		H	-3.870294	1.891286	-3.232344
	H	4.888832	6.040762	1.506048		H	-1.256472	5.395078	-1.182599
	H	4.068718	6.365921	-0.027570		H	0.485347	5.589789	-1.418201
	H	3.121031	6.078626	1.441305		H	-0.562840	5.141895	-2.777734
	H	5.242259	1.903101	-1.709885		H	2.948197	3.172912	-1.741697
	H	3.510977	1.723417	-2.007162		H	2.661564	1.514182	-2.258685
	H	1.232600	5.905210	-0.692196		H	-3.544875	4.566361	-1.739754
	H	-0.359639	5.847387	-1.484721		H	-4.895163	3.425937	-1.548937
	H	4.577912	-0.320829	-2.717476		H	5.001892	1.750636	-1.640391
	H	3.639959	-0.685745	-1.277600		H	4.225246	0.667069	-0.501109

	H	8.702955	-0.911847	0.275042		H	6.119720	3.505111	3.062443
	H	7.724629	-2.108264	1.138489		H	6.267108	4.879524	1.955273
	H	8.384122	-2.489842	-0.460359		H	4.742666	4.588470	2.806814
INT1d’	C	2.715536	3.514345	-0.719904	COM1d	C	0.751423	2.913960	-1.201302
	C	2.651453	4.780781	0.179042		C	0.701349	4.399467	-1.251239
	C	1.100138	4.724114	0.096489		C	0.489792	5.041985	0.127726
	C	-1.240020	0.857766	-2.231944		C	-0.781705	4.494076	0.792290
	C	-2.722999	1.039061	-1.835438		C	-0.793042	3.010841	0.901097
	C	-3.326854	2.449932	-2.053314		C	-1.152889	1.935321	1.462727
	C	-3.124403	3.415240	-0.960737		C	-1.938260	1.309798	2.555844
	C	-3.008852	4.220422	-0.058377		C	1.137929	1.792383	-1.641208
	C	-2.801119	5.174636	1.038389		C	1.948277	1.063894	-2.648573
	Ni	0.417427	0.719456	0.217551		Ni	-0.008482	1.487185	-0.071665
	O	1.047715	2.339304	0.664392		C	-0.008828	-0.446429	0.015570
	C	-3.028050	-4.703574	-1.154831		N	1.048293	-1.315541	0.252895
	C	-0.232671	1.540783	-1.339937		C	0.630424	-2.647094	0.239276
	C	0.309983	2.768203	-1.531835		C	-0.690421	-2.645289	-0.040655
	C	1.195189	3.240061	-0.411853		N	-1.082233	-1.311040	-0.156624
	C	0.174347	-1.201108	0.268634		C	-2.465314	-0.945046	-0.389129
	N	-0.830771	-2.064100	0.635757		C	-3.453677	-1.323697	0.557839
	C	-0.329518	-3.322179	0.958003		C	-4.782190	-0.951844	0.299345
	C	1.016316	-3.269531	0.775445		C	-5.131329	-0.243810	-0.847836
	N	1.304742	-1.978662	0.352038		C	-4.152224	0.070006	-1.788085
	C	2.649753	-1.517421	0.073665		C	-2.810607	-0.286132	-1.592946
	C	3.136348	-1.612616	-1.246730		C	-3.179810	-2.189726	1.793929
	C	4.456563	-1.203865	-1.481406		C	-3.627859	-3.649359	1.537995
	C	5.257114	-0.722623	-0.445134		C	-3.867696	-1.695698	3.084375
	C	4.748102	-0.636735	0.850367		C	-1.809279	-0.063891	-2.724087
	C	3.433651	-1.029081	1.140253		C	-1.993966	1.275812	-3.456941
	C	2.287182	-2.126697	-2.405860		C	-1.868308	-1.248112	-3.715076
	C	2.870698	-3.420980	-3.009158		C	2.439126	-0.965054	0.461502
	C	2.096904	-1.042141	-3.485769		C	3.419702	-1.442136	-0.449946
	C	2.910358	-0.913753	2.570148		C	4.757874	-1.094098	-0.211680
	C	2.981392	0.537243	3.091721		C	5.125925	-0.316581	0.883847
	C	3.647269	-1.883296	3.517808		C	4.153396	0.098766	1.789906
	C	-2.243704	-1.756635	0.688360		C	2.800631	-0.225247	1.611894
	C	-2.733839	-0.951832	1.739158		C	3.124184	-2.383840	-1.624166
	C	-4.112763	-0.694703	1.767569		C	3.532977	-3.834240	-1.269512
	C	-4.970249	-1.231907	0.808772		C	3.827238	-1.996500	-2.942888
	C	-4.462140	-2.044781	-0.204063		C	1.808199	0.135693	2.714461
	C	-3.090822	-2.323426	-0.292142		C	1.968842	1.579707	3.222086
	C	-1.851374	-0.399679	2.856844		C	1.919587	-0.875564	3.877264
	C	-2.205665	-1.055252	4.208926		H	-1.373795	-3.468112	-0.173347
	C	-1.914746	1.138279	2.946213		H	1.298405	-3.469604	0.436034
	C	-2.586442	-3.244426	-1.405115		H	-5.558837	-1.222343	1.010041
	C	-3.029328	-2.791021	-2.810546		H	-4.439657	0.588964	-2.698175
	C	0.068123	3.669125	-2.724255		H	-6.167073	0.044367	-1.018361
	H	1.780699	-4.023125	0.907564		H	5.528102	-1.440225	-0.896040
	H	-0.964701	-4.132651	1.285903		H	4.453129	0.673079	2.662467
	H	4.863695	-1.258432	-2.488731		H	6.170095	-0.052083	1.040685
	H	5.380966	-0.252001	1.646778		H	2.048552	-2.372418	-1.817958

	H	6.279316	-0.408545	-0.649349		H	3.090914	-4.183128	-0.331899
	H	-4.522964	-0.068827	2.556696		H	3.227863	-4.523942	-2.065007
	H	-5.143724	-2.463049	-0.941286		H	4.620544	-3.909400	-1.159211
	H	-6.037041	-1.019476	0.852777		H	4.914691	-2.105745	-2.873828
	H	-0.814016	-0.662074	2.636432		H	3.488938	-2.662569	-3.744830
	H	-2.126073	-2.147066	4.158668		H	3.611141	-0.971100	-3.245491
	H	-1.524312	-0.700874	4.991042		H	0.803032	0.063685	2.302420
	H	-3.226770	-0.808682	4.520697		H	1.911759	2.288444	2.391888
	H	-1.620506	1.604381	2.001418		H	1.159204	1.817704	3.920620
	H	-2.921175	1.486209	3.205035		H	2.914764	1.731176	3.754664
	H	-1.229572	1.494275	3.723974		H	1.744095	-1.901719	3.535105
	H	-1.493429	-3.227666	-1.398866		H	2.913399	-0.843034	4.339139
	H	-2.701333	-1.770648	-3.024321		H	1.179903	-0.647097	4.653928
	H	-2.593879	-3.452266	-3.568352		H	-0.811535	-0.039895	-2.289552
	H	-4.117236	-2.829086	-2.929966		H	-1.988906	2.109882	-2.749996
	H	-2.699493	-5.067523	-0.175729		H	-1.165835	1.428580	-4.157419
	H	-4.119125	-4.797122	-1.191123		H	-2.922034	1.311316	-4.039052
	H	-2.608859	-5.366916	-1.920020		H	-1.667013	-2.201169	-3.213339
	H	1.856047	-1.205171	2.572934		H	-2.854548	-1.321456	-4.188712
	H	2.470197	1.234419	2.420088		H	-1.122191	-1.119997	-4.508531
	H	2.512640	0.599433	4.081039		H	-2.103530	-2.193801	1.985056
	H	4.019620	0.871760	3.200263		H	-3.199399	-4.071622	0.624576
	H	3.562263	-2.921539	3.177875		H	-3.337751	-4.292352	2.377095
	H	4.713699	-1.641377	3.585746		H	-4.717454	-3.702775	1.435484
	H	3.226423	-1.821802	4.527961		H	-3.621154	-0.658964	3.316986
	H	1.294431	-2.369394	-2.018954		H	-4.958014	-1.777927	3.024280
	H	2.967046	-4.208066	-2.253054		H	-3.545885	-2.315982	3.928726
	H	2.219070	-3.795256	-3.807145		H	2.121895	1.676444	-3.543383
	H	3.862509	-3.251717	-3.442747		H	1.477529	0.127477	-2.966418
	H	1.420978	-1.404613	-4.269201		H	2.924714	0.807003	-2.225741
	H	1.671001	-0.131196	-3.055122		H	1.628909	4.777308	-1.701798
	H	3.047637	-0.780812	-3.963968		H	-0.118884	4.709835	-1.915199
	H	-1.117832	1.194809	-3.273182		H	-2.937919	1.050314	2.192265
	H	-1.035788	-0.219684	-2.243200		H	-1.479884	0.387599	2.927918
	H	2.902929	3.764842	-1.770655		H	-2.059769	1.995234	3.405706
	H	3.382469	2.702421	-0.416082		H	1.356630	4.831328	0.765578
	H	0.698214	5.414245	-0.653087		H	0.415913	6.131408	0.024146
	H	0.538902	4.834829	1.028740		H	-0.900259	4.931445	1.793127
	H	0.998610	4.153872	-3.046713		H	-1.654546	4.816834	0.205868
	H	-0.334453	3.129072	-3.585891					
	H	-0.640929	4.470194	-2.477167					
	H	-2.869552	0.740970	-0.793628					
	H	-3.314761	0.345533	-2.445517					
	H	3.135621	5.686356	-0.203068					
	H	3.018124	4.588924	1.191762					
	H	-4.409473	2.339017	-2.198922					
	H	-2.941872	2.875385	-2.989577					
	H	-3.687465	5.246958	1.678867					
	H	-1.955464	4.866690	1.662823					
	H	-2.583944	6.177817	0.653668					
TS1d	C	0.718210	3.029874	-0.907498	INT1d	C	-2.438923	-1.369504	-3.884852

	C	0.879845	4.504936	-1.160847		C	-0.210920	2.345571	0.744555
	C	0.494322	5.286277	0.097634		C	0.377895	3.544751	0.571647
	C	-0.802348	4.630505	0.575630		C	1.434737	3.599411	-0.452379
	C	-0.662332	3.133313	0.515212		C	1.655333	2.423650	-1.075915
	C	-1.187794	2.117168	1.136327		C	0.188465	4.928989	1.175386
	C	-2.189691	2.031648	2.239810		C	0.825453	5.857807	0.102844
	C	1.237724	1.932312	-1.375864		C	1.966509	5.022180	-0.542363
	C	2.285828	1.674288	-2.406780		C	-1.327835	2.027697	1.692964
	Ni	0.007177	1.265938	-0.081743		Ni	0.559736	0.994660	-0.372428
	C	-0.019742	-0.587307	0.027621		C	-0.225488	-0.789435	0.083563
	N	1.024895	-1.453454	0.300490		N	-1.453785	-1.400043	-0.018740
	C	0.598366	-2.782302	0.303739		C	-1.358287	-2.775615	0.182052
	C	-0.720335	-2.774727	0.004209		C	-0.051099	-3.048689	0.429543
	N	-1.096810	-1.439486	-0.146329		N	0.621662	-1.834041	0.362886
	C	-2.464894	-1.050558	-0.401602		C	2.058480	-1.707445	0.488276
	C	-3.444624	-1.314984	0.587661		C	2.862044	-2.060640	-0.618816
	C	-4.770980	-0.955523	0.306073		C	4.252825	-1.960765	-0.469185
	C	-5.118977	-0.359499	-0.905041		C	4.818573	-1.525257	0.728980
	C	-4.141162	-0.133776	-1.872102		C	4.000633	-1.184564	1.805848
	C	-2.800473	-0.481371	-1.650591		C	2.604084	-1.270121	1.713512
	C	-3.140479	-2.024348	1.910399		C	2.280029	-2.558603	-1.941028
	C	-3.649336	-3.484188	1.879820		C	2.600939	-4.051841	-2.165041
	C	-3.727538	-1.309739	3.144215		C	2.748458	-1.713228	-3.141927
	C	-1.792377	-0.311724	-2.785618		C	1.745060	-0.905352	2.920048
	C	-1.831993	1.095388	-3.409726		C	1.961686	0.560350	3.346581
	C	-2.003671	-1.402613	-3.858260		C	1.986575	-1.875745	4.095213
	C	2.408608	-1.090019	0.502932		C	-2.706796	-0.749842	-0.340241
	C	3.370885	-1.512564	-0.448192		C	-3.703287	-0.660310	0.661038
	C	4.712012	-1.173830	-0.214399		C	-4.919681	-0.055237	0.314875
	C	5.090720	-0.446928	0.913096		C	-5.137766	0.449697	-0.966752
	C	4.128501	-0.064677	1.845943		C	-4.143847	0.338017	-1.936697
	C	2.774005	-0.383907	1.671043		C	-2.913339	-0.274391	-1.653464
	C	3.033316	-2.365745	-1.674804		C	-3.523665	-1.215494	2.075228
	C	3.495253	-3.826994	-1.469009		C	-4.324808	-2.523656	2.261944
	C	3.632803	-1.824165	-2.988345		C	-3.913536	-0.206957	3.175455
	C	1.780498	-0.033395	2.777062		C	-1.895569	-0.438265	-2.780213
	C	1.885139	1.435666	3.225919		C	-1.452915	0.919964	-3.359716
	C	1.949304	-0.994651	3.974103		C	2.669449	2.213761	-2.175116
	H	-1.414928	-3.591203	-0.119113		H	0.450512	-3.983551	0.639274
	H	1.262415	-3.604715	0.520776		H	-2.213653	-3.432427	0.121338
	H	-5.545384	-1.143848	1.045993		H	4.903775	-2.222335	-1.300528
	H	-4.428227	0.310190	-2.822207		H	4.456294	-0.843639	2.732786
	H	-6.153667	-0.081739	-1.099036		H	5.900534	-1.449911	0.822936
	H	5.473754	-1.482735	-0.926382		H	-5.706663	0.032205	1.060122
	H	4.438457	0.481904	2.733276		H	-4.330757	0.724430	-2.936109
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	H	3.091015	-4.266286	-0.551717		H	-4.056177	-3.281695	1.519228
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	H	1.748166	2.109404	2.375854		H	-1.022537	1.558528	-2.581063
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	H	-1.929485	-2.407417	-3.427438		H	1.798740	-2.915087	3.803054
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	H	-4.742555	-3.514458	1.808762		H	3.680291	-4.217590	-2.254977
	H	-3.392710	-0.273294	3.208888		H	2.508809	-0.655321	-3.002585
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	C	1.118671	2.671678	-0.119448		C	2.726169	-2.391286	0.505885
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	C	3.852934	-2.827021	1.323800		C	5.411877	-0.331570	-0.636048
	C	3.260333	-1.919315	2.200374		C	4.747940	0.579714	-1.458081
	C	1.903042	-1.582899	2.089701		C	3.510117	1.122259	-1.085150
	C	0.930912	-3.800922	-0.947247		C	3.067045	-0.591489	2.375453
	C	0.644780	-5.274509	-0.585338		C	3.855801	0.127556	3.492466
	C	1.611294	-3.705195	-2.326323		C	3.054426	-2.114599	2.604850
	C	1.282302	-0.628494	3.106460		C	2.836339	2.170759	-1.966283
	C	1.971156	0.750110	3.100621		C	2.978124	1.881901	-3.472221
	C	1.279387	-1.247189	4.520592		C	3.371491	3.584123	-1.644799
	H	-3.422750	-2.438674	1.526853		H	-0.167292	3.297682	2.350421
	H	-0.975267	-3.643398	2.005213		H	2.505725	2.930463	1.741322
	H	-4.704260	2.852934	1.092243		H	-4.757410	2.882507	0.322676
	H	-5.558405	0.342064	-2.270905		H	-4.092667	-0.399161	2.989526
	H	-6.026479	2.363743	-0.933792		H	-5.634946	1.148941	1.846982
	H	3.569157	-4.132161	-0.357642		H	5.385353	-1.413182	1.217483
	H	3.861387	-1.469592	2.987478		H	5.203267	0.874003	-2.399892
	H	4.907499	-3.076092	1.429267		H	6.372192	-0.741789	-0.944251
	H	-0.032816	-3.291218	-1.030164		H	2.029292	-0.257469	2.436011
	H	0.110292	-5.360943	0.366495		H	3.838827	1.215836	3.368043
	H	0.031019	-5.746985	-1.361024		H	3.424760	-0.106105	4.472853
	H	1.574711	-5.847468	-0.497417		H	4.904924	-0.189829	3.503150
	H	1.838584	-2.667581	-2.582241		H	2.448526	-2.607542	1.840770
	H	2.544960	-4.276927	-2.361535		H	4.065352	-2.538500	2.603519
	H	0.950017	-4.112045	-3.099874		H	2.612173	-2.333316	3.584187
	H	0.238478	-0.465695	2.827579		H	1.768956	2.161257	-1.734599
	H	1.939764	1.202604	2.105747		H	2.681445	0.857381	-3.716503
	H	1.464405	1.425417	3.799833		H	2.339850	2.564567	-4.043480
	H	3.019124	0.676542	3.412735		H	4.005146	2.029589	-3.823906
	H	0.757448	-2.210485	4.535748		H	3.212038	3.849090	-0.595046
	H	2.297468	-1.413125	4.889976		H	4.446483	3.650947	-1.848397
	H	0.774771	-0.577353	5.226370		H	2.863463	4.334810	-2.261530
	H	-2.727271	-2.015565	-1.564959		H	-0.507665	-0.725982	2.253788
	H	-2.901489	-0.519314	-3.592129		H	-2.420050	-2.334827	2.387198
	H	-3.323426	-2.210471	-3.907717		H	-1.208944	-2.509953	3.658890
	H	-4.597265	-0.997986	-3.769425		H	-2.761444	-1.756564	4.034208
	H	-4.804836	-2.937779	-0.508280		H	-0.313525	1.136739	3.951731
	H	-5.766644	-2.307518	-1.851677		H	-1.672935	0.445360	4.851374
	H	-4.567311	-3.579421	-2.142307		H	-0.150267	-0.451488	4.711725
	H	-1.818602	0.762797	2.269030		H	-1.137676	3.226739	-0.587409

