Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

On the Formation of Phenyldiacetylene (C_6H_5CCCCH) and D5-Phenyldiacetylene (C_6D_5CCCCH) Studied under Single Collision Conditions

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Electronic Supplementary Information

Table S1. Optimized Cartesian coordinates, total energies, ZPE, rotational constants, and vibrational frequencies of various structures involved in the $C_6H_5 + C_4H_2$ reaction.

Species	Total Energy (a.u)	ZPE correction (a.u)	Rotational Constants (x,y,z) in GHz	Cartesian Coordinates (x,y,z) in Å	Harmonic Frequencies (cm^{-1})
i1	-384.2475022	0.127747	4.47680, 0.64992, 0.56753	6 0.390070 -0.426673 0.000001 6 0.577725 0.965647 0.000001 6 2.802875 -0.712283 -0.000001 6 1.521883 -1.255437 0.000000 6 1.856214 1.505403 0.000000 6 2.975226 0.669702 -0.000001 6 -0.947053 -1.034909 0.000002 6 -2.103240 -0.403927 -0.000002 6 -3.328830 0.070589 -0.000004 6 -4.464134 0.553044 0.000001 1 -0.289496 1.616573 0.000002 1 3.666181 -1.368231 -0.000001 1 1.391125 -2.332682 0.000000 1 1.984923 2.582064 0.000000 1 3.972376 1.094897 -0.000002 1 -0.959957 -2.128446 0.000006 1 -5.449566 0.948876 0.000007	37 803 1484 52 829 1523 196 855 1618 233 934 1638 248 952 1780 305 981 1987 366 1004 3051 400 1016 3159 414 1049 3165 472 1104 3174 515 1182 3181 596 1198 3191 601 1223 3468 633 1292 704 1349 745 1366
i2	-384.240000	0.152215	4.40944, 0.61309, 0.56804	6 1.068952 -1.226009 0.062132 6 2.431917 -1.210659 -0.160304 6 3.127306 -0.000005 -0.273565 6 2.431920 1.210656 -0.160310 6 1.068958 1.226014 0.062127 6 0.339158 0.000007 0.185456 6 -1.014464 -0.000010 0.393305 6 -2.263294 0.000007 0.788995 6 -3.394504 0.000004 -0.083008 6 -4.375120 -0.000004 -0.781290 1 0.532292 -2.162850 0.147085 1 2.967243 -2.149645 -0.248006 1 4.196332 -0.000006 -0.449397 1 2.967256 2.149635 -0.248022 1 0.532303 2.162859 0.147079 1 -2.489490 0.000025 1.860536 1 -5.230903 -0.000019 -1.410495	21 775 1454 73 812 1483 157 826 1561 168 890 1589 255 953 1860 383 973 2206 386 988 3026 413 993 3165 474 1032 3171 517 1100 3188 596 1149 3193 626 1174 3198 640 1205 3476 680 1291 685 1333 750 1347

