

Global CHIPR Potential Energy Surface for Ground-State C₃H and Exploratory Dynamics Study of Reaction C₂+CH→C₃+H

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Electronic Supplementary Information

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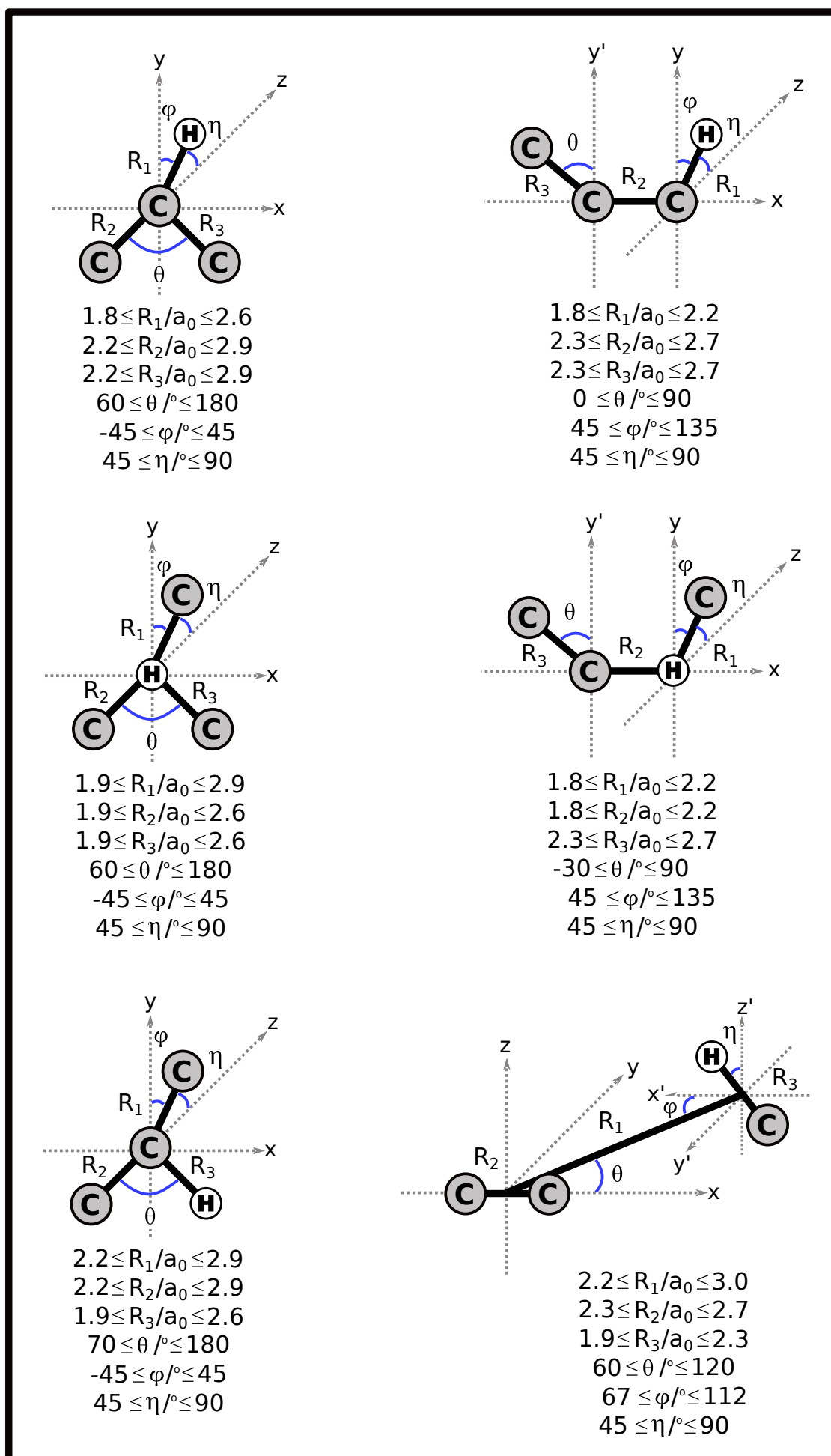


Figure S1: C_3H geometries covered in the *ab initio* calculations.