	H -3.892095 -0.006512 3.424048 H -3.025300 1.211086 4.378298 H -4.484406 1.661095 3.479914 H -1.572007 3.112633 1.456345 H -3.034762 3.572450 2.362714 H -1.607598 2.990372 3.222346 H 0.569476 -0.437013 -3.722638 H -0.423607 -1.162733 -2.438245 H -0.816112 0.432212 -3.058309 H 2.681096 -0.686523 -3.547713 H 3.362110 0.935021 -3.727849 H 2.044046 4.137324 -2.558699 H 0.468244 3.290962 -2.575371 H 0.789553 4.907934 0.938685 H 2.270124 5.356140 0.045873 H 4.190138 -1.223981 -1.729937 H 5.259474 -0.309206 -2.801447 H 5.235123 1.582862 -1.337613 H 4.782209 0.392604 -0.121421 H 4.269465 4.206350 0.059282 H 3.389484 3.632080 1.469909 H 4.670911 2.638679 0.767929 H -0.534931 5.109207 -1.181630 H 0.784396 6.148797 -1.773841		H -1.677389 4.828675 1.264647 H -1.861618 5.585927 -0.325756 H -3.291105 5.069147 0.584814 H -2.970095 2.487642 -2.171844 H -3.986708 3.802394 -1.559766 H -2.468732 4.175312 -2.378672 H -5.359256 -1.383382 -2.671919 H -4.708732 -0.314611 -1.417473 H -3.374545 0.324388 -3.347602 H -3.223049 -1.352423 -3.878251 H -4.121835 -3.273060 -1.818889 H -4.369792 -2.403427 -0.310631 H 0.243433 0.709206 -3.595865 H -0.431271 1.896052 -2.498059 H -1.460941 1.141409 -3.727690 H -2.329495 -5.016588 -0.454533 H -1.497649 -4.476778 1.006678 H -3.134233 -3.916528 0.660009 H 1.048156 -4.752802 0.122684 H 0.015021 -4.968148 -1.321041 H 2.037700 -4.211650 -2.566935 H 2.552846 -3.254877 -1.158343 H 0.027233 -2.692821 -2.851608 H 1.279033 -1.525998 -2.371478
INT3d	C -1.871164 -0.413209 -2.088438 C -3.057436 -1.053910 -1.865295 C -3.453516 -1.968603 -0.773354 C -2.724650 -2.834970 -0.010869 C -1.273955 -3.127547 -0.175894 C -0.680949 -3.395028 -1.559486 C 0.698239 -2.749090 -1.754222 C 0.629372 -1.272180 -2.142729 C -4.330739 -0.809600 -2.687524 Ni -0.405686 -0.205570 -0.917903 O -0.574562 -3.360758 0.818946 C -5.451379 -0.844074 -1.634805 C -4.974889 -1.897862 -0.617619 C -3.391502 -3.627479 1.104986 C -1.770346 0.441618 -3.353760 C 0.872291 0.629219 0.378968 N 2.217865 0.604045 0.661220 C 2.563037 1.562414 1.613092 C 1.420555 2.211014 1.951413 N 0.406328 1.634375 1.195151 C 3.216859 -0.269860 0.081851 C 3.565441 -1.450066 0.772731 C 4.576364 -2.249014 0.216741 C 5.217487 -1.883057 -0.965746 C 4.868192 -0.698925 -1.616008 C 3.864174 0.136408 -1.106637 C 2.945043 -1.832499 2.115852	TS3d	C -1.291433 -0.664984 -1.871965 C -2.449478 -1.346072 -1.583544 C -2.601482 -2.656044 -0.933642 C -1.635144 -3.407700 -0.343279 C -0.238104 -2.895285 -0.144050 C 0.872334 -3.582067 -0.968926 C 1.440946 -2.521892 -1.922852 C 0.288987 -1.625854 -2.468368 C -3.835302 -0.853089 -2.009821 Ni -0.040356 -0.962296 -0.511134 O 0.094019 -2.265397 0.952282 C -4.821745 -1.757101 -1.248462 C -4.062046 -3.084260 -1.069743 C -1.869255 -4.821453 0.150546 C -1.334379 0.572479 -2.741748 C 0.554275 0.742210 0.327597 N 1.857582 1.053650 0.647960 C 1.941080 2.163499 1.486282 C 0.669290 2.575383 1.707388 N -0.163449 1.716384 0.989740 C 3.029809 0.343606 0.189294 C 3.611939 -0.627759 1.032491 C 4.774814 -1.267979 0.576952 C 5.337751 -0.951607 -0.658759 C 4.751910 0.025043 -1.465164 C 3.590223 0.696756 -1.059060 C 3.062788 -0.948753 2.421085

	C	3.909122	-1.477431	3.270633		C	3.931557	-0.281536	3.510911
	C	2.530582	-3.313390	2.198405		C	2.931085	-2.460177	2.683566
	C	3.541006	1.459210	-1.800184		C	3.008718	1.812879	-1.924737
	C	3.445510	1.338434	-3.333338		C	2.987502	1.472078	-3.426612
	C	4.571324	2.542370	-1.410602		C	3.767854	3.136978	-1.685262
	C	-0.972187	2.067522	1.237648		C	-1.600776	1.890097	0.962637
	C	-1.373604	3.130669	0.399253		C	-2.139362	2.957210	0.206412
	C	-2.712993	3.539638	0.469167		C	-3.532771	3.124351	0.216749
	C	-3.608906	2.921185	1.340737		C	-4.355181	2.272405	0.951520
	C	-3.179426	1.888897	2.175119		C	-3.795209	1.246099	1.712871
	C	-1.850710	1.441655	2.149014		C	-2.409414	1.036528	1.747732
	C	-0.395165	3.876813	-0.505352		C	-1.272324	3.966917	-0.549259
	C	-0.045219	5.255627	0.096323		C	-1.169359	5.292984	0.239007
	C	-0.907313	4.028923	-1.949411		C	-1.766403	4.264115	-1.979280
	C	-1.374742	0.373293	3.130652		C	-1.810721	-0.022757	2.671830
	C	-2.366602	-0.791544	3.284248		C	-2.697401	-1.266496	2.847511
	C	-1.063122	1.006031	4.505261		C	-1.480693	0.598824	4.048189
	H	3.578207	1.694115	1.959304		H	2.882572	2.552912	1.846655
	H	1.243762	3.018040	2.648241		H	0.287553	3.387230	2.308531
	H	4.870279	-3.168105	0.717592		H	5.248403	-2.023710	1.198763
	H	5.997482	-2.519819	-1.379927		H	6.238619	-1.463601	-0.993031
	H	5.385858	-0.422723	-2.531253		H	5.208766	0.268871	-2.421025
	H	2.035407	-1.241412	2.249177		H	2.056201	-0.530718	2.491286
	H	4.181442	-0.416772	3.265884		H	4.002348	0.802293	3.369841
	H	3.443260	-1.701271	4.237235		H	3.503393	-0.464251	4.503335
	H	4.835727	-2.059118	3.201965		H	4.951075	-0.684589	3.505692
	H	1.807192	-3.570601	1.421618		H	2.271701	-2.919976	1.944669
	H	3.393126	-3.985167	2.124832		H	3.902053	-2.968622	2.673278
	H	2.052142	-3.504400	3.165760		H	2.488575	-2.623133	3.673144
	H	2.561694	1.792390	-1.446712		H	1.971666	1.968287	-1.617317
	H	2.736026	0.561281	-3.631525		H	2.495557	0.513128	-3.614407
	H	3.105050	2.289265	-3.758573		H	2.441481	2.246859	-3.976443
	H	4.414549	1.108963	-3.789786		H	3.995326	1.423152	-3.853247
	H	4.610076	2.692218	-0.326854		H	3.735406	3.433715	-0.632090
	H	5.577122	2.265669	-1.746869		H	4.820638	3.043613	-1.975842
	H	4.312693	3.501492	-1.874469		H	3.324616	3.946192	-2.277574
	H	-3.060834	4.353676	-0.162455		H	-3.981673	3.932462	-0.355873
	H	-4.645936	3.250865	1.376292		H	-5.434672	2.414361	0.939836
	H	-3.888228	1.428312	2.858372		H	-4.449042	0.603439	2.295187
	H	0.530373	3.297612	-0.555884		H	-0.264015	3.552779	-0.635983
	H	0.368192	5.162167	1.106219		H	-0.789782	5.141111	1.253784
	H	0.697434	5.766961	-0.526934		H	-0.495700	5.990659	-0.271945
	H	-0.931891	5.896871	0.157514		H	-2.150914	5.773051	0.322668
	H	-1.145556	3.056901	-2.387095		H	-1.858648	3.354804	-2.576871
	H	-1.802973	4.657325	-2.004175		H	-2.737829	4.769942	-1.980322
	H	-0.138287	4.503235	-2.569875		H	-1.056171	4.929173	-2.483928
	H	-0.446318	-0.052647	2.742142		H	-0.881269	-0.380014	2.226812
	H	-2.617798	-1.221655	2.312806		H	-2.971870	-1.695591	1.880427
	H	-1.917643	-1.582691	3.893809		H	-2.138573	-2.030446	3.397661
	H	-3.292844	-0.480853	3.781092		H	-3.611197	-1.054317	3.415705
	H	-0.309074	1.796284	4.428726		H	-0.785660	1.440132	3.959642
	H	-1.964598	1.445701	4.947473		H	-2.388631	0.963281	4.544062

	H -0.684221 0.245119 5.197336 H -0.581008 -4.490861 -1.595625 H -1.369457 -3.103187 -2.354352 H 1.241168 -3.294804 -2.543235 H 1.275801 -2.884833 -0.835523 H 1.626415 -0.822856 -2.103765 H 0.255968 -1.171217 -3.166651 H -4.316140 0.126850 -3.249866 H -4.474556 -1.621028 -3.418738 H -5.521531 0.137001 -1.150578 H -6.435860 -1.077002 -2.054879 H -5.411775 -2.882745 -0.834497 H -5.273770 -1.651678 0.407842 H -3.956164 -4.479173 0.698707 H -2.636901 -4.019218 1.789311 H -4.098451 -3.028133 1.687161 H -2.027262 -0.117956 -4.264534 H -2.459772 1.296088 -3.308843 H -0.765743 0.850999 -3.492760		H -1.017419 -0.150642 4.700600 H 1.649813 -3.995876 -0.316134 H 0.444810 -4.409360 -1.547487 H 1.948081 -2.985841 -2.784204 H 2.196989 -1.921811 -1.409120 H 0.700080 -0.852020 -3.119024 H -0.354909 -2.269560 -3.072906 H -3.998225 0.206647 -1.786865 H -3.963328 -0.970625 -3.097502 H -5.028840 -1.320274 -0.264485 H -5.779904 -1.878406 -1.765517 H -4.191064 -3.716263 -1.961205 H -4.424248 -3.659397 -0.212475 H -1.042666 -5.482882 -0.137963 H -1.911136 -4.845477 1.248888 H -2.792792 -5.263358 -0.232757 H -1.440944 0.321566 -3.807734 H -2.188362 1.201579 -2.475315 H -0.426641 1.171289 -2.630503
3a	C -1.194708 0.207645 0.145766 C -0.941830 1.467557 -0.295456 C -0.362246 -1.007836 -0.040445 C 0.990895 -1.222768 -0.054499 C 2.049270 -0.226645 0.283894 C 1.722722 1.078819 0.993924 C 1.467195 2.217261 -0.009665 C 0.341641 1.849722 -0.997831 C -1.320899 -2.195416 -0.160048 C -2.741798 -1.612384 -0.036225 C -2.534486 -0.273515 0.696387 C 1.512357 -2.612955 -0.378807 C -1.911943 2.614857 -0.121385 O 3.235215 -0.472272 0.029384 H 2.602033 -2.612332 -0.399533 H 1.152295 -2.966315 -1.351837 H 1.182574 -3.345469 0.368961 H 0.852043 0.962207 1.644964 H 2.384603 2.431651 -0.570185 H 1.210519 3.128444 0.544892 H 0.685117 1.022690 -1.630311 H 0.153213 2.702619 -1.661392 H -2.741332 2.397096 0.552498 H -2.328154 2.916516 -1.092538 H -1.386998 3.494393 0.272382 H -2.461379 -0.444456 1.780246 H -3.358948 0.421210 0.529198 H -3.159854 -1.420387 -1.030814 H -3.428461 -2.284608 0.487363 H -1.172583 -2.746913 -1.095257 H -1.114039 -2.908540 0.649313 H 2.590604 1.324323 1.613320	Ni-IPr	Ni 0.000204 -0.013185 -1.901113 C 0.000182 -0.005250 -0.128024 N 1.084829 0.002072 0.735750 C 0.679331 0.003270 2.069619 C -0.678828 -0.002027 2.069572 N -1.084404 -0.006158 0.735711 C -2.465718 -0.005613 0.323567 C -3.125749 1.230543 0.157327 C -4.475727 1.205042 -0.221915 C -5.144443 -0.002807 -0.424460 C -4.470379 -1.212038 -0.249615 C -3.120198 -1.240522 0.128853 C -2.403657 -2.578590 0.285875 C -2.236505 -3.278083 -1.078546 C -3.104282 -3.498381 1.305873 -2.411943 2.567280 0.336331 -3.119918 3.474400 1.362435 C -2.235745 3.282445 -1.018893 C 2.466094 0.007210 0.323302 C 3.114424 1.245436 0.128447 C 4.464142 1.223645 -0.251997 C 5.143863 0.017739 -0.427835 C 4.481714 -1.193440 -0.223621 C 3.132102 -1.225789 0.156524 C 2.390759 2.579666 0.286417 C 2.202292 3.267873 -1.081149 C 3.095796 3.511979 1.291582 C 2.426361 -2.566252 0.340264 C 3.137495 -3.465025 1.371400 C 2.258164 -3.288212 -1.012387 H -1.384736 -0.002018 2.889251 H 1.385604 0.008217 2.889078

			H -5.011480 2.140694 -0.366536 H -5.002374 -2.146506 -0.414536 H -6.192061 -0.001725 -0.721091 H 5.022495 -2.126321 -0.367357 H 4.991417 2.160649 -0.417508 H 6.191207 0.021842 -0.725411 H 1.422034 -2.368172 0.721938 H 3.237466 -2.961442 2.339328 H 2.565501 -4.386997 1.527154 H 4.141092 -3.753090 1.039697 H 1.700508 -2.658411 -1.714499 H 3.228314 -3.531056 -1.461460 H 1.705416 -4.225750 -0.878705 H 1.392057 2.375821 0.679683 H 1.648047 2.614339 -1.764126 H 1.637589 4.200573 -0.964700 H 3.165659 3.513556 -1.543203 H 3.212533 3.031070 2.269113 H 4.091506 3.809393 0.944775 H 2.509838 4.427515 1.432697 H -1.398962 -2.379326 0.665853 H -1.685796 -2.633502 -1.772735 H -1.676924 -4.213791 -0.961830 H -3.206667 -3.520573 -1.527757 H -3.201079 -3.011670 2.282708 H -4.108477 -3.785367 0.974974 H -2.526917 -4.420024 1.442772 H -1.409645 2.364455 0.720758 H -3.224217 2.975526 2.332339 H -2.543338 4.394022 1.515255 H -4.121479 3.766033 1.027648 H -1.680910 2.645852 -1.717034 H -3.202930 3.530341 -1.471483 H -1.676748 4.216608 -0.887808

Table S12. Frequencies of some stationary points for reaction **d**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

Species	Frequencies (cm^{-1})
COM2d	10 12 14 19 21 23 24 26 29 31 37 39 45 46 48 50 50 55 60 62 64 68 70 73 81 88100 106 115 131 132 139 155 161 173 196 201 205 213 231 234 235 237 240 248 253 255 258 263 270 271 275 280 283 300 307 309 318 320 321 342 366 370 376 376 416 420 421 442 443 456462 484 499 527 530 537 560 587 591 595 622 642 644 645 653 670 676 694 700 707 738 745 755 760 770 776 790 807 815 816 819 821 858 865 895 896 914 920 923 936 937 939 940 942 954 955 967 967 968 969 970 973 975 980 983 988 1047 1048 1050 1051 1058 1059 1063 1073 1079 1082 1082 1087 1097 1107 1126 1127 1129 1130 1134 1141 1141 1153 1157 1173 1175 1185 1188 1197 1201 1202 1203 1213 1217 1223 1242 1249 1254

	1260 1279 1279 1285 1286 1308 1310 1311 1323 1328 1340 1351 1352 1354 1357 1366 1371 1395 1397 1397 1400 1405 1406 1406 1408 1419 1421 1422 1426 1426 1427 1428 1440 1452 1488 1491 1493 1494 1494 1494 1496 1496 1496 1497 1501 1501 1502 1503 1503 1503 1504 1505 1507 1509 1515 1516 1517 1519 1524 1524 1527 1528 1598 1634 1635 1637 1638 1720 2332 2332 3021 3021 3023 3023 3032 3032 3033 3033 3034 3034 3036 3039 3051 3056 3060 3081 3086 3092 3092 3093 3095 3096 3106 3106 3106 3107 3110 3111 3111 3112 3113 3113 3114 3114 3114 3115 3115 3116 3116 3117 3119 3123 3124 3124 3125 3160 3160 3172 3176 3179 3185 3199 3247 3270
TS1d’	**-290i** 15 18 24 26 31 35 38 41 46 47 52 55 58 59 65 68 70 74 78 83 86 98109 117 130 132 139 145 149 151 161 166 175 189 195 212 221 228 231 233 236 242 246 249 251 254 257 262 268 276 280 284288 305 310 311 316 317 318 327 345 372 405 415 421 428 431 444 445 453 477 483 498 527 528 553 560 586 590 600 622 641 644 647 660 668 681 690 718 720 735 738 747 755 774 779 781 815 815 821 823 823 856 866 894 895 920 922 927 933 937 939 940 946 950 954 957 964 965 966 967 969 971 983 989 9901003 1044 1048 1050 1054 1055 1059 1062 1063 1079 1081 1089 1097 1098 1104 1112 1124 1126 1126 1130 1135 1141 1152 1174 1175 1186 1186 1188 1192 1201 1202 1207 1220 1229 1230 1251 1252 1258 1272 1277 1279 1285 1292 1302 1311 1317 1319 1338 1348 1349 1352 1352 1366 1368 1382 1395 1397 1400 1407 1408 1408 1409 1411 1421 1422 1428 1429 1429 1432 1456 1470 1487 1491 1492 14931494 1495 1495 1496 1497 1498 1499 1502 1503 1503 1505 1505 1505 1506 1509 1510 1515 1516 1517 1518 1524 1525 1527 1530 1604 1606 1633 1633 1636 1637 1976 2332 2546 2974 3026 3030 3032 3033 3034 3034 3034 3036 3036 3037 3037 3039 3044 3058 3064 3071 3080 3087 3095 3097 3097 3101 3103 3109 3110 3110 3112 3114 3114 3115 3115 3116 3117 3117 3119 3123 3124 3126 3128 3136 3136 3137 3147 3148 3161 3161 3176 3177 3185 3186 3255 3279
INT1d’	14 18 24 25 31 38 41 46 50 57 58 60 65 67 70 73 75 78 81 85 98 114 116 128 133 142 148 155 161 166 175 195 208 214 224 229236 238 243 245 251 253 253 256 262 268 277 280 286 302 303 308 310 315 316 320 347 361 363 367 384420 421 430 435 445 446 454 478 490 517 525 527 532 556 583 587 592 600 622 631 641 643 646 670 672701 712 727 737 739 755 767 772 777 814 816 821 823 825 835 855 865 894 895 919 922 925 938 939 939 942 942 946 948 951 954 956 964 965 966 967 972 977 978 991 992 1028 1037 1048 1053 1061 1063 1064 1068 1070 1079 1081 1094 1097 1113 1124 1125 1126 1127 1135 1137 1144 1159 1164 1175 1177 1186 1188 1188 1196 1202 1203 1227 1235 1241 1257 1260 1264 1265 1268 1279 1280 1282 1288 1308 1312 1331 1338 1341 1347 1348 1350 1353 1357 1365 1376 1390 1393 1395 1397 1406 1410 1410 1411 1411 1421 1428 1431 1432 1434 1437 1467 1478 1482 1489 1489 1491 1493 1493 1496 1497 1498 1500 1501 1503 1504 1505 1505 1506 1506 1507 1508 1510 1516 1517 1520 1520 1524 1525 1528 1533 1597 1634 1636 1637 1638 1652 2335 2998 3019 3024 3028 3031 3031 3032 3033 3035 3037 3037 3045 3046 3046 3053 3061 3065 3067 3079 3080 3090 3090 3092 3106 3107 3109 3112 3112 3114 3115 3115 3116 3116 3120 3121 3121 3122 3124 3124 3124 3125 3128 3134 3137 3138 3147 3164 3164 3181 3181 3189 3189 3256 3283
COM1d	20 24 26 42 42 46 50 54 66 71 73 80 89 94 108 114 118 125 132 136 141 148 154 162 169 174 185 194 205 218 227 233 234 237 242 252 256 258 263 268 273 282 289 292 302 304 311 314 322 332 338 344 389 403 404 418 420 421 437 443 452 461 477 505 530 533 541 558 572 581 590 606 620 642643 645 656 697 719 737 751 756 769 773 784 813 814 818 820 824 866 886 893 893 913 917 934 934 935 937 942 943 945 961 961 966 967 969 979 983 9851027 1037 1043 1060 1061 1063 1071 1073 1080 1080 1086 1093 1104 1113 1118 1125 1127 1132 1133 1143 1150 1162 1172 1173 1184 1185 1200 1201 1205 1219 1240 1253 1274 1275 1279 1284 1287 1304 1318 1327 1335 1338 1340 1345 1354 1356 1369 1378 1388 1395 1397 1405 1407 1408 1409 1413 1416 1417 1427 1428 1432 1432 1474 1481 1481 1482 1494 1496 1496 1497 1498 1500 1501 1501 1502 1504 1504 1506 1507 1509 1510 1519 1520 1521 1522 1524 1524 1528 1528 1624 1630 1632 1638 1641 2010