i3	-384.1919617	0.128679	2.92640, 1.34010, 0.93926	6 0.125707 0.777229 0.140009 6 0.131864 -0.742297 0.399773 6 -2.302450 0.721970 -0.073563 6 -1.129449 1.425569 0.059239 6 -1.150045 -1.414842 -0.006532 6 -2.289359 -0.711949 -0.178508 6 1.336640 1.490274 -0.040047 6 2.438487 0.663433 -0.108800 6 2.406675 -0.597082 -0.175002 6 1.404805 -1.482794 -0.088742 1 0.175437 -0.827581 1.513751 1 -3.242088 1.252055 -0.175626 1 -1.145388 2.510641 0.029325 1 -1.143789 -2.496709 -0.085800 1 -3.212986 -1.227870 -0.418487 1 1.330091 2.564994 -0.181864 1 1.401469 -2.552591 -0.248268	112 854 1400 140 867 1443 254 950 1467 345 975 1499 395 996 1636 428 1000 1816 448 1034 2734 496 1051 3155 515 1131 3158 561 1165 3173 603 1187 3175 640 1212 3189 660 1230 3199 696 1271 779 1304 820 1322
i4	-384.2297167	0.128599	3.03656 0.96050 0.72969	6 1.037502 1.227028 -0.001591 6 2.381518 0.880242 -0.001795 6 2.761121 -0.463257 -0.000223 6 1.782859 -1.452745 0.001547 6 0.433302 -1.106753 0.001755 6 0.043901 0.236881 0.000261 6 -1.396860 0.616124 0.000858 6 -1.830243 1.872116 0.002553 6 -2.397357 -0.414022 -0.000990 6 -3.255403 -1.259517 -0.002329 1 0.745284 2.271326 -0.002983 1 3.136985 1.657992 -0.003282 1 3.811153 -0.732875 -0.000442 1 2.067420 -2.498967 0.002742 1 -0.324154 -1.881115 0.003123 1 -2.786436 2.372166 0.004383 1 -4.012293 -2.005109 -0.003816	26 737 1477 133 785 1525 144 851 1591 249 856 1627 289 937 1644 408 984 2191 412 1005 3161 428 1017 3168 450 1035 3177 589 1060 3187 612 1106 3194 635 1183 3253 641 1203 3476 664 1260 687 1328 707 1356
i5	-384.203412	0.128187	3.71220 0.84264 0.68675	6 0.152739 1.635303 0.000000 6 1.420903 2.199365 0.000000 6 2.552393 1.380778 0.000000 6 2.410251 -0.005621 0.000000 6 1.142341 -0.576927 0.000000 6 0.000000 0.237968 0.000000 6 -1.310070 -0.361135 0.000000 6 -2.626197 -0.267692 0.000000 6 -2.095768 -1.612621 0.000000 6 -2.231521 -2.901407 0.000000 1 -0.727755 2.267738 0.000000 1 1.532045 3.277715 0.000000 1 3.541414 1.824597 0.000000 1 3.288180 -0.641369 0.000000 1 1.021903 -1.653637 0.000000 1 -3.506732 0.355594 0.000000 1 -1.639485 -3.798706 0.000000	56 796 1477 100 855 1518 122 894 1614 279 934 1637 305 938 1639 408 985 1849 414 1009 3166 430 1016 3173 475 1047 3182 517 1049 3190 561 1104 3196 632 1184 3238 693 1195 3283 703 1218 747 1324 761 1353

p2 + H	-384.1908557	0.121726	3.13639 1.35680 0.94709	6 2.435722 0.626558 0.000062 6 1.363635 1.464512 -0.000057 6 2.435790 -0.626559 0.000062 6 1.363654 -1.464480 -0.000057 6 0.128231 -0.723010 -0.000033 6 0.128217 0.723021 -0.000033 6 -1.121168 1.400161 0.000003 6 -2.305918 0.706895 0.000020 6 -2.305907 -0.706925 0.000020 6 -1.121144 -1.400168 0.000003 1 1.366795 2.547603 -0.000005 1 1.366812 -2.547573 -0.000006 1 -1.122498 2.484967 0.000004 1 -3.247672 1.243958 0.000030 1 -3.247651 -1.244003 0.000031 1 -1.122454 -2.484975 0.000004	190 894 1506 201 897 1561 360 966 1648 372 996 1979 416 1042 3160 464 1091 3165 485 1146 3177 520 1175 3184 570 1215 3187 607 1223 3190 638 1254 3196 750 1310 3238 752 1331 3283 780 1374 852 1454 862 1486
p1 + H	-384.1871344	0.119371	5.69030 0.57297 0.52056	6 -0.389044 -0.000011 -0.000045 6 -1.103035 1.212390 -0.000020 6 -2.492223 -1.206751 0.000030 6 -1.103051 -1.212398 -0.000020 6 -2.492205 1.206765 0.000030 6 -3.190883 0.000011 0.000056 6 1.031978 -0.000015 -0.000092 6 2.245622 -0.000002 -0.000093 6 3.606766 0.000008 0.000006 6 4.815155 0.000001 0.000099 1 -0.556494 2.147514 -0.000041 1 -3.031943 -2.146864 0.000049 1 -0.556528 -2.147534 -0.000041 1 -3.031914 2.146884 0.000049 1 -4.274838 0.000020 0.000096 1 5.877233 -0.000002 0.000183	71 778 1608 74 854 1640 198 937 2160 226 980 2317 366 983 3167 374 1006 3176 409 1016 3186 485 1051 3194 511 1102 3198 584 1184 3478 587 1201 3196 633 1304 3238 639 1311 3283 651 1353 704 1473 705 1524
i1-p1ts	-384.1788665	0.120274	5.26030 0.57638 0.52138	6 0.409230 0.120849 0.051756 6 1.256186 1.237591 -0.041238 6 2.357524 -1.324143 0.023581 6 0.978944 -1.166213 0.083541 6 2.634001 1.069029 -0.104257 6 3.189482 -0.208982 -0.070978 6 -1.014055 0.247348 0.091254 6 -2.218147 0.052147 0.003608 6 -3.568002 -0.065090 -0.053153 6 -4.771365 -0.177444 -0.108040 1 0.821709 2.229072 -0.061715 1 2.783911 -2.320371 0.051100 1 0.329100 -2.029629 0.155640 1 3.276580 1.938896 -0.177441 1 4.265012 -0.335697 -0.117310 1 -1.170943 2.081242 1.048473 1 -5.828154 -0.274067 -0.155192	-574 649 1352 40 703 1473 82 709 1521 103 774 1609 195 853 1638 245 937 2132 360 983 2250 388 984 3167 410 1006 3177 442 1016 3187 485 1051 3195 507 1103 3199 562 1184 3476 575 1202 632 1288 636 1315