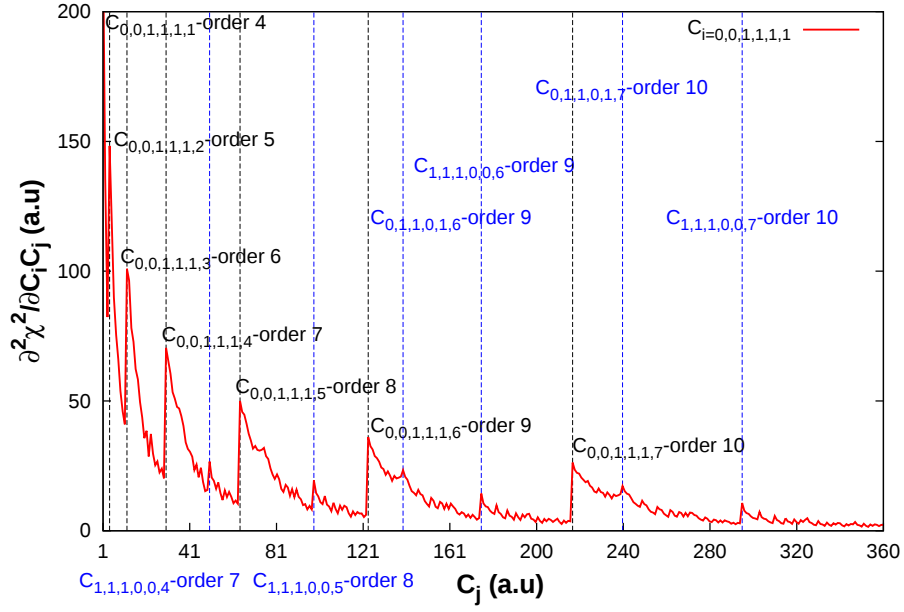


Figure S2: Second derivative of χ^2 with respect to $C_{0,0,1,1,1,1}$ and other coefficients (this is the first row of the matrix $\partial^2 \chi^2 / \partial C_i C_j$ that defines the sensitivity of χ^2 (sum of the least-squares-fit squared deviations) with respect to the various coefficients in the polynomial fit). Corresponding similarly looking profiles are obtained for other rows.

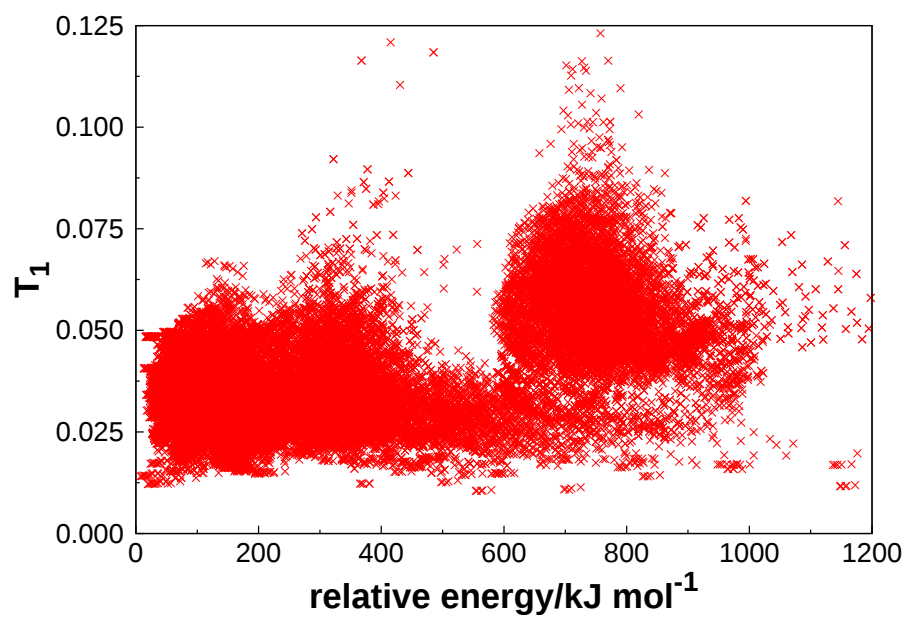


Figure S3: Scatter plot of T_1 values at CCSD(T)/AVTZ level for all *ab initio* data points. Energies defined relative to the *c*-C₃H global minimum.