	2020 3006 3008 3015 3017 3026 3026 3037 3037 3039 3039 3039 3048 3048 3054 3060 3089 3090 3091 3092 3096 3105 3107 3108 3109 3112 3112 3112 3113 3113 3113 3122 3123 3127 3130 3140 3142 3150 3154 3166 3166 3167 3167 3189 3190 3195 3199 3298 3321
TS1d	**-156i** 17 23 28 36 42 44 49 56 58 66 70 76 84 86 94 98119 120 131 133 155 167 175 176 184 191 196 202 211 213 222 226 232 238 245 251 257 259 265 267 273 281 283 304 305 308 312 317 328 330 390 401 413 421 423 425 440 445 450 462 478489 528 535 555 560 582 590 606 608 611 621 642 643 646 655 697 719 738 756 771 775 797 813 814 819 821 822 843 893 894 909 917 917 918 934 936 936 937 944 946 948 962 964 965 966 968 976 985 9851017 1037 1042 1059 1061 1064 1070 1072 1079 1080 1091 1098 1114 1119 11211125 1126 1132 1134 1140 1147 1160 1172 1174 1185 1186 1200 1201 1202 1215 1247 1255 1274 1275 1278 1281 1297 1308 1328 1332 1335 1339 1341 1344 1345 1348 1358 1369 1393 1396 1398 1406 1407 1407 1408 1410 1411 1421 1428 1429 1429 1432 1482 1486 1488 1490 1492 1495 1496 1497 1499 1500 1501 1501 1502 1503 1506 1506 1507 1508 1509 1517 1518 1521 1522 1523 1524 1527 1528 1619 1632 1632 1637 1639 1748 1833 2994 2996 3007 3010 3027 3028 3035 3035 3037 3038 3046 3046 3047 3069 3070 3073 3077 3092 3094 3096 3101 3103 3103 3106 3107 3107 3111 3112 3113 3113 3122 3122 3125 3126 3132 3132 3141 3142 3162 3163 3164 3166 3182 3183 3190 3191 3283 3306
INT1d	20 25 28 33 39 44 47 51 56 60 68 73 76 80 95 107 112 127 132 140 147 155 164 167 175 177 183 201 215 226 230 234 242 243 249 251 254 256 259 264 270 277 279 297 302 305 311 316 320 321 331 349 412 421 423 431 444 445 452 461 477 527 529 532 555 585 591 599 601 603 622 640 642 646 655 668 700 733 738 754 756 772 778 814 816 821 823 834 855 864 894 895 904 922 923 933 934 936 938 941 949 951 952 962 965 966 967 973 991 992 993 1007 1023 1035 1041 1057 1062 1064 1079 1081 1092 1096 1103 1113 1120 1125 1127 1127 1128 1138 1145 1148 1174 1176 1187 1188 1191 1201 1203 1225 1236 1257 1263 1279 1281 1286 1288 1303 1307 1313 1320 1328 1336 1338 1342 1344 1349 1352 1366 1395 1395 1395 1397 1402 1409 1410 1410 1412 1425 1430 1432 1432 1434 1481 1486 1487 1488 1491 1492 1496 1497 1498 1499 1501 1501 1502 1504 1506 1506 1507 1507 1513 1517 1518 1519 1521 1525 1526 1526 1528 1599 1634 1635 1637 1638 1684 1687 2973 2992 3002 3007 3028 3030 3032 3033 3034 3034 3035 3039 3042 3045 3046 3057 3074 3078 3081 3086 3090 3093 3095 3096 3110 3111 3114 3115 3115 3116 3119 3120 3122 3123 3124 3125 3126 3131 3140 3152 3164 3165 3181 3181 3189 3189 3259 3289
TS1-2d’	**-370i** 3 23 24 34 40 45 46 56 57 59 63 65 68 75 81 88 92 103 108 114 120 131 134 136 151 160 163 169 176 182 202 218 225 226 230 231 240 243 248 251 256 259 268 275 282 286 290 292 298 307 310 312 313 319 338 355 360 389 400 415 419 420 440 442 444 459 470 478 492 526 530 532 553 558 575 582 590 596 602 619 641 641 645 671 688 693 711 736 738 756 769 775 775 778 809 815 816 817 819 834 850 868 893 895 896 910 911916 933 936 937 938 942 947 947 953 957 963 966 967 972 972 973 974 983 988 1012 1023 1027 1036 1054 1058 1062 1066 1067 1081 1083 1089 1096 1107 1109 1117 1122 1125 1127 1128 1138 1148 1151 1170 1171 1176 1186 1186 1199 1202 1204 1206 1210 1219 1231 1250 1255 1259 1261 1262 1280 1281 1284 1296 1304 1315 1316 1328 1332 1335 1340 1345 1351 1351 1359 1367 1391 1393 1394 1399 1408 1408 1409 1409 1410 1422 1429 1430 1431 1432 1473 1475 1481 1484 14861495 1496 1496 1497 1498 1498 1502 1503 1504 1505 1506 1507 1508 1508 1509 1515 1516 1518 1522 15251527 1528 1530 1537 1539 1570 1607 1633 1639 1640 1640 1934 3019 3023 3024 3030 3030 3032 3034 3034 3039 3041 3043 3046 3046 3048 3049 3059 3071 3079 3080 3084 3085 3094 3096 3100 3100 3101 3107 3109 3110 3110 3115 3115 3118 3119 3121 3122 3125 3129 3129 3131 3135 3137 3138 3138 3145 3152 3163 3169 3178 3188 3193 3203 3261 3290
TS1-2d	**-201i** 19 24 31 40 42 46 49 53 56 61 63 72 76 80 82 87 96110 115 124 131 132 137 153 154

	159 167 177 181 194 202 214 218 223 225 232 238 242 244 252 252 254 258 261 268 275 275283 285 299 305 307 312 316 328 331 349 362 400 414 423 433 440 444 452 458 460 464 476 528 532 542 557 582 589 596 605 611 620 641 643 645 646 659 666 702 726 730 737 740 754 755 772 777 815 815 817 821 828 849 856 870 894 895 905 916 919 934 936 937 938 940 942 945 949 953 962 967 968 969 972 976 989 990 995 997 1005 1018 1038 1054 1059 1062 1065 1067 1077 1081 1083 1088 1095 1096 1109 1116 1124 1126 1129 1135 1139 1148 1155 1170 1176 1186 1187 1189 1198 1202 1203 1214 1222 1231 1236 1251 1257 1258 1270 1279 1280 1282 1295 1303 1307 1311 1328 1334 1338 1338 1343 1350 1351 1352 1367 1391 1396 1399 1402 1405 1405 1408 1408 1411 1423 1427 1430 1431 1434 1459 1469 1482 1484 1487 1488 1492 1492 1496 1496 1497 1500 1501 1502 1502 1503 1506 1506 1507 1508 1509 1512 1517 1520 1520 1521 1523 1525 1527 1527 1523 1525 1527 1527 1531 1607 1610 1630 1631 1633 1636 1638 2995 2997 3005 3006 3029 3030 3031 3036 3037 3037 3040 3044 3046 3046 3058 3059 3066 3076 3077 3081 3086 3087 3094 3097 3101 3105 3106 3108 3109 3112 3113 3114 3115 3122 3123 3124 3125 3127 3133 3140 3142 3143 3143 3150 3156 3158 3163 3165 3181 3189 3189 3205 3262 3294
INT2d	13 24 24 30 36 41 45 49 54 58 63 70 73 75 79 84 96 104 123 126 128 128 138 139 159 162 165 174 187 191 198 219 223 226 230 234 242 248 252 255 257 260 263 268 275 279 285291 301 305 309 313 317 323 327 341 342 364 407 419 432 433 440 443 445 458 478 503 528 533 534 557 586 593 595 598 610 623 630 641 642 646 649 668 689 710 731 733 738 755 771 777 779 788 815 816 820 822 830 850 867 887 895 895 918 922 928 935 936 936 939 943 944 950 951 952 965 966 966 968 968 973 979 990 990 991 1011 1024 1036 1041 1062 1063 1065 1066 1072 1079 1082 1093 1096 1098 11151121 1123 1126 1126 1139 1145 1147 1148 1152 1174 1176 1187 1188 1192 1202 1202 1203 1212 1225 1236 1244 1252 1258 1265 1266 1271 1278 1280 1288 1306 1309 1312 1314 1327 1333 1340 1343 1345 1345 1348 1351 1365 1391 1395 1396 1403 1408 1409 1410 1412 1414 1427 1429 1431 1434 1439 1471 1481 1485 1489 1490 1492 1497 1498 1498 1500 1501 1502 1502 1503 1504 1505 1506 1506 1507 1507 1513 1516 1519 1520 1521 1521 1525 1525 1527 1528 1599 1635 1636 1637 1638 1647 1689 3008 3009 3014 3027 3031 3031 3033 3034 3035 3036 3044 3045 3052 3053 3056 3067 3068 3072 3080 3082 3086 3087 3091 3091 3103 3110 3110 3114 3115 3115 3116 3116 3116 3119 3120 3122 3123 3124 3125 3129 3132 3138 3138 3143 3145 3149 3163 3166 3180 3185 3188 3192 3260 3282
TS2-3d	**-218i** 13 20 27 33 36 40 48 53 61 64 71 73 79 83 87 99 112 117 130 132 136 149 156 163 166 170 173 186 204 217 220 220 223 226 231 242 246 259 260 265 269 271 273 277 284 284295 299 303 308 311 313 323 327 333 339 363411 415 422 429 438 440 443 453 461 475 489 522 528 535 558 560582 588 595 612 616 619 637 639 643 646 666 693 703 727 737 738 754 770 772 775 787 815 815 817 819 828 862 877 894 895 913 915 917 933 935 936 939 940 942 947 950 952 958 964 966 968 969 979 984 987 989 997 1013 1018 1023 1040 1042 1063 1064 1067 1081 1082 1083 1092 1096 1098 1117 1120 1122 1125 1128 1134 1142 1143 1148 1154 1170 1172 1173 1186 1187 1200 1203 1203 1209 1222 1237 1246 1259 1259 1264 1270 1279 1280 1286 1304 1308 1311 1317 1320 1327 1331 1339 1342 1343 1348 1351 1354 1368 1391 1395 1398 1405 1406 1406 1408 1409 1412 1425 1427 1428 1429 1429 1454 1484 1485 1486 1488 1490 1495 1497 1497 1498 1499 1502 1503 1503 1504 1506 1506 1508 1508 1509 1514 1517 1518 1518 1521 1521 1524 1525 1526 1531 1609 1610 1634 1635 1637 1638 1660 3000 3010 3012 3016 3023 3030 3030 3033 3034 3034 3040 3041 3043 3047 3049 3059 3072 3074 3084 3086 3090 3098 3098 3099 3100 3107 3108 3109 3112 3112 3113 3115 3120 3123 3123 3126 3126 3127 3128 3129 3130 3132 3148 3150 3151 3153 3163 3164 3185 3187 3196 3203 3263 3288
INT3d	13 19 23 30 34 38 38 42 47 54 59 61 68 68 78 83 89 107 114 120 125 129 130 137 153 158 163 169 178 185 205 210218 220 227 229 234 241 251 252 256 259 263 266 272 278 279286 299 301 307 311 313 321 327 331 355 365 398 417 420 421 434 441 444 457 468

	477 512 528 528 543 551 558 586 587 589 595 621 623 641 643 644 645 669 698 709 728 735 737 753 771776 779 815 816 820 821 821 834 858 878 892 895 897 915 916 918 936 938 939 940 946 950 950 951 954 958 966 967 967 969 974 982 989 9911025 1026 1034 10551060 1062 1065 1070 1080 1082 1083 1091 1096 1103 1110 1121 1124 1124 1128 1129 1139 1145 1148 1154 1173 1175 1187 1188 1196 12021203 1218 1226 1251 1257 1258 1263 1269 1278 1279 1286 1291 1309 13131316 1326 1328 1336 1340 1345 1346 1348 1353 1359 1369 1386 1393 1393 1397 14001406 1408 1409 1410 1410 1426 1430 1430 1433 1436 1475 1479 1486 1489 14921496 1496 1497 1498 1499 15001501 1501 1502 1505 1506 1506 1507 1508 1513 1516 1519 1520 1521 1522 1523 1524 15251526 1528 1567 1604 1633 1634 1636 1637 1638 1675 2987 2997 3001 3016 3017 3023 3032 3032 3033 3033 3041 3041 3043 3044 3048 3060 3062 3075 3089 3091 3091 3092 3093 3102 3102 3110 3111 3112 3113 3113 3116 3119 3119 3120 3120 3122 3123 3124 3124 3125 3133 3138 3153 3153 3157 3160 3165 3165 3185 3186 3193 3194 3261 3285
TS3d	**-249i** 21 25 34 36 43 46 50 56 58 60 63 68 70 81 84 94 100 112 116 130 133 135 153 156 160 167 173 177 205 212 224 226 226 234 235 238 243 251 253 255 260 266 271 276 281 284287 300 301 307 311 313 326 332 334 341 385 397 414 419 423 434 442 445 453 459 476 499 514 528 530 533 559 583 586 590 596 619 621 626 640 643 644 666 682 698 728 736 747 754 771776 788 804 814 815 818 820 828 848 871 880 894 895 904 914 915 935 936 937 938 945 946 948 950 955 964 966 969 969 971 987 988 9881010 1025 1035 1042 1052 1062 1064 1065 1067 1081 1083 1087 1088 1095 1106 11191122 1125 1127 1134 1138 1145 1149 1158 1168 1171 1174 1186 1186 1201 1202 1205 1220 1225 1255 12591261 1270 1274 1276 1277 1282 1284 1302 1308 1320 1322 1330 1333 1335 1342 1344 1345 1351 13511359 1371 1396 1396 1398 1406 1407 1408 1408 1411 1414 1422 1425 1429 1429 1430 1432 1468 1484 14851490 1490 1493 1496 1496 1498 1499 1500 1501 1501 1502 1504 1505 1507 1507 1508 15121513 1517 1518 1519 1520 1523 1524 1525 1527 1528 1553 1609 1631 1633 1636 1637 1666 2994 2995 30083010 3012 3028 3031 3032 3036 3037 3038 3041 3042 3046 3047 3073 3076 3081 3087 3090 3092 3095 30953098 3103 3106 3107 3108 3112 3112 3113 3117 3119 3120 3121 3124 3126 3127 3129 3134 3135 3136 31433148 3154 3156 3163 3164 3185 3185 3192 3203 3263 3290
3a	57 84 101 118 130 146 169 205 258 289 307 338 362 372 418 447 480 531 569 590 614 635 670 768 783 819 855 864 891 916 944 973 9841014 1030 1038 1042 1048 1067 1082 1097 1134 11491157 1194 1208 1224 1259 1273 1293 13081324 1332 1347 1355 1376 1381 1409 1419 1476 1491 1496 1497 1500 1507 1511 1516 1517 1518 16121676 1687 3021 3023 3029 3032 3037 3043 3055 3071 3082 3083 3086 3093 3099 3115 3132 3133 3162 3168
Ni-IPr	17 23 35 40 45 47 48 54 54 62 77 82 116 128 128 141 158 178 210 235 236 240 241 244 248 249 252 253 268 273 274 289 301 305 313 317 317 375 411 418 419 443 443 460 481 526 526 560 587 590 593 623 643 643 643 652 665 709 737 754 770 775 815 815 819 819 821 894 895 914 914 935935 936 937 940 951 952 966 967 967 968 979 987 987 1057 1062 1077 1079 1087 1097 1118 1126 1127 1128 1129 1133 1139 1173 1175 1185 1186 1201 1202 1219 1249 1257 1279 1279 1285 1308 1309 1317 1338 1347 1348 1349 1349 1362 1389 1392 1396 1404 1405 1406 1407 1418 1426 1426 1427 1428 1491 1494 1495 1496 1499 1499 1500 1501 1503 1503 1507 1507 1516 1516 1517 1518 1522 1523 1524 1525 1599 1633 1634 1636 1637 3023 3023 3024 3024 3034 3034 3034 3034 3093 3094 3094 3094 3108 3108 3109 3109 3112 3112 3113 3113 3116 3116 3117 3117 3124 3125 3125 3125 3162 3162 3179 3179 3187 3187 3248 3271

Table S13. Some optimized Cartesian Coordinates of stationary points for reaction **e**.