i1-i3ts	-384.1692752	0.127846	2.83555 1.28937 0.92922	6 -0.072212 -0.740887 0.302842 6 -0.034127 0.711126 0.509530 6 2.286961 -0.707875 -0.301968 6 1.117841 -1.403286 -0.046412 6 1.213928 1.383540 0.248225 6 2.321089 0.700268 -0.182503 6 -1.330118 -1.463118 0.222256 6 -2.416394 -0.741000 -0.150798 6 -2.408194 0.554167 -0.362023 6 -1.580713 1.530314 -0.333943 1 -0.531175 1.043468 1.424828 1 3.177189 -1.244238 -0.609224 1 1.092373 -2.480996 -0.171998 1 1.268303 2.452524 0.426007 1 3.241548 1.234085 -0.391168 1 -1.303289 -2.549142 0.231315 1 -1.533314 2.604808 -0.340977	-571 835 1442 135 847 1451 168 881 1523 260 954 1552 338 982 1613 420 985 1741 437 1023 3033 460 1049 3143 508 1097 3157 567 1120 3161 574 1168 3176 619 1192 3189 650 1202 3285 710 1284 740 1338 756 1349
i3-Hts	-384.1680358	0.123427	3.02625 1.34149 0.94316	6 0.126378 0.747295 0.033810 6 0.127997 -0.718396 0.130437 6 -2.306838 0.717168 -0.031538 6 -1.124403 1.414063 0.019450 6 -1.133003 -1.397167 -0.041378 6 -2.306191 -0.700468 -0.094443 6 1.357109 1.480715 -0.025999 6 2.433466 0.643434 -0.054225 6 2.430301 -0.611194 -0.092404 6 1.376501 -1.461077 -0.064122 1 0.127862 -0.746937 1.821008 1 -3.248859 1.252714 -0.057735 1 -1.131046 2.498866 0.022429 1 -1.128728 -2.480584 -0.082025 1 -3.246351 -1.231039 -0.194127 1 1.360915 2.562904 -0.071445 1 1.378303 -2.542164 -0.115639	-1045 792 1358 181 834 1447 186 860 1478 340 884 1492 360 898 1541 407 966 1641 451 992 1936 475 1033 3162 502 1077 3168 518 1141 3180 565 1163 3185 576 1198 3191 614 1220 3194 637 1241 726 1295 746 1326
i1-i2ts	-384.1644494	0.122376	4.83014 0.58181 0.53646	6 -0.403533 -0.000013 0.217978 6 -1.113584 -1.215576 0.090373 6 -2.476548 1.206294 -0.167378 6 -1.113561 1.215566 0.090403 6 -2.476571 -1.206273 -0.167401 6 -3.168224 0.000019 -0.296593 6 0.983527 -0.000028 0.540213 6 2.266501 0.000023 0.402856 6 3.501673 0.000004 -0.178311 6 4.663874 0.000013 -0.536220 1 -0.580148 -2.153491 0.188978 1 -3.004914 2.147500 -0.272164 1 -0.580106 2.153468 0.189035 1 -3.004956 -2.147466 -0.272207 1 -4.233389 0.000032 -0.495558 1 1.760989 -0.000245 1.587633 1 5.661200 0.000023 -0.901235	-2065 695 1466 27 699 1504 55 757 1587 182 839 1619 191 904 1954 235 942 2151 317 973 2271 392 992 3163 405 1007 3169 434 1043 3183 467 1099 3187 492 1179 3194 520 1194 3474 541 1245 634 1301 682 1351
i1-i4ts	-384.1869485	0.125508	3.08555 0.84628	6 0.011692 -0.000020 0.299189 6 -0.701437 1.230847 0.054696	-591 699 1443 80 725 1469