Species	Cartesian coordinates			Species	Cartesian coordinates		
1c	C	0.685983	0.001888 -0.000948	COM1e	Ni	-0.209888	1.354199 -0.543123
	C	-0.465490	1.028050 -0.000953		C	0.052964	-0.372463 0.268223
	C	-1.796705	0.402780 -0.000719		N	-0.940051	-1.278465 0.592808
	C	-2.889997	-0.127079 0.000274		C	-0.439589	-2.356567 1.323112
	C	-4.215313	-0.761370 0.000567		C	0.886841	-2.140349 1.479807
	C	2.061985	0.699580 0.001451		N	1.185973	-0.947419 0.817420
	C	3.186892	-0.246001 0.000735		C	2.546550	-0.469847 0.684909
	C	4.105584	-1.038689 -0.000557		C	3.462632	-1.226913 -0.090495
	H	4.921050	-1.735716 -0.001045		C	4.781136	-0.757908 -0.187013
	H	-4.791555	-0.468722 -0.883840		C	5.186359	0.408055 0.460776
	H	-4.789434	-0.472613 0.887633		C	4.277267	1.115038 1.244477
	H	-4.127127	-1.853226 -0.001917		C	2.947418	0.690337 1.384510
	H	-0.375550	1.680808 -0.879623		C	3.110483	-2.557936 -0.762507
	H	-0.375446	1.680912 0.877642		C	3.674038	-3.746099 0.052044
	H	0.601574	-0.645202 0.878122		C	3.609565	-2.673516 -2.217802
	H	0.603434	-0.643140 -0.881714		C	2.029235	1.440398 2.345612
	H	2.146938	1.349224 0.882315		C	2.042690	2.962490 2.114672
	H	2.148476	1.352723 -0.876668		C	2.388630	1.095607 3.807799
					C	-2.337052	-1.187908 0.226938
					C	-3.296008	-0.918788 1.232473
					C	-4.648482	-0.904881 0.861634
					C	-5.041636	-1.146389 -0.453594
					C	-4.080011	-1.419663 -1.424223
					C	-2.713987	-1.454433 -1.108365
					C	-2.931362	-0.674356 2.697197
					C	-3.215526	-1.921136 3.565219
					C	-3.664275	0.543316 3.300445
					C	-1.713642	-1.842615 -2.193919
					C	-1.883184	-1.006218 -3.475940
					C	-1.801536	-3.353983 -2.497874
					C	-1.253963	2.098733 0.925778
					C	-1.191237	2.974234 0.016195
					C	-1.466537	4.307264 -0.579033
					C	-1.457437	4.297153 -2.116105
					C	-0.127503	3.753692 -2.661937
					C	0.200605	2.394053 -2.155765
					C	0.749972	1.256665 -2.251744
					C	1.604367	0.338096 -3.044963
					H	-1.591879	1.804078 1.904559
					H	1.634128	-2.719264 2.000235
					H	-1.062273	-3.175223 1.652060
					H	5.505335	-1.314191 -0.777085
					H	4.610932	2.007171 1.768737
					H	6.213411	0.756417 0.365515
					H	-5.408260	-0.698575 1.611497
					H	-4.398615	-1.621105 -2.444350
					H	-6.097104	-1.127134 -0.719919
					H	-1.857662	-0.473031 2.750014
					H	-2.680034	-2.805154 3.206687

			H -2.910717 -1.741746 4.602871 H -4.285163 -2.159813 3.565787 H -4.730517 0.341431 3.448832 H -3.241929 0.784334 4.282672 H -3.580361 1.428071 2.663690 H -0.710446 -1.638535 -1.817773 H -1.781846 0.060086 -3.255824 H -1.110361 -1.277253 -4.204450 H -2.854117 -1.175628 -3.954850 H -1.631788 -3.953815 -1.596790 H -2.785513 -3.624022 -2.898475 H -1.047411 -3.639000 -3.241041 H 1.006156 1.110028 2.168149 H 1.784119 3.196774 1.078408 H 1.299096 3.442448 2.760259 H 3.017029 3.407791 2.346110 H 2.324185 0.017286 3.992090 H 3.406987 1.416273 4.056498 H 1.700488 1.598250 4.497822 H 2.021810 -2.654583 -0.786173 H 3.339990 -3.734554 1.093336 H 3.359684 -4.697603 -0.392419 H 4.769610 -3.724580 0.060205 H 3.263119 -1.845091 -2.837735 H 4.702832 -2.704085 -2.274692 H 3.238316 -3.605238 -2.659468 H -2.433459 4.675829 -0.212540 H -0.704872 5.016082 -0.222780 H -2.282697 3.673498 -2.479687 H -1.624046 5.314388 -2.491171 H -0.156156 3.736263 -3.759968 H 0.679823 4.446142 -2.381540 H 2.605645 0.278200 -2.605098 H 1.200958 -0.679372 -3.067138 H 1.712269 0.682400 -4.082495
TS1e	Ni -0.140854 1.246488 -0.221822 C 0.063610 -0.537728 0.190135 N -0.935523 -1.481122 0.310041 C -0.428199 -2.713215 0.724845 C 0.907669 -2.554501 0.883014 N 1.202317 -1.232269 0.542978 C 2.549416 -0.710690 0.531263 C 3.424820 -1.119937 -0.501496 C 4.740405 -0.634100 -0.472827 C 5.172474 0.220237 0.540929 C 4.294095 0.595922 1.556572 C 2.968896 0.137097 1.579652 C 3.014104 -2.102953 -1.598464 C 3.610966 -3.503421 -1.332375 C 3.402584 -1.630782 -3.012758 C 2.064160 0.500749 2.754087	INT1e	Ni 0.414522 1.042258 -0.138553 C 0.005877 -0.867856 0.055508 N 1.089582 -1.701122 0.174849 C 0.714557 -3.035398 0.289485 C -0.644102 -3.051314 0.241252 N -1.059369 -1.726722 0.099785 C -2.453087 -1.352708 0.015930 C -3.166241 -1.134199 1.212734 C -4.519970 -0.784465 1.105275 C -5.134216 -0.660363 -0.141501 C -4.404726 -0.887741 -1.308254 C -3.048396 -1.241848 -1.257675 C -2.511963 -1.229767 2.589071 C -3.253044 -2.213797 3.516816 C -2.379885 0.163679 3.239475 C -2.267477 -1.452592 -2.552204

C	2.098270	2.002932	3.090026	C	-2.032045	-0.111405	-3.278514
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C	-2.342411	-1.261415	0.066444	C	2.447738	-1.206668	0.169876
C	-3.205349	-1.091152	1.172345	C	3.136167	-1.126134	-1.060838
C	-4.577612	-0.959010	0.915717	C	4.452828	-0.643019	-1.036617
C	-5.074094	-0.983421	-0.387472	C	5.054088	-0.253941	0.160281
C	-4.200702	-1.144194	-1.462140	C	4.348907	-0.337507	1.360789
C	-2.819857	-1.289018	-1.260987	C	3.031303	-0.816038	1.395784
C	-2.701469	-1.071064	2.613968	C	2.497273	-1.523571	-2.389149
C	-2.970416	-2.416437	3.323392	C	3.299319	-2.629256	-3.104813
C	-3.305201	0.085551	3.435858	C	2.298739	-0.294290	-3.300167
C	-1.905172	-1.518041	-2.461446	C	2.281424	-0.882100	2.723414
C	-2.109055	-0.456848	-3.558861	C	2.018936	0.531165	3.285788
C	-2.085184	-2.944119	-3.024476	C	3.011988	-1.769910	3.751326
C	-0.983435	2.177022	1.194541	C	-1.270917	1.911025	-0.092888
C	-0.846773	3.137214	0.322407	C	-1.170151	3.245527	-0.223570
C	-1.166830	4.609911	0.259379	C	0.200168	3.778509	-0.352350
C	-1.328952	5.028977	-1.203612	C	1.163911	2.832412	-0.328207
C	-0.163424	4.349531	-1.925233	C	-2.160364	4.398335	-0.237202
C	-0.035069	2.930058	-1.433116	C	-1.272688	5.616442	0.145647
C	0.460030	1.825298	-1.927375	C	0.134911	5.296540	-0.434080
C	1.127316	1.541034	-3.233648	C	2.642437	3.125312	-0.433213
H	-1.411796	2.201524	2.191390	H	-2.203906	1.360232	0.031789
H	1.666539	-3.252878	1.204146	H	-1.345848	-3.873108	0.292631
H	-1.056875	-3.581073	0.863457	H	1.432266	-3.838371	0.393255
H	5.439916	-0.928918	-1.251386	H	-5.100704	-0.597303	2.005715
H	4.649096	1.249234	2.349872	H	-4.896678	-0.780408	-2.272458
H	6.197448	0.587484	0.543428	H	-6.184713	-0.380997	-0.203570
H	-5.268918	-0.829839	1.745152	H	5.013190	-0.563079	-1.965468
H	-4.600271	-1.164491	-2.473362	H	4.829292	-0.018192	2.283065
H	-6.143073	-0.877441	-0.565001	H	6.075098	0.124118	0.156408
H	-1.619887	-0.916399	2.586901	H	1.504633	-1.930875	-2.181085
H	-2.502207	-3.255382	2.799475	H	3.422268	-3.510462	-2.465427
H	-2.574214	-2.396159	4.345452	H	2.778678	-2.942737	-4.016898
H	-4.046023	-2.619002	3.383515	H	4.297436	-2.285319	-3.395494
H	-4.369536	-0.071246	3.642989	H	3.257762	0.162638	-3.569976
H	-2.795240	0.162781	4.402934	H	1.794801	-0.587772	-4.228012
H	-3.200954	1.041050	2.915272	H	1.687424	0.469168	-2.806673
H	-0.872420	-1.423427	-2.120893	H	1.306122	-1.338936	2.540310
H	-1.955121	0.548836	-3.156987	H	1.462968	1.144792	2.568927
H	-1.389513	-0.613812	-4.370733	H	1.431131	0.466277	4.208566
H	-3.111403	-0.507004	-3.998512	H	2.955758	1.048673	3.521577
H	-1.897506	-3.703672	-2.257532	H	3.175969	-2.780559	3.362386
H	-3.101861	-3.097417	-3.404686	H	3.987859	-1.355129	4.027306
H	-1.387851	-3.119845	-3.852100	H	2.417767	-1.851608	4.668315
H	1.035916	0.269889	2.472393	H	-1.284350	-1.855026	-2.292591
H	1.839727	2.602454	2.212875	H	-1.512120	0.603176	-2.633119
H	1.365502	2.224435	3.874270	H	-1.426665	-0.270692	-4.179038
H	3.078885	2.323388	3.459910	H	-2.981268	0.340505	-3.588924
H	2.345305	-1.423218	3.776670	H	-3.103899	-3.437605	-2.974082
H	3.441995	-0.149463	4.333399	H	-3.912895	-2.126839	-3.846602
H	1.738078	-0.125160	4.820347	H	-2.311175	-2.663896	-4.358835

	H	1.925234	-2.198148	-1.579901		H	-1.498293	-1.616713	2.458336
	H	3.326001	-3.890510	-0.349157		H	-3.333429	-3.208456	3.063840
	H	3.264994	-4.217569	-2.088735		H	-2.713975	-2.316200	4.465538
	H	4.705922	-3.475930	-1.371540		H	-4.266502	-1.870610	3.750880
	H	3.004474	-0.636453	-3.225127		H	-1.806856	0.843410	2.601507
	H	4.488787	-1.599492	-3.151417		H	-3.363069	0.613676	3.419503
	H	3.000596	-2.325289	-3.759488		H	-1.867497	0.082295	4.205366
	H	-2.059951	4.812553	0.859728		H	0.935918	5.809081	0.111738
	H	-0.338058	5.177799	0.706421		H	0.192766	5.638992	-1.478705
	H	2.212030	1.458184	-3.089600		H	-1.204681	5.679482	1.238814
	H	0.794871	0.589748	-3.663293		H	-1.679230	6.568911	-0.213683
	H	0.954876	2.330016	-3.981140		H	-3.012875	4.260226	0.436649
	H	-2.283747	4.660267	-1.597316		H	-2.565645	4.537035	-1.250198
	H	-1.309832	6.117725	-1.323010		H	3.043693	2.825695	-1.413747
	H	-0.285434	4.347896	-3.014977		H	2.875169	4.193522	-0.301828
	H	0.764452	4.898309	-1.706317		H	3.227076	2.565513	0.311253
TSee’	Ni	-0.477918	1.051475	-0.072379	INT1e’	Ni	0.615444	1.025776	-0.436766
	C	0.239945	-0.880433	0.041681		C	-0.145869	-0.754304	0.031121
	N	1.459150	-1.497842	0.106435		N	-1.356166	-1.402200	-0.043588
	C	1.333323	-2.883295	0.195933		C	-1.204150	-2.781283	0.084854
	C	0.000977	-3.152820	0.186722		C	0.121897	-3.019372	0.259623
	N	-0.646448	-1.924601	0.092884		N	0.747216	-1.778737	0.225184
	C	-2.083372	-1.765334	0.053066		C	2.181304	-1.596384	0.302489
	C	-2.782700	-1.623921	1.270119		C	-2.593961	-1.314580	-3.848706
	C	-4.176182	-1.480401	1.202762		C	-0.156703	2.370271	0.692276
	C	-4.841338	-1.475845	-0.023447		C	0.416236	3.576008	0.508539
	C	-4.122937	-1.610980	-1.211514		C	1.456756	3.636509	-0.534795
	C	-2.728391	-1.758062	-1.201763		C	1.675997	2.463501	-1.163689
	C	-2.080827	-1.592107	2.625415		C	0.220982	4.959741	1.110860
	C	-2.593070	-2.700511	3.567432		C	0.836377	5.891236	0.026361
	C	-2.201732	-0.199538	3.278865		C	1.976984	5.061500	-0.625475
	C	-1.967674	-1.869923	-2.520077		C	-1.253484	2.040623	1.659430
	C	-2.042479	-0.548515	-3.313634		C	2.945053	-1.770037	-0.872077
	C	-2.450761	-3.063542	-3.368492		C	4.335256	-1.615185	-0.770194
	C	2.733593	-0.817863	0.092035		C	4.936597	-1.300343	0.448107
	C	3.373873	-0.612043	-1.147728		C	4.156069	-1.132733	1.592031
	C	4.608849	0.052393	-1.133940		C	2.762482	-1.277371	1.547257
	C	5.181821	0.481498	0.063691		C	2.318807	-2.097925	-2.226639
	C	4.531941	0.250220	1.276356		C	2.866071	-3.416850	-2.808767
	C	3.294073	-0.408298	1.319509		C	2.496350	-0.933727	-3.223298
	C	2.757590	-1.060006	-2.471658		C	1.938536	-1.069698	2.813856
	C	3.740989	-1.881640	-3.328204		C	2.043920	0.387812	3.308646
	C	2.198121	0.140630	-3.263362		C	2.327279	-2.069981	3.921601
	C	2.593461	-0.633484	2.657743		C	-2.645461	-0.783893	-0.270027
	C	2.040874	0.689192	3.229027		C	-3.574411	-0.739139	0.796301
	C	3.503306	-1.345141	3.679017		C	-4.830101	-0.170295	0.540686
	C	-2.078261	2.070716	-0.088148		C	-5.148766	0.343019	-0.716513
	C	-1.926757	3.401999	-0.220960		C	-4.218180	0.277506	-1.751613
	C	-0.514602	3.810628	-0.302450		C	-2.952371	-0.297128	-1.559020
	C	0.350496	2.778002	-0.232144		C	-3.279517	-1.304510	2.186567
	C	-2.808295	4.636164	-0.276373		C	-4.018961	-2.642939	2.408826

	C	-1.825610	5.776559	0.118215		C	-3.628632	-0.321822	3.322954
	C	-0.430443	5.324074	-0.406757		C	-2.001453	-0.407864	-2.749011
	C	1.851026	2.871072	-0.277680		C	-1.616978	0.975554	-3.310759
	H	-3.046538	1.560221	0.005503		H	0.666032	-3.943840	0.398958
	H	-0.535370	-4.091057	0.237537		H	-2.039463	-3.464050	0.026888
	H	2.190917	-3.540083	0.256981		H	4.956284	-1.735557	-1.655162
	H	-4.748827	-1.360424	2.119559		H	4.638964	-0.878553	2.532920
	H	-4.654692	-1.591070	-2.160047		H	6.017153	-1.181102	0.505401
	H	-5.923253	-1.358505	-0.053765		H	-5.568512	-0.119361	1.337254
	H	5.129535	0.241691	-2.069930		H	-4.483015	0.671355	-2.730249
	H	4.992506	0.592450	2.200339		H	-6.126311	0.789540	-0.890117
	H	6.139640	0.998836	0.051751		H	-2.206300	-1.503647	2.253617
	H	1.911187	-1.714192	-2.246569		H	-3.770149	-3.383262	1.641744
	H	4.136035	-2.739476	-2.772964		H	-3.755520	-3.067068	3.384508
	H	3.232496	-2.261243	-4.221627		H	-5.105043	-2.498738	2.387435
	H	4.591878	-1.281336	-3.667766		H	-4.707390	-0.145521	3.392219
	H	2.992133	0.849397	-3.525442		H	-3.305717	-0.738222	4.283910
	H	1.735060	-0.203437	-4.195675		H	-3.136298	0.644100	3.188562
	H	1.439064	0.677005	-2.685829		H	-1.078219	-0.881228	-2.407476
	H	1.736694	-1.290075	2.485586		H	-1.134095	1.593161	-2.546220
	H	1.329680	1.154315	2.539035		H	-0.914927	0.860645	-4.144675
	H	1.522154	0.504327	4.176993		H	-2.493706	1.514719	-3.687501
	H	2.847107	1.406074	3.422799		H	-2.850290	-2.305141	-3.456640
	H	3.896236	-2.286129	3.278465		H	-3.501622	-0.882824	-4.284745
	H	4.356545	-0.724024	3.972474		H	-1.868607	-1.447799	-4.659598
	H	2.937738	-1.574453	4.589251		H	0.889135	-1.251490	2.569149
	H	-0.913742	-2.046363	-2.291161		H	1.749655	1.092269	2.524432
	H	-1.669896	0.291328	-2.717639		H	1.389959	0.540986	4.175214
	H	-1.438790	-0.620108	-4.226022		H	3.067292	0.629880	3.617755
	H	-3.072369	-0.319974	-3.610766		H	2.225086	-3.106200	3.580204
	H	-2.379253	-4.005174	-2.812857		H	3.361956	-1.927923	4.252606
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	H	-1.837826	-3.155956	-4.272312		H	1.243829	-2.235612	-2.084451
	H	-1.016220	-1.777873	2.461803		H	2.716705	-4.252208	-2.115946
	H	-2.488873	-3.692360	3.113678		H	2.353183	-3.658671	-3.746577
	H	-2.022061	-2.694376	4.502917		H	3.937701	-3.350977	-3.025348
	H	-3.648483	-2.560066	3.825127		H	2.062888	-0.005521	-2.836548
	H	-1.804498	0.581746	2.622380		H	3.554507	-0.742513	-3.433189
	H	-3.246097	0.046511	3.502092		H	2.003672	-1.169237	-4.173754
	H	-1.643512	-0.175002	4.222120		H	-1.533443	2.920503	2.257387
	H	0.394278	5.772068	0.159498		H	-0.953580	1.247978	2.358264
	H	-0.307494	5.637645	-1.454311		H	-2.155815	1.684855	1.147561
	H	-1.787267	5.853031	1.211943		H	-0.821687	5.210918	1.335589
	H	-2.129092	6.756428	-0.268335		H	0.785930	5.056695	2.050045
	H	-3.686601	4.587318	0.377216		H	0.073276	6.110639	-0.730760
	H	-3.175721	4.800630	-1.300278		H	1.179096	6.849214	0.434615
	H	2.265332	2.426779	-1.192529		H	2.207695	5.385119	-1.646893
	H	2.182347	3.919855	-0.244060		H	2.898964	5.172536	-0.035060
	H	2.329153	2.346112	0.558730		H	2.417398	2.386467	-1.973618
TS1-2e	Ni	-0.267628	0.722221	-0.548589	TS1-2e’	Ni	0.642926	0.827276	-0.141418
	C	0.162996	-0.914804	0.392854		C	-0.570312	-0.674796	0.330204