			0.82251	6 -2.035193 -1.213697 -0.288430 6 -0.701452 -1.230855 0.054584 6 -2.035178 1.213735 -0.288321 6 -2.724412 0.000031 -0.453582 6 1.103028 -0.000103 1.713088 6 1.510576 -0.000020 0.484654 6 2.622641 0.000019 -0.373317 6 3.544002 0.000062 -1.149421 1 -0.169652 2.168124 0.171420 1 -2.557591 -2.151904 -0.443145 1 -0.169677 -2.168149 0.171220 1 -2.557566 2.151962 -0.442950 1 -3.773895 0.000049 -0.721566 1 1.300447 -0.000170 2.773289 1 4.362340 0.000095 -1.827103	83 753 1546 185 799 1583 248 847 1776 313 891 2207 374 966 3159 419 977 3163 428 1002 3181 498 1020 3182 590 1095 3193 617 1163 3246 662 1166 3475 666 1204 672 1292 697 1336
i5-i2ts	-384.1915927	0.126097	3.82405 0.76944 0.65678	6 -1.079650 -1.219488 0.188115 6 -2.444934 -0.981528 0.278835 6 -2.948899 0.306111 0.092409 6 -2.076920 1.360850 -0.176817 6 -0.708453 1.135754 -0.255555 6 -0.190079 -0.161161 -0.087056 6 1.218693 -0.400205 -0.170797 6 2.277727 -1.129481 -0.422229 6 2.895468 0.047239 0.069092 6 3.686429 0.941025 0.449041 1 -0.687375 -2.219032 0.334665 1 -3.119758 -1.802498 0.493869 1 -4.015305 0.487030 0.162933 1 -2.465105 2.363312 -0.316678 1 -0.025264 1.953661 -0.449933 1 2.589362 -2.083410 -0.835421 1 3.947151 1.906248 0.820337	-651 768 1471 18 795 1511 78 852 1604 117 932 1632 256 951 1774 325 982 1878 405 1005 3147 411 1012 3165 426 1046 3173 485 1101 3183 503 1132 3190 533 1183 3196 555 1196 3400 633 1212 703 1309 752 1351
i4-i5ts	-384.1927374	0.125811	3.50529 0.87687 0.70141	6 0.011692 -0.000020 0.299189 6 -0.701437 1.230847 0.054696 6 -2.035193 -1.213697 -0.288430 6 -0.701452 -1.230855 0.054584 6 -2.035178 1.213735 -0.288321 6 -2.724412 0.000031 -0.453582 6 1.103028 -0.000103 1.713088 6 1.510576 -0.000020 0.484654 6 2.622641 0.000019 -0.373317 6 3.544002 0.000062 -1.149421 1 -0.169652 2.168124 0.171420 1 -2.557591 -2.151904 -0.443145 1 -0.169677 -2.168149 0.171220 1 -2.557566 2.151962 -0.442950 1 -3.773895 0.000049 -0.721566 1 1.300447 -0.000170 2.773289 1 4.362340 0.000095 -1.827103	-707 721 1480 58 751 1523 114 785 1620 127 858 1643 285 940 1710 290 985 1914 405 1008 3163 414 1016 3171 440 1037 3179 493 1056 3186 495 1107 3193 524 1184 3241 572 1198 3418 633 1237 654 1330 709 1355
i2-Hts	-384.1793927	0.120252	5.32269 0.56937 0.52065	6 0.011692 -0.000020 0.299189 6 -0.701437 1.230847 0.054696 6 -2.035193 -1.213697 -0.288430 6 -0.701452 -1.230855 0.054584 6 -2.035178 1.213735 -0.288321 6 -2.724412 0.000031 -0.453582 6 1.103028 -0.000103 1.713088 6 1.510576 -0.000020 0.484654 6 2.622641 0.000019 -0.373317 6 3.544002 0.000062 -1.149421 1 -0.169652 2.168124 0.171420 1 -2.557591 -2.151904 -0.443145 1 -0.169677 -2.168149 0.171220 1 -2.557566 2.151962 -0.442950 1 -3.773895 0.000049 -0.721566 1 1.300447 -0.000170 2.773289 1 4.362340 0.000095 -1.827103	-706 660 1353 64 701 1472 72 708 1520 83 774 1604 209 852 1634 241 935 2131 326 976 2265 378 984 3168 408 1006 3177 444 1014 3187 479 1049 3196 513 1103 3199 562 1184 3478 581 1201 637 1302 644 1311
C_6H_5+C_4H_2-i4ts	-384.1622376	0.124294	2.56933 0.85755 0.67975	6 1.010194 1.180388 -0.406626 6 2.380980 0.899820 -0.458681 6 2.856533 -0.344641 -0.046476 6 1.973058 -1.320216 0.415330	-404 669 1465 15 686 1476 68 728 1580 98 827 1630