N	-0.741841	-1.903552	0.675490	N	0.014227	-1.748522	0.955769
C	-0.150066	-2.958993	1.366079	C	-0.928698	-2.664830	1.411299
C	1.156256	-2.628265	1.530862	C	-2.142214	-2.169184	1.066104
N	1.334413	-1.381846	0.929835	N	-1.915376	-0.961915	0.402042
C	-2.119859	-1.908300	0.234382	C	1.438190	-1.929267	1.153175
C	-2.408317	-2.393916	-1.058621	C	2.020901	-1.471093	2.354850
C	-3.752417	-2.410601	-1.460490	C	3.388520	-1.717221	2.545973
C	-4.765410	-1.978002	-0.605879	C	4.141196	-2.393915	1.586847
C	-4.452735	-1.521020	0.674746	C	3.537419	-2.841660	0.412145
C	-3.125534	-1.473380	1.123792	C	2.174855	-2.621044	0.168329
C	-1.335822	-2.932636	-2.003083	C	1.214198	-0.776624	3.450137
C	-1.278376	-2.146208	-3.327278	C	1.893284	0.505037	3.967705
C	-1.532363	-4.442291	-2.258510	C	0.923943	-1.749291	4.614153
C	-2.818477	-1.003544	2.543474	C	1.536571	-3.162251	-1.107858
C	-3.175767	-2.096803	3.574002	C	1.371803	-4.695650	-1.034497
C	-3.516887	0.324142	2.892966	C	2.312857	-2.751665	-2.373729
C	2.627870	-0.734138	0.848409	C	-3.014399	-0.167763	-0.115527
C	3.475705	-1.056651	-0.234432	C	-3.478928	0.931938	0.643002
C	4.741310	-0.452783	-0.267337	C	-4.558343	1.665250	0.128961
C	5.148938	0.426507	0.735701	C	-5.171139	1.308592	-1.071927
C	4.299084	0.711068	1.803959	C	-4.725668	0.191828	-1.776000
C	3.023096	0.134455	1.888304	C	-3.645561	-0.576259	-1.314327
C	3.096152	-2.076459	-1.306154	C	-2.904678	1.276143	2.016003
C	3.792552	-3.428515	-1.033897	C	-3.638427	0.480355	3.119784
C	3.396010	-1.592262	-2.737039	C	-2.944379	2.778981	2.342877
C	2.146960	0.408072	3.108171	C	-3.254664	-1.843537	-2.076644
C	2.076973	1.902874	3.474007	C	-3.234096	-1.660530	-3.607972
C	2.622721	-0.425425	4.318467	C	-4.203929	-3.011662	-1.721813
C	-0.732003	1.747310	0.994176	C	0.824046	0.694559	-2.052855
C	-1.228453	2.974241	0.693328	C	1.931639	1.316965	-2.540380
C	-1.580966	3.164404	-0.709505	C	2.840347	1.822862	-1.523587
C	-1.140566	2.219171	-1.587044	C	2.357594	1.790529	-0.254581
C	-1.732707	4.154770	1.501712	C	2.553417	1.509475	-3.914991
C	-2.936043	4.646581	0.648243	C	4.073198	1.568641	-3.581735
C	-2.559953	4.324627	-0.827027	C	4.163000	2.206574	-2.166557
C	-1.827368	1.976342	-2.914586	C	-0.250862	0.124525	-2.933461
C	0.963325	1.806955	-2.096725	C	0.669912	3.013025	0.803813
C	1.886228	2.680447	-1.207163	C	0.085490	3.885804	-0.328573
C	1.882964	3.764446	-2.324613	C	1.166911	4.958854	0.004686
C	1.131833	2.795944	-3.283012	C	1.565346	4.169735	1.288163
O	0.922864	0.529178	-2.178322	O	0.175331	2.058313	1.463215
H	-0.529468	1.484194	2.037808	H	3.011236	1.966604	0.605299
H	-0.700879	-3.839549	1.666013	H	-0.655273	-3.571558	1.932312
H	1.964298	-3.160693	2.012206	H	-3.134734	-2.557429	1.239138
H	-5.254848	-1.194735	1.332471	H	4.135960	-3.371147	-0.325450
H	-4.011216	-2.772025	-2.453352	H	3.872536	-1.378947	3.458872
H	-5.802570	-2.001265	-0.936308	H	5.201371	-2.574983	1.756326
H	5.421016	-0.675923	-1.086111	H	-4.933216	2.523566	0.679143
H	4.636355	1.387543	2.585439	H	-5.227700	-0.089268	-2.698082
H	6.135253	0.885301	0.688749	H	-6.006424	1.894374	-1.452153
H	2.017694	-2.239313	-1.249673	H	-1.853266	0.988906	2.023519
H	3.552662	-3.817084	-0.038462	H	-3.549083	-0.600379	2.973380

	H	3.477670	-4.175571	-1.771849		H	-3.216732	0.719367	4.103164
	H	4.882319	-3.329923	-1.099598		H	-4.705959	0.730331	3.140504
	H	2.883405	-0.649167	-2.937723		H	-2.501898	3.374219	1.539782
	H	4.470239	-1.464124	-2.912449		H	-3.963676	3.141146	2.520963
	H	3.037248	-2.335363	-3.458902		H	-2.366986	2.968221	3.253599
	H	1.130182	0.088243	2.869697		H	-2.245674	-2.128457	-1.765861
	H	1.758243	2.505372	2.619031		H	-2.646238	-0.791525	-3.910460
	H	1.353042	2.054412	4.282729		H	-2.794969	-2.547074	-4.079050
	H	3.041458	2.284491	3.826455		H	-4.243954	-1.547005	-4.016976
	H	2.623646	-1.497493	4.094746		H	-4.216303	-3.225774	-0.649516
	H	3.640091	-0.145394	4.614895		H	-5.231529	-2.783028	-2.026440
	H	1.963689	-0.261201	5.179010		H	-3.893705	-3.925117	-2.242373
	H	-0.362659	-2.812478	-1.522007		H	0.255212	-0.472226	3.024934
	H	-1.044453	-1.093909	-3.148224		H	2.082031	1.202017	3.148247
	H	-0.493567	-2.557260	-3.972841		H	1.236227	1.006605	4.687123
	H	-2.225523	-2.207597	-3.875030		H	2.838551	0.292515	4.479518
	H	-1.544842	-5.009302	-1.321049		H	0.394329	-2.644402	4.270600
	H	-2.473537	-4.643245	-2.782321		H	1.852118	-2.075852	5.097373
	H	-0.716820	-4.831262	-2.879030		H	0.302735	-1.261228	5.374204
	H	-1.742586	-0.824985	2.611588		H	0.537537	-2.728439	-1.193689
	H	-2.644538	-3.033022	3.371435		H	0.779598	-4.996105	-0.163172
	H	-2.909478	-1.770462	4.586133		H	0.865668	-5.069487	-1.932279
	H	-4.249961	-2.314514	3.562907		H	2.344623	-5.195973	-0.965297
	H	-3.269108	1.099157	2.162781		H	2.422967	-1.665067	-2.427336
	H	-4.606531	0.215950	2.932633		H	3.310066	-3.204730	-2.406320
	H	-3.188697	0.668177	3.880757		H	1.773659	-3.087783	-3.267177
	H	-2.014977	3.901071	2.529215		H	-1.226468	0.558881	-2.679471
	H	-0.967894	4.943868	1.556682		H	-0.354336	-0.959703	-2.795039
	H	-2.062568	5.186913	-1.296207		H	-0.069847	0.310606	-4.002171
	H	-3.439991	4.099745	-1.440431		H	2.314987	0.717158	-4.632992
	H	1.492262	2.972680	-0.231648		H	2.233502	2.461095	-4.365902
	H	2.851791	2.180491	-1.066265		H	4.237864	3.301208	-2.247018
	H	1.789982	2.328784	-4.027110		H	5.040072	1.869264	-1.602412
	H	0.247193	3.175410	-3.792753		H	0.091664	3.455073	-1.332316
	H	-3.827521	4.071139	0.925385		H	-0.936798	4.198846	-0.079588
	H	-3.169206	5.705746	0.805708		H	1.125391	4.591464	2.202440
	H	1.290271	4.643545	-2.060774		H	2.624290	3.975446	1.469025
	H	2.868488	4.090318	-2.669314		H	4.468135	0.546268	-3.540862
	H	-1.228215	1.353811	-3.587008		H	4.654502	2.113922	-4.334138
	H	-2.774910	1.442975	-2.751456		H	1.968068	4.987350	-0.736274
	H	-2.074551	2.905528	-3.448223		H	0.793291	5.972479	0.172473
INT2e	Ni	-0.250692	0.741837	-0.037077	INT2e’	Ni	-0.100387	0.939766	-0.184804
	C	-0.500377	-1.128152	0.213786		C	-0.589456	-0.831466	0.339735
	N	0.327174	-2.176934	0.524604		N	0.152218	-1.822707	0.934231
	C	-0.403854	-3.314822	0.860341		C	-0.663081	-2.811187	1.478267
	C	-1.718484	-2.987740	0.751444		C	-1.946397	-2.451210	1.216869
	N	-1.759670	-1.656175	0.352880		N	-1.887892	-1.251306	0.514755
	C	-2.978165	-0.915260	0.109473		C	-3.063744	-0.524977	0.080231
	C	-3.579774	-0.222093	1.180778		C	-3.549864	0.527303	0.886319
	C	-4.775353	0.463027	0.917970		C	-4.710646	1.188533	0.458970
	C	-5.340459	0.463371	-0.356512		C	-5.364618	0.814655	-0.713773

C	-4.717119	-0.221587	-1.400178	C	-4.870602	-0.237576	-1.484970
C	-3.523603	-0.926368	-1.192080	C	-3.712048	-0.931394	-1.107339
C	-2.982840	-0.187405	2.585493	C	-2.903067	0.928863	2.210869
C	-3.897029	-0.899101	3.604416	C	-3.747938	0.425404	3.401607
C	-2.663090	1.254686	3.033010	C	-2.647897	2.445846	2.312263
C	-2.845774	-1.635188	-2.361097	C	-3.226262	-2.110289	-1.948391
C	-2.282049	-0.610143	-3.367765	C	-3.186668	-1.796497	-3.456731
C	-3.781764	-2.646162	-3.053001	C	-4.088848	-3.365180	-1.688149
C	1.773519	-2.140954	0.564665	C	1.593421	-1.836979	1.072654
C	2.492224	-2.728586	-0.499281	C	2.347247	-2.659277	0.208262
C	3.891830	-2.725077	-0.417133	C	3.737021	-2.691771	0.390589
C	4.547731	-2.154669	0.673914	C	4.350672	-1.935691	1.389244
C	3.811826	-1.583089	1.710858	C	3.579622	-1.142992	2.238095
C	2.409589	-1.567766	1.684926	C	2.184440	-1.082176	2.107708
C	1.807077	-3.379226	-1.700478	C	1.706294	-3.529892	-0.870431
C	1.924449	-4.917748	-1.641416	C	1.706569	-5.017240	-0.454617
C	2.341571	-2.852903	-3.047645	C	2.376199	-3.356953	-2.247219
C	1.644614	-0.963671	2.859637	C	1.374977	-0.257856	3.105753
C	1.972540	0.530410	3.053315	C	1.791721	1.225986	3.112015
C	1.890840	-1.763219	4.156579	C	1.461505	-0.866345	4.521984
C	1.237894	0.737325	-1.133357	C	0.915749	0.639638	-1.727052
C	2.215443	1.662262	-1.225218	C	2.156121	1.158964	-1.857747
C	2.416516	2.928709	-0.480130	C	2.856931	2.106554	-0.958355
C	1.477005	3.822514	-0.094920	C	2.336625	3.196072	-0.361809
C	0.004187	3.624855	-0.439411	C	0.904109	3.663875	-0.472880
O	-0.509590	2.479720	0.180952	O	-0.033848	2.708085	-0.062942
C	3.504522	1.423782	-2.013483	C	3.202767	0.760491	-2.904734
C	4.586734	1.934396	-1.041778	C	4.502248	0.685219	-2.072047
C	3.930224	3.146957	-0.338422	C	4.354959	1.793036	-0.997853
C	1.848902	5.065841	0.683035	C	0.471213	4.312100	-1.848284
C	-0.415089	3.703997	-1.955896	C	-0.228835	5.456188	-1.063440
C	-1.692879	4.475081	-1.531996	C	0.568102	5.037636	0.202882
C	-1.003836	4.801959	-0.179934	H	3.013351	3.838626	0.207766
H	1.329461	-0.155799	-1.756099	C	0.241170	-0.188166	-2.793633
H	-2.612141	-3.574014	0.917764	H	-2.880420	-2.932255	1.471533
H	0.070981	-4.240999	1.151900	H	-0.263702	-3.666506	2.004756
H	-5.267228	1.011027	1.718359	H	-5.110045	2.007067	1.052807
H	-5.162368	-0.199341	-2.392098	H	-5.394882	-0.521326	-2.394152
H	-6.266330	1.005916	-0.539756	H	-6.263202	1.343103	-1.027600
H	4.479148	-3.170028	-1.217264	H	4.350005	-3.314283	-0.256927
H	4.336323	-1.144594	2.556929	H	4.069753	-0.567344	3.020004
H	5.635617	-2.157024	0.715875	H	5.432184	-1.969427	1.509386
H	0.743108	-3.130102	-1.661211	H	0.663230	-3.221138	-0.980265
H	1.509147	-5.320435	-0.711478	H	1.189268	-5.172948	0.498010
H	1.385036	-5.375776	-2.478472	H	1.204985	-5.627325	-1.214714
H	2.971278	-5.236090	-1.702089	H	2.729350	-5.394443	-0.342315
H	2.262995	-1.763797	-3.112779	H	2.399865	-2.306280	-2.546509
H	3.390479	-3.125142	-3.205859	H	3.404285	-3.734429	-2.251083
H	1.763647	-3.284184	-3.872928	H	1.819871	-3.916773	-3.007659
H	0.576446	-1.027520	2.640224	H	0.324925	-0.293990	2.806263
H	1.760901	1.103743	2.146433	H	1.696106	1.671197	2.117903
H	1.365555	0.943828	3.867146	H	1.152353	1.790238	3.800915

	H	3.025971	0.679264	3.317279		H	2.828060	1.350783	3.446450
	H	1.623404	-2.818800	4.034202		H	1.130205	-1.910717	4.532047
	H	2.941300	-1.718325	4.465192		H	2.486265	-0.837254	4.909049
	H	1.287177	-1.353511	4.974693		H	0.827518	-0.302760	5.216161
	H	-1.996436	-2.201356	-1.970019		H	-2.203100	-2.344013	-1.641148
	H	-1.597307	0.086452	-2.873767		H	-2.618168	-0.885826	-3.662980
	H	-1.735038	-1.122674	-4.167768		H	-2.711147	-2.623097	-3.996601
	H	-3.085090	-0.026194	-3.831821		H	-4.191146	-1.671173	-3.875260
	H	-4.168748	-3.384782	-2.342299		H	-4.089318	-3.646472	-0.630127
	H	-4.639619	-2.153124	-3.523007		H	-5.129186	-3.193848	-1.986946
	H	-3.240699	-3.184304	-3.839712		H	-3.708722	-4.217298	-2.263462
	H	-2.036227	-0.734664	2.567478		H	-1.929111	0.436974	2.279728
	H	-4.096715	-1.935157	3.309012		H	-3.884710	-0.661134	3.367346
	H	-3.424892	-0.913454	4.593425		H	-3.257376	0.675258	4.349473
	H	-4.861423	-0.388596	3.703800		H	-4.741453	0.887936	3.405753
	H	-2.008646	1.763739	2.318435		H	-2.035625	2.803861	1.479608
	H	-3.575428	1.852647	3.139535		H	-3.585074	3.013259	2.329857
	H	-2.163024	1.240140	4.008566		H	-2.115305	2.668049	3.244277
	H	3.645339	0.378016	-2.301895		H	0.863989	-0.328020	-3.686194
	H	3.508405	2.031226	-2.931280		H	-0.057470	-1.175677	-2.422916
	H	0.268410	4.335437	-2.535603		H	-0.680028	0.310951	-3.118413
	H	-0.535714	2.740908	-2.455929		H	2.986443	-0.178302	-3.421181
	H	-1.595125	4.703165	0.735690		H	3.294376	1.543385	-3.672612
	H	-0.529028	5.787658	-0.202714		H	1.326209	4.670700	-2.431969
	H	4.805159	1.149031	-0.309448		H	-0.155686	3.667993	-2.470461
	H	5.526585	2.195806	-1.541066		H	0.021353	4.960698	1.147829
	H	4.231383	4.085007	-0.823425		H	1.463773	5.652933	0.349368
	H	4.246053	3.221981	0.709114		H	4.559828	-0.296028	-1.588537
	H	-2.548074	3.806590	-1.402847		H	5.403399	0.807353	-2.683049
	H	-1.995331	5.325431	-2.152989		H	4.930871	2.687061	-1.265586
	H	1.765695	5.975516	0.070954		H	4.723178	1.455153	-0.021927
	H	1.173331	5.204234	1.536290		H	-1.302661	5.282778	-0.950362
	H	2.869670	5.026132	1.070440		H	-0.074392	6.477218	-1.429344
TS2-3e	Ni	0.219430	-0.837378	-0.573474	TS2-3e’	Ni	0.224030	-0.870194	-0.724705
	C	0.448973	0.763210	0.374939		C	0.364044	0.665503	0.351393
	N	-0.397206	1.594457	1.059109		N	-0.538374	1.369279	1.107353
	C	0.306690	2.641918	1.657371		C	0.098555	2.376048	1.836279
	C	1.614723	2.472552	1.341434		C	1.417843	2.310904	1.535046
	N	1.687379	1.321488	0.560002		N	1.569858	1.261772	0.630825
	C	-1.835268	1.465367	1.172394		C	-1.959847	1.116288	1.251724
	C	-2.645287	2.342401	0.420889		C	-2.867761	2.013481	0.649702
	C	-4.035347	2.250382	0.590328		C	-4.237305	1.808642	0.877629
	C	-4.591174	1.320737	1.466207		C	-4.683754	0.753375	1.669065
	C	-3.764972	0.465828	2.198203		C	-3.764163	-0.116272	2.256852
	C	-2.369539	0.519273	2.076836		C	-2.383654	0.044704	2.073508
	C	-2.074394	3.390526	-0.532911		C	-2.426311	3.202879	-0.201591
	C	-2.242133	4.815659	0.037297		C	-2.588795	4.532917	0.567104
	C	-2.691126	3.300397	-1.942532		C	-3.176745	3.276465	-1.546239
	C	-1.475658	-0.377781	2.932881		C	-1.397560	-0.874758	2.793370
	C	-2.139727	-1.704905	3.334364		C	-1.952093	-2.284883	3.058775
	C	-0.995788	0.373424	4.195543		C	-0.928894	-0.238852	4.122144

C	2.923359	0.775088	0.046252	C	2.863879	0.807621	0.163592
C	3.685515	-0.070340	0.880402	C	3.597368	-0.083300	0.977569
C	4.897343	-0.560267	0.370732	C	4.866339	-0.476385	0.525975
C	5.330637	-0.222076	-0.910784	C	5.383715	-0.002968	-0.678432
C	4.559601	0.621857	-1.710871	C	4.644609	0.890274	-1.454637
C	3.340783	1.141041	-1.251554	C	3.373399	1.320714	-1.049552
C	3.264495	-0.430182	2.303425	C	3.097449	-0.570864	2.335730
C	4.196567	0.240768	3.335452	C	3.828221	0.172892	3.475818
C	3.191656	-1.953585	2.524946	C	3.223077	-2.096187	2.508373
C	2.546042	2.101867	-2.132471	C	2.615498	2.356625	-1.875151
C	2.298156	1.538977	-3.545172	C	2.750941	2.140737	-3.393799
C	3.236986	3.480675	-2.203006	C	3.060457	3.788014	-1.499926
C	-0.821765	-0.170616	-1.976049	C	-0.973334	-0.257037	-2.046937
C	-1.928684	-0.928294	-2.155570	C	-2.066245	-1.065476	-2.081571
C	-2.366385	-2.095436	-1.332096	C	-2.299706	-2.282208	-1.254692
C	-1.644915	-2.942761	-0.550975	C	-1.422250	-3.085337	-0.605217
C	-0.131834	-2.933159	-0.350202	C	0.083055	-2.998485	-0.514565
O	0.368848	-2.268091	0.720502	O	0.638302	-2.296387	0.509120
C	-3.043640	-0.656393	-3.164272	C	-3.333145	-0.864214	-2.924012
C	-4.315190	-1.058712	-2.396384	C	-4.449132	-1.431129	-2.026173
C	-3.871361	-2.279847	-1.562894	C	-3.787209	-2.640553	-1.339349
C	-2.325185	-4.083973	0.189102	C	-0.770594	0.892148	-2.997170
C	0.579813	-4.298634	-0.584189	C	0.838534	-4.322625	-0.810219
C	1.688985	-3.689442	-1.445037	C	1.820520	-3.650634	-1.777492
C	0.835605	-2.499974	-1.906455	C	0.863885	-2.494187	-2.119792
H	-0.674791	0.698885	-2.623226	H	-1.831279	-3.973984	-0.114279
H	-0.183728	3.399898	2.250975	H	-0.440008	3.031436	2.504837
H	2.488597	3.053043	1.602461	H	2.252798	2.900931	1.885098
H	-4.691147	2.911152	0.027818	H	-4.963591	2.481650	0.428245
H	-4.217830	-0.250770	2.876927	H	-4.130545	-0.931037	2.874212
H	-5.672275	1.260786	1.581383	H	-5.750505	0.607242	1.831043
H	5.512066	-1.214736	0.984656	H	5.460034	-1.161755	1.125931
H	4.915294	0.882602	-2.705185	H	5.068268	1.258809	-2.385242
H	6.274360	-0.613973	-1.286613	H	6.369139	-0.324882	-1.011253
H	2.257761	-0.040354	2.470876	H	2.034005	-0.335326	2.413031
H	4.223016	1.329131	3.209867	H	3.707452	1.258881	3.397733
H	3.852065	0.026355	4.353683	H	3.432958	-0.140800	4.448900
H	5.224344	-0.129265	3.245917	H	4.902687	-0.043896	3.464152
H	2.464846	-2.405508	1.844489	H	2.661258	-2.612166	1.726452
H	4.167692	-2.432474	2.384019	H	4.267686	-2.427411	2.491794
H	2.870337	-2.161537	3.552653	H	2.804604	-2.390160	3.478257
H	1.565765	2.250368	-1.673980	H	1.555310	2.265780	-1.628290
H	1.801865	0.565424	-3.500182	H	2.521184	1.109184	-3.676993
H	1.654410	2.220851	-4.112498	H	2.057956	2.800532	-3.926882
H	3.229376	1.422777	-4.110474	H	3.759480	2.373215	-3.752937
H	3.368827	3.914338	-1.205769	H	2.899216	3.996466	-0.437610
H	4.226700	3.405938	-2.667965	H	4.125442	3.935072	-1.713143
H	2.637796	4.178875	-2.799072	H	2.494483	4.528446	-2.077315
H	-0.603341	-0.651260	2.335433	H	-0.529920	-1.016301	2.145979
H	-2.536849	-2.229486	2.461890	H	-2.353106	-2.731026	2.144752
H	-1.392543	-2.355843	3.799858	H	-1.140492	-2.928690	3.413121
H	-2.950559	-1.565773	4.059572	H	-2.734489	-2.290915	3.827231

	H	-0.443474	1.284997	3.948095	H	-0.454894	0.735310	3.969473
	H	-1.845052	0.656284	4.829546	H	-1.773279	-0.099004	4.808288
	H	-0.332254	-0.267433	4.787993	H	-0.198733	-0.890877	4.615787
	H	-1.003234	3.204021	-0.642922	H	-1.364117	3.081616	-0.430820
	H	-1.770355	4.918790	1.020218	H	-2.027195	4.534377	1.506649
	H	-1.786582	5.552597	-0.634298	H	-2.230272	5.372128	-0.040289
	H	-3.301176	5.073937	0.149495	H	-3.640884	4.719782	0.810298
	H	-2.585017	2.292908	-2.351680	H	-3.121306	2.327643	-2.084555
	H	-3.755922	3.557437	-1.940387	H	-4.233925	3.528112	-1.408913
	H	-2.186783	4.001425	-2.617745	H	-2.736188	4.055159	-2.179319
	H	-5.167711	-1.278936	-3.048712	H	-5.355163	-1.699380	-2.581213
	H	-4.606389	-0.241858	-1.725881	H	-4.723163	-0.681986	-1.274622
	H	-3.055827	0.378360	-3.520172	H	-3.511360	0.178160	-3.201660
	H	-2.923246	-1.303758	-4.046581	H	-3.276422	-1.442833	-3.859040
	H	-4.055558	-3.212209	-2.116060	H	-3.914799	-3.541360	-1.955304
	H	-4.433271	-2.359027	-0.625789	H	-4.217079	-2.860687	-0.356320
	H	0.878824	-4.778754	0.352931	H	0.125438	0.716853	-3.607572
	H	-0.048144	-4.985326	-1.162139	H	-0.590361	1.834128	-2.464373
	H	2.092031	-4.314171	-2.251297	H	-1.604625	1.053501	-3.692404
	H	2.519408	-3.343655	-0.824101	H	1.255436	-4.779113	0.093315
	H	0.153264	-2.743222	-2.721954	H	0.189916	-5.043583	-1.320449
	H	1.410828	-1.609026	-2.188610	H	2.160135	-4.243664	-2.634838
	H	-3.303644	-3.790704	0.580792	H	2.697207	-3.275462	-1.243609
	H	-2.489310	-4.957019	-0.458889	H	0.138562	-2.743556	-2.895286
	H	-1.718833	-4.418827	1.036652	H	1.370035	-1.558654	-2.397309
INT3e	Ni	-0.399021	-0.178889	-0.954333	INT3e'	Ni	-0.437740	-0.409497	-0.912483
	C	0.879217	0.662135	0.326887		C	0.704430	0.645302	0.347626
	N	2.220564	0.646538	0.620806		N	2.040741	0.822162	0.618235
	C	2.554810	1.628458	1.552719		C	2.250171	1.864630	1.519955
	C	1.407033	2.283517	1.863645		C	1.028638	2.362730	1.837077
	N	0.402221	1.683904	1.112927		N	0.103127	1.612706	1.119529
	C	3.214612	-0.253403	0.076662		C	3.151629	0.067070	0.076173
	C	3.527122	-1.426958	0.794756		C	3.671710	-1.006312	0.830064
	C	4.532673	-2.255234	0.272993		C	4.784077	-1.684588	0.307247
	C	5.201505	-1.923775	-0.904582		C	5.357981	-1.302433	-0.904262
	C	4.883282	-0.747978	-1.585104		C	4.835284	-0.223404	-1.618804
	C	3.885786	0.115380	-1.110170		C	3.723885	0.487207	-1.145644
	C	2.872970	-1.776235	2.131070		C	3.121011	-1.393532	2.201776
	C	3.839006	-1.464822	3.296504		C	4.049459	-0.864712	3.318395
	C	2.383375	-3.234733	2.207376		C	2.892789	-2.907999	2.364732
	C	3.593245	1.425468	-1.840302		C	3.200862	1.699703	-1.915644
	C	3.497904	1.262381	-3.369710		C	3.155654	1.483504	-3.440456
	C	4.645977	2.496228	-1.477934		C	4.031198	2.958046	-1.578165
	C	-0.984211	2.091088	1.139841		C	-1.323799	1.844095	1.164430
	C	-1.425725	3.058970	0.211219		C	-1.886728	2.773995	0.261755
	C	-2.774080	3.439765	0.265776		C	-3.269680	2.992560	0.337033
	C	-3.640163	2.887983	1.209371		C	-4.053300	2.321175	1.275802
	C	-3.172316	1.947144	2.126888		C	-3.467284	1.426601	2.171691
	C	-1.834575	1.527501	2.115788		C	-2.088997	1.169665	2.141951
	C	-0.490208	3.724213	-0.795349		C	-1.033838	3.584778	-0.711846
	C	-0.273221	5.211729	-0.443716		C	-0.803769	5.011915	-0.166709

C	-0.981562	3.562681	-2.246717	C	-1.620018	3.639065	-2.134073
C	-1.335173	0.540453	3.167962	C	-1.451720	0.254578	3.185446
C	-2.183726	-0.742906	3.224957	C	-2.254726	-1.033386	3.438587
C	-1.257268	1.215481	4.554741	C	-1.230139	1.021299	4.508681
C	-1.855104	-0.407747	-2.101967	C	-1.852844	-0.848174	-2.074448
C	-3.065871	-1.017093	-2.000668	C	-2.964920	-1.573539	-1.741988
C	-3.568146	-1.918610	-0.944449	C	-3.180828	-2.403245	-0.549542
C	-2.895004	-2.780981	-0.132044	C	-2.315782	-3.117152	0.225516
C	-1.438548	-3.089039	-0.233838	C	-0.893177	-3.441760	0.053462
C	-0.792203	-3.384426	-1.588461	C	-0.276156	-3.657247	-1.327808
C	0.603547	-2.762078	-1.750239	C	0.999657	-2.827233	-1.556357
C	0.590526	-1.290707	-2.168381	C	0.732259	-1.410507	-2.063777
C	-4.258984	-0.715554	-2.910581	C	-4.320105	-1.490082	-2.456723
C	-5.447894	-0.699500	-1.931055	C	-5.328570	-1.506664	-1.290726
C	-5.091988	-1.792988	-0.900822	C	-4.684099	-2.456972	-0.263116
C	-3.621954	-3.520724	0.980344	O	-0.213346	-3.727791	1.052739
O	-0.782753	-3.307955	0.792840	C	-1.873252	-0.095589	-3.401752
H	-1.762746	0.205042	-3.012767	H	-2.720875	-3.556781	1.138849
H	3.565739	1.767179	1.909462	H	3.237326	2.152417	1.852042
H	1.218982	3.104770	2.541639	H	0.742816	3.170399	2.495486
H	4.800897	-3.169429	0.796883	H	5.209146	-2.520499	0.857188
H	5.977354	-2.582177	-1.291855	H	6.219293	-1.843870	-1.291993
H	5.420441	-0.500576	-2.497421	H	5.299886	0.067295	-2.557522
H	1.992563	-1.140713	2.254864	H	2.147871	-0.911197	2.325158
H	4.161269	-0.418024	3.289955	H	4.193603	0.218878	3.250824
H	3.350956	-1.661502	4.258051	H	3.624821	-1.087741	4.303885
H	4.737717	-2.090014	3.242203	H	5.037504	-1.336029	3.263738
H	1.644344	-3.451254	1.432606	H	2.185809	-3.293435	1.626366
H	3.209861	-3.949207	2.122442	H	3.828985	-3.472769	2.291012
H	1.901484	-3.408687	3.176299	H	2.470177	-3.108817	3.355793
H	2.620386	1.789890	-1.499778	H	2.172685	1.882222	-1.591870
H	2.768002	0.496274	-3.646549	H	2.601024	0.577833	-3.702250
H	3.183726	2.209041	-3.823461	H	2.659156	2.334664	-3.919720
H	4.461299	0.993325	-3.816389	H	4.157710	1.407333	-3.876392
H	4.685057	2.675080	-0.398493	H	4.021960	3.173331	-0.505006
H	5.646540	2.188452	-1.802635	H	5.075529	2.831307	-1.885978
H	4.409947	3.447552	-1.969060	H	3.629422	3.834112	-2.100553
H	-3.152724	4.178458	-0.436951	H	-3.741692	3.699324	-0.341283
H	-4.683950	3.196659	1.233521	H	-5.125930	2.503410	1.315644
H	-3.858053	1.535004	2.863439	H	-4.092233	0.924680	2.905924
H	0.482673	3.230749	-0.732861	H	-0.056787	3.100870	-0.788679
H	0.114424	5.330947	0.574057	H	-0.336533	4.995735	0.823400
H	0.445499	5.666026	-1.135402	H	-0.148903	5.577246	-0.839793
H	-1.208210	5.779002	-0.512827	H	-1.750202	5.557659	-0.079712
H	-1.107091	2.506049	-2.499116	H	-1.789487	2.635713	-2.531322
H	-1.938808	4.069328	-2.412981	H	-2.568432	4.186105	-2.167868
H	-0.252996	3.998149	-2.940364	H	-0.923452	4.156592	-2.803464
H	-0.321398	0.236860	2.896137	H	-0.471327	-0.051503	2.811328
H	-2.203246	-1.245705	2.255442	H	-2.437619	-1.573532	2.507098
H	-1.755817	-1.440453	3.953418	H	-1.690223	-1.695777	4.103514
H	-3.214942	-0.536244	3.532614	H	-3.217261	-0.829168	3.920962
H	-0.619368	2.106115	4.535561	H	-0.611566	1.913194	4.364600

	H	-2.249609	1.523711	4.903170		H	-2.185146	1.343262	4.939830
	H	-0.844145	0.519114	5.293417		H	-0.728645	0.378869	5.241531
	H	-0.700553	-4.481580	-1.599160		H	-0.019895	-4.725907	-1.344308
	H	-1.446768	-3.105450	-2.415532		H	-1.001428	-3.477068	-2.124638
	H	1.158700	-3.335458	-2.510621		H	1.632611	-3.344713	-2.295713
	H	1.149943	-2.892113	-0.811655		H	1.574711	-2.809956	-0.625693
	H	1.604251	-0.878603	-2.129424		H	1.658140	-0.827407	-2.069186
	H	0.220206	-1.184925	-3.194557		H	0.352773	-1.446160	-3.089843
	H	-4.141076	0.219030	-3.466981		H	-4.426314	-0.605810	-3.090045
	H	-4.394937	-1.524107	-3.646040		H	-4.474881	-2.369293	-3.101519
	H	-5.494504	0.277264	-1.434970		H	-5.408696	-0.497553	-0.869877
	H	-6.415289	-0.874383	-2.414406		H	-6.332897	-1.824680	-1.590572
	H	-5.545710	-2.756262	-1.175308		H	-5.039997	-3.485126	-0.411425
	H	-5.462371	-1.557051	0.103421		H	-4.911836	-2.191223	0.775118
	H	-4.210826	-4.358566	0.579769		H	-2.073870	-0.758579	-4.255225
	H	-2.903235	-3.925035	1.695886		H	-2.664024	0.667241	-3.411178
	H	-4.316734	-2.872652	1.525305		H	-0.928185	0.418736	-3.596746
TS3e	Ni	-0.085751	-0.930154	-0.531114	TS3e’	Ni	0.031020	-1.082694	-0.484351
	C	0.590926	0.728378	0.308659		C	0.435443	0.677129	0.320479
	N	1.897451	1.062423	0.582604		N	1.703904	1.112339	0.636121
	C	1.988847	2.217650	1.357287		C	1.682282	2.247202	1.444120
	C	0.717453	2.634433	1.579627		C	0.377483	2.546976	1.652001
	N	-0.120157	1.727279	0.931302		N	-0.371258	1.598292	0.954759
	C	3.057293	0.308155	0.165205		C	2.937942	0.508301	0.187681
	C	3.570241	-0.680691	1.031970		C	3.613545	-0.385032	1.048156
	C	4.721825	-1.369307	0.620985		C	4.835276	-0.912688	0.603256
	C	5.337925	-1.083549	-0.596585		C	5.364268	-0.564737	-0.639358
	C	4.816401	-0.093287	-1.430263		C	4.683218	0.331217	-1.463730
	C	3.668357	0.626075	-1.068808		C	3.459409	0.890251	-1.068263
	C	2.958712	-0.973887	2.400494		C	3.094809	-0.731639	2.442223
	C	3.819573	-0.345251	3.518707		C	3.850307	0.081859	3.517183
	C	2.743124	-2.477800	2.653376		C	3.168118	-2.236544	2.758497
	C	3.148166	1.745694	-1.968625		C	2.770447	1.922458	-1.958802
	C	3.189690	1.392858	-3.467811		C	2.729651	1.511077	-3.442735
	C	3.920696	3.058664	-1.710928		C	3.436491	3.307282	-1.800623
	C	-1.560257	1.858603	0.950618		C	-1.818250	1.644934	0.918689
	C	-2.163440	2.787834	0.075816		C	-2.442759	2.648689	0.141928
	C	-3.554041	2.954005	0.158702		C	-3.845403	2.698492	0.147958
	C	-4.311681	2.221890	1.072036		C	-4.594813	1.794394	0.898328
	C	-3.690005	1.306998	1.922036		C	-3.952372	0.831157	1.676835
	C	-2.302963	1.104304	1.884757		C	-2.553914	0.738051	1.715740
	C	-1.359433	3.628384	-0.915008		C	-1.661386	3.710899	-0.635346
	C	-1.241669	5.091405	-0.434933		C	-1.668749	5.057569	0.124276
	C	-1.936977	3.582022	-2.343748		C	-2.177399	3.935282	-2.071010
	C	-1.640483	0.140854	2.867476		C	-1.870542	-0.252041	2.657341
	C	-2.433145	-1.163072	3.066486		C	-2.654429	-1.559096	2.859822
	C	-1.386944	0.840518	4.221207		C	-1.589886	0.420204	4.020794
	C	-1.324455	-0.494239	-1.852878		C	-1.275198	-0.934910	-1.800412
	C	-2.532946	-1.104372	-1.683588		C	-2.355731	-1.723130	-1.466943
	C	-2.799538	-2.419800	-1.081929		C	-2.319586	-3.044220	-0.847575
	C	-1.887168	-3.251638	-0.516398		C	-1.249114	-3.673455	-0.296408

C	-0.449474	-2.846304	-0.327349	C	0.075814	-3.044860	-0.047302
C	0.594096	-3.544759	-1.229139	C	1.256245	-3.613624	-0.853422
C	1.297228	-2.451478	-2.050260	C	1.632016	-2.547456	-1.898881
C	0.263267	-1.386091	-2.522573	C	0.355581	-1.817431	-2.421999
C	-3.857707	-0.508075	-2.160384	C	-3.799878	-1.411477	-1.869718
C	-4.926965	-1.317183	-1.402224	C	-4.641329	-2.483171	-1.145766
C	-4.291321	-2.713000	-1.235008	C	-3.690279	-3.689725	-1.021536
O	-0.057047	-2.344662	0.817991	O	0.323700	-2.330215	1.013746
C	-2.207187	-4.657093	-0.053903	C	-1.467036	0.256688	-2.710552
H	-1.295454	0.448914	-2.399437	H	-1.316837	-4.749828	-0.107414
H	2.934562	2.629678	1.680422	H	2.582933	2.729999	1.795462
H	0.339582	3.479999	2.136755	H	-0.078678	3.335671	2.231628
H	5.144452	-2.138579	1.262769	H	5.383325	-1.604291	1.238381
H	6.229183	-1.632082	-0.896993	H	6.313030	-0.988693	-0.964257
H	5.312159	0.119443	-2.374031	H	5.113403	0.601711	-2.424994
H	1.972350	-0.506547	2.437332	H	2.039514	-0.454123	2.485821
H	3.937168	0.735139	3.380923	H	3.774379	1.160227	3.342969
H	3.353682	-0.511293	4.496951	H	3.438811	-0.127043	4.511505
H	4.821684	-0.789079	3.544305	H	4.915120	-0.178725	3.532258
H	2.081937	-2.903644	1.895064	H	2.603381	-2.811398	2.021968
H	3.687699	-3.033232	2.668081	H	4.200360	-2.603212	2.792213
H	2.266404	-2.620475	3.630187	H	2.723038	-2.426199	3.741942
H	2.100967	1.922662	-1.708604	H	1.734423	2.015606	-1.624470
H	2.702605	0.434712	-3.671699	H	2.294238	0.515734	-3.570630
H	2.672326	2.166540	-4.046091	H	2.120787	2.223298	-4.010977
H	4.214920	1.336772	-3.849548	H	3.726837	1.504062	-3.896181
H	3.845913	3.372489	-0.665238	H	3.414505	3.646576	-0.759883
H	4.983592	2.940301	-1.951263	H	4.483923	3.278836	-2.122039
H	3.521390	3.867291	-2.334357	H	2.916540	4.055363	-2.410542
H	-4.052091	3.664298	-0.497399	H	-4.359439	3.455310	-0.439700
H	-5.390179	2.363386	1.120810	H	-5.682355	1.845942	0.884666
H	-4.295404	0.744099	2.627642	H	-4.551689	0.146058	2.269391
H	-0.348458	3.215168	-0.965540	H	-0.622429	3.379300	-0.714888
H	-0.791988	5.155130	0.561072	H	-1.277280	4.960523	1.141197
H	-0.619012	5.673274	-1.124529	H	-1.056451	5.798004	-0.403394
H	-2.226599	5.569594	-0.386376	H	-2.687098	5.455285	0.199890
H	-2.045038	2.553397	-2.699522	H	-2.198019	3.007627	-2.647074
H	-2.918827	4.063404	-2.404968	H	-3.185333	4.363569	-2.081658
H	-1.270872	4.112357	-3.033991	H	-1.521413	4.641995	-2.592098
H	-0.675581	-0.154054	2.451793	H	-0.915658	-0.541315	2.216427
H	-2.613209	-1.659397	2.109835	H	-2.892580	-2.030045	1.902781
H	-1.850857	-1.850315	3.689579	H	-2.036955	-2.264073	3.425856
H	-3.392388	-0.995793	3.570137	H	-3.582815	-1.409042	3.423874
H	-0.763452	1.733533	4.105135	H	-0.968755	1.315448	3.914377
H	-2.329705	1.147959	4.689452	H	-2.524270	0.715511	4.513591
H	-0.874240	0.160318	4.911516	H	-1.063407	-0.275559	4.684578
H	1.311316	-4.117454	-0.628592	H	2.103775	-3.846230	-0.199093
H	0.085998	-4.245673	-1.902383	H	0.945453	-4.541136	-1.349688
H	1.788271	-2.873599	-2.941551	H	2.145530	-2.995293	-2.764767
H	2.089679	-1.989577	-1.453681	H	2.336445	-1.834061	-1.461383
H	0.761205	-0.544561	-3.008225	H	0.647402	-1.056457	-3.148822
H	-0.378918	-1.868081	-3.262816	H	-0.253773	-2.565224	-2.935452