				6 0.598310 -1.058662 0.466563 6 0.176416 0.184147 0.049454 6 -2.059193 0.721445 0.181913 6 -2.120187 1.890081 0.554173 6 -2.567203 -0.499530 -0.207984 6 -3.004997 -1.572225 -0.541580 1 0.626236 2.145074 -0.720166 1 3.071744 1.654616 -0.820372 1 3.919248 -0.555417 -0.085560 1 2.348090 -2.287036 0.735262 1 -0.100254 -1.812788 0.811773 1 -1.926590 2.882591 0.884320 1 -3.401947 -2.510685 -0.841776	144 896 1983 237 900 2230 254 965 3153 402 975 3159 407 993 3171 436 1018 3174 526 1050 3185 529 1078 3451 610 1176 3477 612 1179 648 1312 664 1325
C_6H_5+C_4H_2-i1ts	-384.1686775	0.124564	3.27818 0.60731 0.51239	6 -0.639976 0.494558 -0.000226 6 -0.604362 -0.880219 -0.000891 6 -3.007844 0.571283 0.000879 6 -1.785366 1.257346 0.000661 6 -1.835283 -1.548167 -0.000659 6 -3.027192 -0.822775 0.000217 6 1.613809 1.634198 -0.001022 6 2.499307 0.800580 -0.000391 6 3.415519 -0.203919 0.000363 6 4.237040 -1.091190 0.001020 1 0.331372 -1.428226 -0.001565 1 -3.938027 1.130180 0.001572 1 -1.762800 2.342435 0.001188 1 -1.858288 -2.633090 -0.001163 1 -3.976058 -1.347085 0.000393 1 1.049708 2.535022 -0.001734 1 4.960175 -1.869411 0.001602	-195 680 1464 5 685 1475 40 723 1576 60 821 1630 105 894 2063 237 921 2224 267 963 3150 401 977 3158 428 993 3167 501 1018 3175 527 1050 3186 582 1077 3456 607 1176 3476 633 1178 636 1309 659 1325

Table S2. Rate constants (s^{-1}) of various unimolecular reaction steps calculated using RRKM theory at different collision energies in the C_6H_5 + C_4H_2 reaction.

Collision energy (KJ/mole)	0	10	20	30	40	46	50	60
i1=>i3	1.07E-06	9.69E-05	1.36E-03	1.01E-02	5.18E-02	1.21E-01	2.06E-01	6.83E-01
i3=>i1	4.17E+04	1.49E+06	9.57E+06	3.51E+07	9.55E+07	1.57E+08	2.13E+08	4.16E+08
i1=>i2	3.58E-03	1.63E-02	7.56E-02	3.48E-01	1.53E+00	3.54E+00	6.09E+00	2.17E+01
i2=>i1	2.44E-02	1.04E-01	4.56E-01	1.99E+00	8.30E+00	1.86E+01	3.14E+01	1.07E+02
i1=>i4	1.14E+02	4.00E+02	1.19E+03	3.12E+03	7.39E+03	1.18E+04	1.60E+04	3.23E+04
i4=>i1	6.20E+04	1.84E+05	4.71E+05	1.07E+06	2.21E+06	3.28E+06	4.26E+06	7.58E+06
i1=>P1+H	1.83E+00	1.44E+01	7.79E+01	3.25E+02	1.13E+03	2.21E+03	3.37E+03	8.95E+03
i3=>P2+H	3.75E+04	5.45E+05	3.09E+06	1.10E+07	2.96E+07	4.87E+07	6.61E+07	1.30E+08
i2=>i5	7.80E+04	2.00E+05	4.58E+05	9.57E+05	1.86E+06	2.68E+06	3.38E+06	5.84E+06
i5=>i2	1.89E+11	2.88E+11	4.10E+11	5.57E+11	7.29E+11	8.44E+11	9.25E+11	1.14E+12
i2=>P1+H	2.09E+01	1.39E+02	6.65E+02	2.51E+03	7.97E+03	1.49E+04	2.20E+04	5.45E+04
i5=>i4	7.78E+10	1.14E+11	1.57E+11	2.08E+11	2.67E+11	3.06E+11	3.33E+11	4.06E+11
i4=>i5	2.55E+06	5.70E+06	1.15E+07	2.15E+07	3.77E+07	5.12E+07	6.24E+07	9.87E+07