	H -3.931198 0.568158 -1.975910 H -3.967904 -0.660853 -3.245342 H -5.088749 -0.869359 -0.414739 H -5.892648 -1.346884 -1.918874 H -4.471583 -3.318455 -2.135845 H -4.711847 -3.263864 -0.388354 H -2.093975 -4.739991 1.035879 H -3.219434 -4.974570 -0.317571 H -1.509241 -5.383977 -0.490848		H -4.107938 -0.395929 -1.597276 H -3.921264 -1.496322 -2.961028 H -4.907954 -2.123090 -0.145213 H -5.572370 -2.722833 -1.670755 H -3.710769 -4.278848 -1.950098 H -3.951362 -4.365122 -0.200524 H -1.619019 -0.049155 -3.756350 H -2.353232 0.825142 -2.412885 H -0.606417 0.929915 -2.681086
3e	C 1.039728 -0.950490 0.109021 C 0.278867 -1.963990 -0.359588 C -1.072523 -1.841920 -1.007911 C -2.215224 -1.690693 0.017831 C -1.949159 -0.527605 0.992277 C -1.699854 0.785973 0.262130 C -0.315859 1.271801 -0.027179 C 0.819214 0.509149 -0.020569 C 2.202915 1.156915 -0.119057 C 3.222617 -0.002111 -0.076599 C 2.457967 -1.141621 0.624151 O -2.673519 1.483874 -0.043857 C -0.206096 2.760682 -0.306149 H 0.682660 -2.972840 -0.258073 H -1.261642 -2.720244 -1.634989 H -1.083195 -0.965872 -1.670068 H -2.832854 -0.371070 1.618746 H -1.106350 -0.778691 1.641273 H 2.304508 1.773232 -1.019207 H 2.342508 1.836096 0.733385 H 2.857815 -2.136338 0.407541 H 2.489205 -0.997875 1.713725 H 0.253277 2.957229 -1.281832 H 0.417883 3.258287 0.446727 H -1.192880 3.223788 -0.297773 H 3.482469 -0.310908 -1.095406 H 4.149981 0.273644 0.434564 H -3.157964 -1.521343 -0.515396 H -2.332821 -2.614632 0.597488	3e’	C -1.046095 0.306759 0.148581 C -0.409283 1.450279 -0.217919 C 0.911759 1.456860 -0.956944 C 2.143294 1.410569 -0.030690 C 2.115109 0.195433 0.915138 C 1.959689 -1.121755 0.169620 C 0.627832 -1.650345 -0.180217 C -0.607002 -1.079076 -0.119813 C -1.860005 -1.947620 -0.256672 C -3.049423 -0.975081 -0.137073 C -2.479510 0.212760 0.666350 C -0.977585 2.825038 0.049809 O 2.962476 -1.796745 -0.100951 H 0.674671 -2.701244 -0.471384 H 0.969526 2.363678 -1.571669 H 0.957131 0.604077 -1.643941 H 3.056025 0.140853 1.470801 H 1.295780 0.314512 1.631949 H -1.858671 -2.516405 -1.192719 H -1.873160 -2.681590 0.558957 H -3.061542 1.125356 0.526349 H -2.486821 -0.023258 1.740145 H -3.354164 -0.626759 -1.130537 H -3.922986 -1.431729 0.338061 H 3.048902 1.379236 -0.648126 H 2.203015 2.324293 0.573726 H -1.293381 3.301295 -0.888629 H -1.824635 2.825050 0.736951 H -0.202183 3.473665 0.476661

Table S14. Frequencies of some stationary points for reaction **e**, at SCRF(PCM)-B3LYP/DZVP level in toluene.

Species	Frequencies (cm^{-1})
1c	16 60 78 90 152 212 279 301 334 371 432 541 630 637 739 758 839 951 1036 1039 1048 1052 1078 1158 1181 1267 1302 1330 1355 1400 1421 1483 1486 1492 1493 1509 2200 2336 3024 3031 3037 3066 3067 3075 3117 3117 3125 3421
COM1e	21 26 28 38 43 45 49 58 66 67 74 78 85 96103 115 122 129 130 146 150 162 167 171 186

	191 208 220 229 232 237 241 250 252 259 264 266 270 275 283 285 291 305 306 315 316 329 332 335 371 397 408 418 421 437 442 446 449 459 478 493 524 529 533 559 566 584 589 602 620 640 643 645 659 668 696 718 738 756 757 770 774 777 813 814 819 822 823 844 870 893 894 900 916 917 933 934 936 938 944 946 949 962 962 965 966 970 986 986 996 1043 1054 1058 1060 1062 1065 1078 1080 1088 1095 1106 1116 1119 1126 1127 1133 1140 1147 1163 1172 1173 1186 1186 1200 1201 1212 1221 1246 1255 1277 1279 1280 1282 1296 1306 1324 1330 1337 1343 1344 1347 1352 1354 1366 1382 1390 1392 1395 1403 1407 1408 1409 1412 1418 1426 1427 1430 1430 1473 1481 1485 1488 1493 1496 1496 1499 1500 1501 1502 1502 1503 1505 1506 1507 1509 1517 1519 1520 1522 1524 1526 1527 1528 1615 1631 1634 1638 1640 1922 2011 3006 3013 3016 3028 3028 3035 3038 3038 3039 3041 3042 3048 3056 3065 3085 3089 3092 3098 3103 3107 3108 3109 3111 3112 3113 3113 3114 3120 3122 3129 3131 3134 3140 3140 3141 3146 3163 3164 3165 3183 3185 3190 3192 3276 3301 3328
TS1e	**-198i** 14 16 25 30 38 39 47 53 54 58 68 70 77 80 93 106 120 127 130 156 164 169 181 186 191 198 212 216 225 234 238 241 251 257 260 262 265 274 280 283 296 302 305 311 315 326 328 383 391 410 416 424 427 438 444 444 464 478 500 528 531 561 567 583 588 590 605 615 622 642 644 646 658 696 720 738 748 756 771 776 814 815 816 818 820 822 859 881 894 895 915 917 923 932 933 935 937 940 946 949 950 964 964 966 967 978 985 988 1010 1025 1049 1060 1062 1065 1076 1080 1081 1092 1098 1117 1119 1121 1126 1127 1136 1139 1145 1152 1172 1174 1186 1186 1201 1201 1203 1219 1255 1259 1274 1278 1279 1284 1306 1310 1328 1333 1337 1341 1342 1345 1347 1349 1358 1368 1394 1396 1398 1405 1406 1407 1407 1409 1423 1427 1428 1429 1430 1481 1489 1490 1492 1493 1496 1497 1497 1499 1501 1503 1505 1506 1507 1507 1509 1510 1518 1519 1520 1521 1524 1525 1526 1526 1611 1633 1635 1637 1639 1681 1789 2996 3008 3016 3028 3029 3034 3034 3038 3038 3041 3044 3048 3071 3076 3091 3093 3093 3096 3100 3103 3108 3108 3109 3110 3110 3114 3115 3121 3121 3126 3126 3128 3133 3137 3141 3143 3157 3162 3164 3182 3185 3189 3192 3214 3264 3288
INT1e	9 21 26 29 31 38 44 46 50 55 57 63 67 73 85 110 112 122 129 132 137 158 165 169 175 196 210 225 227 231 237 239 245 249 251 255 258 266 269 276 283 297 306 308 311 317 319 331 361 398 419 422 424 442 444 449 482 495 526 527 556 561 588 591 594 599 621 624 642 643 645 648 666 698 707 729 738 753 756 773 780 814 815 823 825 830 851 873 894 894 901 919 924 935 936 937 939 951 952 953 961 965 968 968 970 976 986 990 997 1006 1040 1048 1061 1063 1079 1081 1093 1096 1097 1112 1124 1126 1127 1128 1128 1135 1136 1142 1174 1176 1187 1188 1194 1201 1203 1230 1236 1259 1272 1280 1280 1289 1290 1306 1312 1314 1321 1334 1335 1342 1348 1349 1351 1354 1365 1394 1396 1397 1402 1408 1409 1410 1410 1429 1430 1431 1431 1432 1485 1486 1491 1491 1495 1496 1496 1497 1500 1500 1503 1503 1504 1504 1507 1508 1510 1516 1516 1518 1519 1523 1524 1528 1529 1595 1633 1636 1636 1638 1644 1675 2975 3000 3015 3028 3029 3029 3031 3035 3036 3036 3036 3036 3040 3051 3072 3084 3086 3089 3093 3094 3099 3109 3110 3113 3114 3116 3117 3118 3118 3119 3121 3123 3124 3126 3128 3129 3131 3149 3163 3164 3180 3181 3188 3189 3248 3270
TSee’	**-59**. 15. 20. 28. 33. 41. 44. 49. 49. 53. 58. 60. 65. 68. 79. 109. 110. 122. 130. 141. 156. 159. 162. 167. 171. 199. 217. 226. 232. 236. 238. 242. 246. 251. 253. 257. 259. 267. 278. 279. 288. 299. 301. 306. 311. 317. 317. 321. 344. 390. 412. 413. 424. 443. 445. 449. 476. 493. 525. 527. 556. 563. 589. 590. 592. 596. 602. 623. 641. 643. 644. 648. 668. 693. 707. 732. 738. 752. 754. 772. 778. 815. 815. 821. 823. 830. 850. 873. 894. 896. 899. 920. 922. 936. 937. 939. 940. 952. 953. 953. 967. 967. 968. 968. 969. 974. 984. 990. 993. 1013. 1031. 1047. 1061. 1064. 1079. 1082. 1090. 1092. 1096. 1111. 1122. 1125. 1127. 1127. 1129. 1131. 1136. 1142. 1173. 1176. 1187. 1187. 1192. 1202. 1203. 1230. 1235. 1260. 1271. 1279. 1280. 1291. 1292. 1305. 1314. 1314. 1329. 1334. 1334. 1343. 1347. 1350. 1351. 1353. 1366. 1396. 1397.

	1402. 1404. 1409. 1410. 1411. 1411. 1427. 1430. 1431. 1432. 1432. 1484. 1484. 1490. 1492. 1496. 1497. 1498. 1499. 1501. 1501. 1503. 1503. 1504. 1505. 1508. 1509. 1510. 1515. 1517. 1519. 1519. 1524. 1525. 1530. 1531. 1596. 1635. 1636. 1637. 1638. 1652. 1685. 2998. 3006. 3010. 3028. 3029. 3031. 3032. 3035. 3035. 3036. 3037. 3041. 3057. 3067. 3076. 3080. 3081. 3087. 3089. 3090. 3092. 3098. 3111. 3111. 3112. 3112. 3117. 3118. 3118. 3119. 3120. 3120. 3123. 3123. 3125. 3126. 3127. 3131. 3164. 3165. 3180. 3183. 3188. 3190. 3248. 3270.
INT1e'	19. 22. 24. 29. 33. 42. 44. 49. 58. 64. 65. 70. 75. 81. 94. 112. 125. 130. 132. 141. 154. 164. 170. 173. 186. 217. 221. 224. 230. 232. 234. 237. 245. 250. 251. 256. 259. 263. 268. 280. 281. 302. 305. 310. 313. 316. 320. 337. 349. 392. 417. 420. 428. 442. 444. 451. 476. 479. 527. 529. 555. 564. 586. 590. 592. 596. 603. 622. 640. 642. 646. 647. 669. 701. 732. 736. 738. 753. 754. 771. 778. 814. 815. 820. 823. 836. 853. 875. 894. 894. 903. 919. 924. 934. 934. 938. 940. 950. 951. 952. 963. 966. 966. 967. 971. 974. 990. 991. 994. 1031. 1041. 1055. 1061. 1063. 1078. 1080. 1092. 1096. 1100. 1109. 1121. 1125. 1127. 1127. 1131. 1133. 1136. 1144. 1174. 1175. 1187. 1188. 1194.1201. 1202. 1226. 1236. 1257. 1264. 1278. 1280. 1287. 1292. 1305. 1306. 1313. 1327. 1329. 1337. 1337. 1344. 1346. 1351. 1352. 1363. 1392. 1394. 1396. 1403. 1409. 1410. 1411. 1412. 1426. 1430. 1431. 1432. 1433. 1481. 1486. 1488. 1490. 1493. 1497. 1497. 1499. 1499. 1501. 1502. 1504. 1504. 1505. 1506. 1508. 1513. 1515. 1517. 1517. 1521. 1523. 1525. 1526. 1529. 1598. 1634. 1635. 1637. 1638. 1646. 1685. 2995. 3006. 3008. 3026. 3029. 3030. 3033. 3033. 3034. 3035. 3037. 3041. 3045. 3062. 3079. 3080. 3083. 3085. 3088. 3091. 3093. 3098. 3110. 3111. 3114. 3114. 3116. 3117. 3119. 3120. 3121. 3122. 3123. 3124. 3125. 3127. 3129. 3150. 3164. 3165. 3178. 3183. 3188. 3191. 3255. 3286.
TS1-2e	**-207i** 13 20 26 32 37 40 45 48 50 57 57 66 70 73 77 88 91 96 114 122 127 132 149 156 159 163 172 190 193 210 222 224 227 232 233 241 247 249 253 256 259 263 267 273 277 281 299 301 304 307 313 317 325 340 352 408 421 425 431 441 442 444 456 467 478 492 528 532 560 562 588 591 595 602 622 624 640 644 645 646 658 669 712 730 733 738 739 754 757 772 777 815 816 820 822 823 829 847 854 876 894 896 905 917 917 935 937 937 939 940 951 952 952 964 966 966 967 971 978 979 989 990 994 997 1010 1043 1058 1062 1064 1065 1072 1079 1082 1094 1097 1098 1116 1121 1124 1126 1128 1130 1138 1145 1152 1174 1176 1187 1187 1190 1201 1201 1202 1217 1225 1232 1236 1252 1258 1268 1270 1279 1280 1289 1296 1306 1309 1311 1330 1336 1336 1341 1342 1350 1351 1353 1366 1393 1395 1398 1404 1407 1407 1408 1408 1427 1428 1429 1429 1432 1461 1467 1477 1482 1489 1491 1493 1496 1497 1498 1499 1500 1501 1503 1506 1506 1507 1508 1508 1512 1516 1518 1518 1520 1520 1523 1525 1526 1529 1596 1602 1624 1634 1636 1637 1638 2997 3008 3009 3031 3031 3031 3032 3038 3038 3039 3040 3044 3051 3054 3062 3077 3079 3087 3090 3092 3096 3097 3097 3102 3106 3107 3109 3111 3111 3116 3116 3118 3118 3122 3124 3125 3126 3130 3141 3142 3144 3149 3154 3163 3163 3166 3180 3185 3189 3191 3258 3283
TS1-2e'	**-136i** 12 19 28 31 37 44 46 53 55 59 63 69 75 81 83 86 102 110 119 129 130 133 138 150 160 167 171 172 183 185 208 211 219 228 237 241 242 252 256 258 261 267 270 277 281 283 298 302 304 307 313 318 329 346 355 402 417 424 429 434 441 444 453 459 476 485 528 531 557 564 584 585 590 594 606 620 641 643 643 646 670 673 706 714 732 735 737 754 755 770 775 815 816 818 819 821 833 854 865 878 894 896 904 914 917 931 935 937 938 940 947 950 952 963 965 966 968 970 973 975 988 988 988 993 1022 1051 1056 1062 1063 1065 1078 1080 1082 1089 1095 1108 1114 1117 1124 1125 1128 1137 1139 1146 1148 1171 1176 1185 1185 1188 1200 1201 1202 1215 1221 1233 1236 1250 1258 1259 1270 1277 1280 1283 1295 1304 1306 1311 1327 1334 1335 1338 1341 1344 1349 1355 1367 1391 1394 1398 1401 1406 1407 1409 1411 1422 1427 1428 1431 1432 1452 1466 1482 1483 1486 1492 1492 1493 1496 1496 1498 1499 1500 1502 1504 1506 1507 1507 1508 1512 1518 1519 1520 1522 1522 1523 1526 1528 1552 1607 1609 1631 1635 1636

	1638 1639 2995 3005 3011 3030 3031 3031 3037 3037 3040 3040 3042 3043 3045 3050 3066 3073 3078 3083 3087 3087 3092 3093 3098 3101 3107 3109 3110 3111 3112 3116 3117 3121 3122 3124 3125 3129 3135 3135 3138 3142 3146 3152 3153 3155 3163 3166 3182 3190 3192 3200 3262 3291
INT2e	12 17 23 29 35 39 46 49 55 56 58 64 69 71 75 80 100 116 126 128 130 133 147 161 162 172 177 182 194 226 227 233 234 239 242 248 251 252 253 255 259 265 277 280 286 297 307 310 315 316 318 323 328 338 350 386 422 422 431 444 445 454 455 481 504 527 531 557 559 589 592 595 602 620 624 634 642 643 647 661 668 689 707 729 731 739 754 773 778 779 789 798 815 815 821 824 828 855 872 891 894 894 920 923 930 938 938 941 941 942 950 953 953 956 966 967 967 968 974 981 990 991 992 996 1023 1034 1062 1062 1065 1066 1076 1079 1082 1096 1098 1110 1119 1124 1124 1126 1128 1138 1143 1145 1149 1160 1174 1176 1187 1188 1191 1201 1202 1203 1228 1234 1246 1250 1258 1259 1271 1272 1277 1280 1281 1292 1307 1312 1314 1316 1332 1338 1344 1346 1348 1351 1351 1354 1367 1395 1397 1399 1409 1409 1411 1411 1415 1429 1431 1431 1432 1436 1470 1483 1491 1492 1494 1497 1497 1498 1501 1502 1502 1503 1504 1505 1505 1506 1507 1507 1513 1516 1517 1519 1519 1519 1525 1526 1527 1529 1597 1621 1635 1637 1638 1639 1687 3008 3011 3025 3030 3031 3032 3034 3034 3035 3036 3042 3050 3052 3056 3068 3069 3075 3083 3087 3089 3093 3100 3108 3110 3110 3113 3115 3115 3115 3116 3117 3118 3120 3122 3123 3124 3124 3129 3129 3132 3134 3136 3137 3143 3163 3165 3180 3182 3188 3190 3255 3281
INT2e’	10 23 27 30 33 41 42 49 55 57 63 69 72 74 78 82 90 99 115 127 128 129 138 145 160 163 165 175 190 218 224 229 236 239 241 242 252 253 257 260 261 264 270 277 280 287 299 303 308 313 318 326 335 337 357 408 419 424 430 441 443 445 450 459 479 528 532 537 557 586 592 594 597 614 623 634 641 642 645 670 680 695 712 735 738 748 754 771 777 777 796 814 815 816 820 824 834 855 865 892 895 895 917 920 926 935 937 940 941 942 950 951 952 963 965 966 966 968 969 979 985 990 991 1004 1017 1030 1056 1060 1061 1065 1068 1078 1081 1094 1098 1100 1116 1122 1125 1126 1127 1138 1143 1147 1149 1174 1176 1181 1187 1188 1193 1201 1202 1202 1211 1226 1238 1246 1248 1257 1265 1269 1278 1279 1288 1289 1303 1308 1310 1311 1333 1339 1341 1343 1343 1348 1350 1363 1379 1390 1393 1394 1403 1408 1409 1410 1410 1428 1430 1430 1433 1439 1469 1479 1485 1488 1491 1492 1496 1496 1497 1499 1501 1502 1503 1504 1506 1507 1507 1507 1508 1517 1517 1519 1520 1522 1525 1526 1526 1530 1599 1634 1636 1636 1638 1644 1694 3009 3016 3030 3031 3033 3034 3035 3035 3036 3044 3044 3045 3053 3055 3064 3078 3083 3084 3086 3086 3092 3092 3103 3105 3110 3110 3110 3114 3114 3114 3116 3116 3119 3120 3121 3123 3124 3124 3125 3137 3138 3138 3143 3148 3163 3166 3181 3185 3189 3192 3259 3282
TS2-3e	**-237i** 16 24 29 34 37 41 45 53 61 61 66 71 74 81 82 92 103 116 120 129 135 146 161 163 169 172 183 212 219 225 226 231 234 239 244 252 258 259 266 274 278 281 286 299 299 306 308 310 311 317 322 330 338 345 369 410 417 423 438 442 443 457 466 476 505 519 528 534 559 582 586 590 596 605 619 624 640 644 646 664 670 688 704 717 734 738 755 771 772 777 791 814 816 818 820 822 826 859 882 895 895 915 916 920 933 936 937 937 940 941 947 952 955 964 965 969 970 978 980 986 987 991 999 1018 1023 1039 1059 1062 1066 1077 1080 1080 1084 1095 1096 1119 1124 1125 1128 1128 1134 1138 1140 1143 1147 1171 1174 1176 1187 1188 1201 1202 1203 1222 1226 1242 1252 1259 1262 1270 1273 1280 1281 1289 1305 1311 1313 1316 1320 1329 1335 1340 1343 1346 1347 1352 1362 1369 1394 1398 1402 1406 1408 1408 1409 1415 1425 1427 1428 1431 1432 1453 1483 1484 1488 1494 1495 1497 1498 1499 1501 1503 1503 1504 1505 1506 1506 1507 1509 1513 1515 1517 1518 1518 1522 1523 1526 1527 1533 1591 1606 1634 1635 1637 1638 1660 3003 3014 3017 3028 3030 3030 3032 3033 3038 3039 3040 3041 3048 3048 3058 3079 3091 3091 3094 3094 3094 3099 3100 3106 3106 3108 3112 3112 3112 3114 3117 3119 3121 3122 3123 3124 3126 3128 3128 3136 3141 3147 3148 3150 3162 3162

	3178 3182 3187 3203 3259 3284
TS2-3e’	**-218i** 18 24 32 39 43 48 51 61 65 73 76 78 81 86 92 98 112 116 130 135 150 161 167 171 173 184 197 214 222 225 227 229 232 239 249 261 264 265 269 276 279 279 283 287 296 300 301 303 310 313 325 334 344 355 406 414 416 425 439 441 445 451 464 473 478 513 528 534 550 559 582 589 596 601 618 620 640 643 643 646 665 690 706 731 738 752 755 769 770 775 798 815 815 817 819 830 831 873 883 895 895 914 915 931 936 936 937 939 942 947 950 952 958 964 965 967 971 975 979 988 989 993 998 1016 1023 1047 1064 1065 1067 1067 1081 1084 1093 1096 1117 1120 1122 1123 1125 1128 1132 1142 1142 1148 1162 1170 1175 1178 1186 1188 1203 1203 1208 1209 1222 1239 1257 1259 1261 1266 1279 1281 1286 1297 1308 1310 1310 1316 1318 1331 1339 1346 1347 1349 1349 1357 1368 1373 1391 1394 1399 1405 1407 1408 1408 1410 1425 1427 1430 1430 1431 1453 1483 1485 1488 1490 1491 1496 1497 1498 1499 1502 1503 1504 1506 1506 1506 1507 1508 1509 1517 1518 1520 1521 1523 1526 1526 1527 1532 1599 1609 1634 1635 1637 1639 1667 3002 3010 3018 3025 3029 3031 3033 3034 3035 3037 3041 3044 3047 3050 3058 3074 3084 3086 3087 3090 3098 3099 3101 3102 3108 3108 3111 3111 3112 3113 3116 3120 3122 3124 3125 3126 3127 3129 3130 3132 3140 3151 3152 3153 3163 3165 3186 3187 3194 3203 3263 3288
INT3e	4 24 26 30 34 39 42 44 50 51 55 56 63 68 75 79 84 99 107 122 124 126 132 150 158 160 170 174 186 208 214 216 223 225 231 239 244 250 250 257 261 264 270 274 279 281 300 303 308 310 314 318 328 335 363 379 411 418 420 430 441 443 455 469 477 498 527 528 546 556 561 587 591 593 610 622 625 641 642 643 645 668 699 706 722 733 737 753 771 776 779 815 816 820 822 823 833 854 864 882 890 894 895 915 916 919 935 936 938 941 942 949 950 951 953 966 966 966 967 974 984 989 991 1019 1036 1051 1061 1064 1064 1071 1079 1082 1088 1092 1096 1110 1121 1124 1125 1126 1127 1129 1137 1143 1145 1159 1173 1175 1187 1188 1201 1201 1202 1227 1249 1252 1256 1258 1265 1277 1278 1279 1287 1300 1310 1312 1316 1330 1333 1339 1343 1345 1347 1351 1354 1360 1368 1388 1395 1397 1401 1405 1407 1408 1409 1409 1427 1428 1429 1433 1436 1476 1479 1485 1490 1493 1494 1496 1496 1497 1498 1500 1501 1502 1502 1505 1506 1506 1507 1514 1516 1516 1519 1520 1520 1523 1524 1524 1526 1583 1601 1634 1635 1637 1638 1644 1677 2987 2998 3009 3015 3017 3020 3031 3032 3032 3032 3038 3041 3042 3042 3043 3047 3076 3088 3089 3092 3094 3095 3099 3100 3108 3110 3112 3112 3113 3114 3116 3117 3118 3120 3122 3123 3124 3125 3137 3138 3138 3149 3153 3155 3163 3165 3181 3185 3189 3192 3254 3279
INT3e’	8 15 22 26 31 35 36 40 46 55 58 63 67 73 74 84 90 107 119 125 129 134 142 145 156 162 167 173 186 202 206 220 226 230 235 239 251 253 256 259 262 263 270 273 279 283 295 301 304 306 310 314 326 332 340 388 411 418 420 433 440 444 458 476 486 513 527 528 543 557 562 585 586 589 595 614 621 640 642 645 662 670 697 721 731 733 737 753 772 778 784 806 814 816 819 822 829 845 872 882 894 895 896 918 919 934 936 937 938 940 949 950 950 950 956 966 967 967 969 973 982 988 991 9931019 1058 1062 1064 1065 1069 1080 1083 1090 1095 1101 1108 1117 1121 1122 1127 1127 1137 1139 1142 1144 1170 1173 1175 1187 1187 1201 1203 1215 1225 1231 1253 1259 1263 1266 1272 1277 1280 1286 1308 1310 1311 1313 1326 1335 1341 1343 1346 1347 1354 1358 1370 1379 1384 1394 1396 1398 1399 1408 1409 1409 1410 1425 1430 1431 1433 1438 1480 1482 1487 1490 1491 1494 1496 1497 1497 1499 1500 1501 1502 1503 1506 1507 1507 1509 1512 1519 1520 1520 1521 1522 1524 1526 1527 1527 1559 1603 1632 1633 1636 1637 1641 1662 2987 3002 3004 3032 3032 3033 3033 3033 3034 3040 3041 3043 3044 3050 3061 3065 3087 3088 3089 3091 3092 3098 3106 3110 3112 3113 3113 3115 3118 3118 3120 3120 3121 3122 3122 3124 3125 3126 3127 3131 3137 3152 3153 3155 3165 3165 3185 3188 3193 3194 3262 3285
TS3e	**-260i** 20 22 27 33 35 43 48 53 56 58 63 70 75 78 81 89 108 113 115 130 133 134 158 160 162 170 188 208 218 222 227 230 233 234 240 248 251 253 258 264 268 270 280 283 291

	300 301 305 314 316 327 330 339 370 395 413 417 420 434 440 443 458 476 487 501 517 528 529 551 560 585 587 594 603 619 621 641 644 645 667 669 689 698 727 736 740 754 772 777 787 798 815 815 816 820 821 826 868 882 894 895 901 905 915 917 930 935 936 936 940 949 950 951 964 966 968 969 971 973 988 989 993 1019 1022 1041 1061 1062 1064 1067 1080 1082 1090 1096 1104 1109 1121 1122 1126 1127 1131 1139 1145 1147 1154 1166 1172 1174 1186 1187 1200 1202 1202 1223 1253 1258 1259 1260 1261 1272 1278 1279 1286 1299 1308 1310 1320 1326 1331 1335 1339 1342 1345 1347 1348 1352 1356 1368 1393 1395 1399 1406 1407 1407 1408 1414 1418 1424 1428 1429 1430 1431 1471 1488 1489 1490 1492 1494 1496 1497 1498 1499 1500 1500 1501 1503 1506 1506 1507 1508 1511 1515 1517 1518 1519 1521 1522 1524 1526 1528 1550 1605 1633 1635 1637 1638 1672 2997 2999 3012 3013 3027 3030 3033 3033 3037 3038 3040 3041 3042 3048 3069 3081 3085 3086 3087 3092 3096 3098 3101 3103 3107 3108 3108 3111 3112 3116 3116 3120 3121 3124 3124 3128 3129 3129 3132 3134 3138 3149 3150 3151 3162 3164 3183 3184 3191 3193 3257 3281
TS3e’	**-247i** 22 27 30 35 42 43 50 56 60 65 68 71 82 86 95 113 114 119 131 135 152 156 164 166 171 177 185 209 214 219 225 228 232 236 241 250 252 256 259 262 264 271 282 286 296 300 302 307 311 320 330 332 338 376 381 410 412 419 432 439 441 444 459 476 493 517 526 528 530 558 583 587 596 601 608 619 622 640 643 643 666 673 694 726 736 754 768 771 776 787 797 814 815 817 819 820 827 855 869 887 893 894 915 917 917 934 935 936 937 938 945 948 949 964 965 967 970 972 984 988 989 1006 1009 1026 1036 1062 1062 1064 1072 1081 1083 1088 1095 1102 1105 1119 1122 1126 1127 1140 1144 1146 1149 1163 1170 1173 1174 1186 1187 1190 1201 1202 1220 1225 1254 1254 1258 1266 1273 1276 1278 1282 1303 1309 1313 1319 1323 1325 1332 1340 1345 1346 1349 1353 1357 1372 1374 1395 1396 1399 1404 1405 1406 1407 1409 1422 1426 1428 1428 1430 1444 1472 1485 1488 1490 1491 1494 1496 1496 1497 1499 1500 1501 1502 1505 1506 1508 1508 1510 1511 1515 1518 1519 1520 1522 1523 1526 1526 1527 1537 1610 1631 1633 1636 1637 1655 2996 2997 3010 3016 3028 3032 3033 3037 3038 3041 3042 3042 3045 3049 3075 3077 3082 3087 3093 3093 3094 3095 3100 3103 3107 3109 3109 3110 3112 3112 3119 3120 3120 3122 3126 3126 3131 3135 3136 3136 3145 3145 3153 3159 3163 3164 3184 3187 3191 3202 3264 3291
3e	66 106 121 137 168 204 236 286 289 330 360 401 429 473 506 543 586 621 644 684 766 807 823 847 857 884 895 936 976 982 1002 1026 1039 1064 1076 1085 1092 1127 1157 1162 1190 1211 1231 1257 1288 1344 1346 1369 1376 1395 1411 1475 1494 1497 1499 1506 1507 1516 1519 1624 1684 1696 3023 3028 3031 3033 3043 3056 3073 3084 3089 3095 3099 3110 3120 3134 3136 3168
3e’	72 102 125 136 143 187 246 248 287 317 358 396 452 462 535 552 594 622 634 698 752 766 836 849 871 890 904 922 939 988 993 1024 1041 1051 1064 1081 1122 1136 1155 1180 1188 1223 1255 1266 1281 1307 1315 1326 1348 1351 1376 1383 1389 1419 1480 1490 1492 1500 1504 1510 1513 1516 1633 1676 1691 3023 3024 3037 3042 3042 3056 3062 3083 3086 3095 3098 3117 3125 3133 3134 3160

Table S15. The total energies (*E*$_{tot}$: a.u), zero-point energies (*ZPE*:a.u.) and gibbs free energies (*G*:a.u) for reaction **a**, computed for the Diels-Alder reaction in toluene, in the absence of catalyst.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1a	-350.098595	0.179625	-349.959494
2a	-231.262168	0.090603	-231.202436
TS	-581.263378	0.272478	-581.034955
3a-six	-581.455636	0.280939	-581.214108

Table S16. The total energies (*E*$_{tot}$: a.u), zero-point energies (*ZPE*:a.u.) and gibbs free energies (*G*:a.u) for reaction **a**, computed for radical reaction in toluene, in the absence of catalyst.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1a	-350.098595	0.179625	-349.959494
2a	-231.262168	0.090603	-231.202436
TS1	-581.254791	0.266315	-581.040304
INT1	-581.334358	0.271743	-581.109372
TS2	-581.331937	0.272226	-581.102778
3a	-581.486727	0.281840	-581.244597

Table S17. The total energies (*E*$_{tot}$: a.u), zero-point energies (*ZPE*:a.u.) and gibbs free energies (*G*:a.u) for reaction **a**.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1a	-350.098595	0.179625	-349.959494
2a	-231.262168	0.090603	-231.202436
Ni	-1507.974017	0.000000	-1507.989755
COM1a	-2089.487175	0.273692	-2089.263394
TS1a’	-2089.447182	0.276097	-2089.214606
INT1a’	-2089.494524	0.278091	-2089.259736
TS1a	-2089.442635	0.273539	-2089.218111
INT1a	-2089.494954	0.275074	-2089.267540
TS1-3a	-2089.437745	0.276801	-2089.203642
TS1-2a	-2089.466162	0.275299	-2089.233619
INT2a	-2089.493295	0.278423	-2089.256765
TS2-3a	-2089.463028	0.277338	-2089.227568
INT3a	-2089.500275	0.278963	-2089.263623
TS3-4a	-2089.185301	0.277230	-2089.227333
INT4a	-2089.505883	0.277113	-2089.272516
TS4a	-2089.480229	0.276892	-2089.244525
3a+Ni	-2089.530394	0.281317	-2089.290846

Table S18. The total energies (*E*$_{tot}$: a.u), zero-point energies (*ZPE:*a.u.) and gibbs free energies (*G:*a.u) for reaction **b**.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1b	-805.911284	0.264944	-805.699478
2b	-501.646578	0.199249	-501.483936
Ni	-1507.974017	0.000000	-1507.989755
COM1b	-2815.687665	0.467156	-2815.290824
TS1b’	-2815.643304	0.469157	-2815.238876
INT1b’	-2815.692066	0.471208	-2815.285650
TS1b’	-2815.648244	0.467188	-2815.250767
INT1b	-2815.701347	0.468458	-2815.302518
TS1-3b	-2815.639597	0.470003	-2815.235166
TS1-2b	-2815.669324	0.468557	-2815.265398
INT2b	-2815.695998	0.471440	-2815.288407
TS2-3b	-2815.667909	0.470192	-2815.261923
INT3b	-2815.690549	0.472936	-2815.281368
TS3-4b	-2815.655983	0.470076	-2815.249677
INT4b	-2815.712453	0.470985	-2815.305120
TS4b	-2815.671704	0.470606	-2815.262778
3b+Ni	-2815.708960	0.473528	-2815.298713

Table S19. The total energies (*E*$_{tot}$: a.u), zero-point energies (*ZPE:*a.u.) and gibbs free energies (*G:*a.u) for reaction **c**.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1a	-350.098595	0.179625	-349.959494
2a	-231.262168	0.090603	-231.202436
Ni-$(P(CH_3)_3)_2$	-2430.292648	0.228823	-2430.11039
COM2c	-3011.691316	0.502985	-3011.26566
TS1c’	-3011.638558	0.502837	-3011.204378
INT1c’	-3011.695404	0.508181	-3011.251258
COM1c	-2780.427966	0.410971	-2780.080451
TS1c	-2780.394063	0.409760	-2780.041830
INT1c	-2780.421511	0.411596	-2780.066817
TS1-2c’	-3011.648411	0.506557	-3011.203023
TS1-2c	-3011.686085	0.506825	-3011.238071
INT2c	-3011.738699	0.509639	-3011.289508
TS2-3c	-3011.701518	0.506813	-3011.259966
INT3c	-3011.756011	0.510946	-3011.304475
TS3c	-3011.733687	0.510435	-3011.281875
3a	-581.486727	0.281840	-581.244597

Table S20. The total energies (E_{tot}: a.u), zero-point energies (*ZPE:*a.u.) and gibbs free energies (*G:*a.u) for reaction **d**.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1a	-350.098595	0.179625	-349.959494
2a	-231.262168	0.090603	-231.202436
Ni-IPr	-2668.215267	0.570400	-2667.710093
COM2d	-3249.607761	0.843508	-3248.862684
TS1d’	-3249.556587	0.842272	-3248.802619
INT1d’	-3249.641620	0.848913	-3248.877985
COM1d	-3018.367041	0.751645	-3017.701259
TS1d	-3018.361765	0.753799	-3017.683033
INT1d	-3018.392069	0.754686	-3017.713094
TS1-2d’	-3249.589691	0.847853	-3248.824141
TS1-2d	-3249.641473	0.847980	-3248.873332
INT2d	-3249.693193	0.851647	-3248.922517
TS2-3d	-3249.663704	0.850261	-3248.892419
INT3d	-3249.683464	0.850149	-3248.916298
TS3d	-3249.685735	0.850884	-3248.913421
3a	-581.486727	0.281840	-581.244597

Table S21. The total energies (E_{tot}: a.u), zero-point energies (*ZPE:*a.u.) and gibbs free energies (*G:*a.u) for reaction **e**.

	E_{tot} /a.u.	ZPE/a.u.	G/a.u.
1c	-310.771907	0.150738	-310.658406
2a	-231.262168	0.090603	-231.202436
Ni-IPr	-2668.215267	0.570400	-2667.710093
COM1e	-2979.062015	0.725560	-2978.409795
TS1e	-2979.044389	0.725108	-2978.394177
INT1e	-2979.077724	0.726046	-2978.428353
TSee’	-2979.069165	0.725994	-2978.417337
INT1e’	-2979.072134	0.726474	-2978.420470
TS1-2e	-3210.328035	0.819785	-3209.588514
TS1-2e’	-3210.325953	0.819629	-3209.586105
INT2e	-3210.380762	0.823912	-3209.636984
INT2e’	-3210.377007	0.823294	-3209.633968
TS2-3e	-3210.348433	0.822066	-3209.604033
TS2-3e’	-3210.348545	0.822791	-3209.601541
INT3e	-3210.382413	0.822649	-3209.642186
INT3e’	-3210.380632	0.823212	-3209.639713
TS3e	-3210.372722	0.822626	-3209.628187
TS3e’	-3210.368201	0.822817	-3209.621699
3e	-542.168842	0.254015	-541.952266
3e’	-542.171307	0.253969	-541.954965