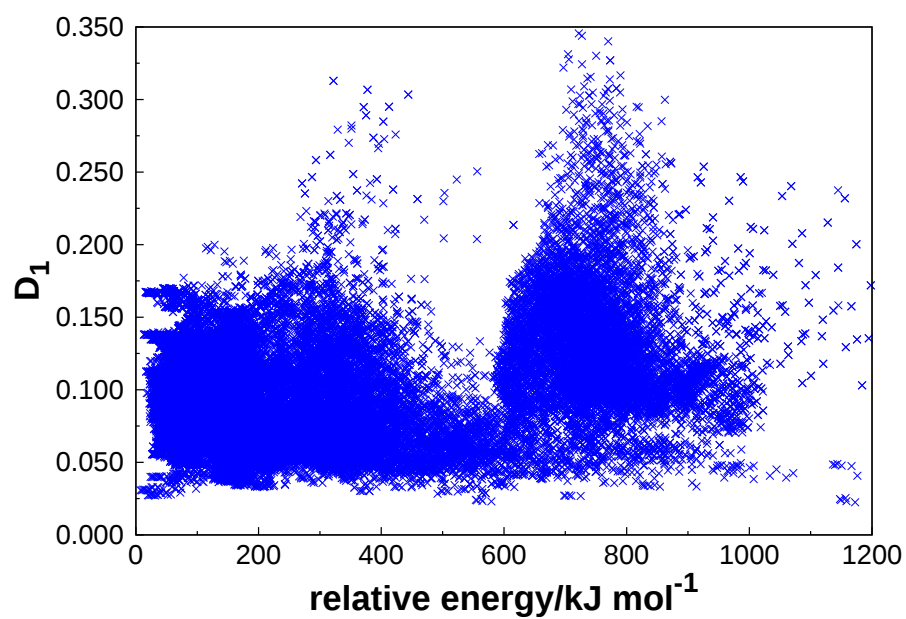


Figure S4: Scatter plot of D_1 values at CCSD(T)/AVTZ level for all *ab initio* data points. Energies defined relative to the *c*-C₃H global minimum.

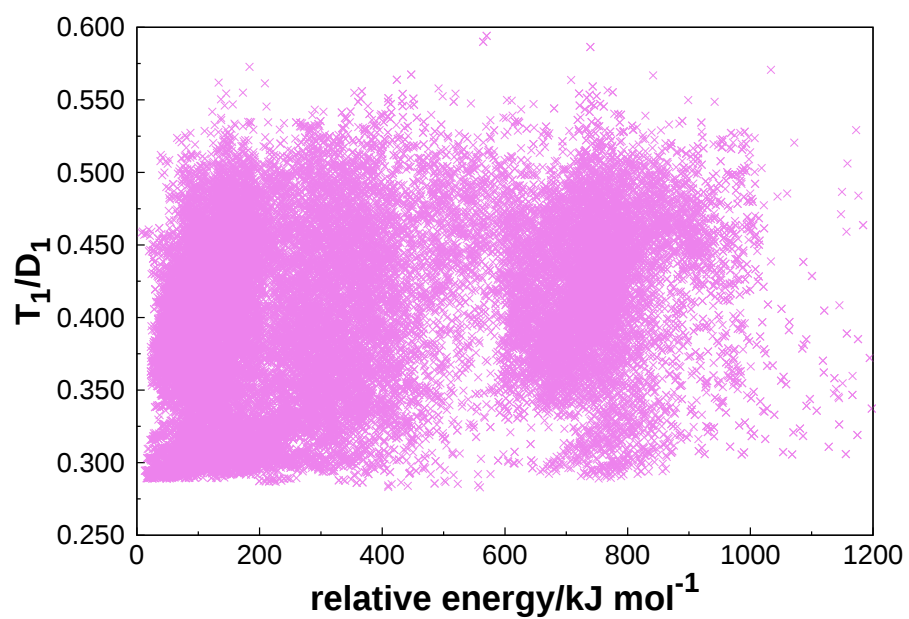


Figure S5: Scatter plot of T_1/D_1 ratios at CCSD(T)/AVTZ level for all *ab initio* data points. Energies defined relative to the *c*-C₃H global minimum.

Table S1: Coefficients of the C-H contracted basis set (in a.u.).

Coefficient	
c_1	$-0.209\,778\,382\,105\,283\,839\text{D}-3$
c_2	$0.108\,762\,784\,340\,722\,035\text{D}0$
c_3	$0.272\,508\,306\,582\,142\,836\text{D}+3$
γ_1	$0.448\,500\,110\,284\,426\,956\text{D}+1$
γ_2	$0.749\,760\,526\,181\,131\,093\text{D}0$
γ_3	$0.235\,508\,110\,035\,697\,493\text{D}+1$
ζ	$0.277\,640\,199\,392\,213\,383\text{D}+1$
R^{ref}	$0.629\,036\,540\,040\,488\,146\text{D}0$

Table S2: Coefficients of the C-C contracted basis set (in a.u.).

Coefficient	
c_1	$-0.236\,213\,374\,985\,701\,566\text{D}-1$
c_2	$0.148\,796\,282\,467\,438\,062\text{D}0$
c_3	$-0.204\,015\,801\,300\,122\,894\text{D}+4$
γ_1	$0.366\,930\,163\,632\,717\,754\text{D}+1$
γ_2	$0.253\,068\,358\,005\,330\,873\text{D}+1$
γ_3	$0.244\,379\,771\,875\,571\,850\text{D}+1$
ζ	$0.236\,647\,527\,057\,571\,638\text{D}+1$
R^{ref}	$0.110\,996\,011\,081\,052\,304\text{D}+1$

Table S3: Non-redundant coefficients of the four-body term $V^{(4)}$ (in a.u.).

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
0	0	1	1	1	1	$C_{0,0,1,1,1,1}$	4	1	0.127 807 702 223 165 066D+3
0	1	1	0	1	1	$C_{0,1,1,0,1,1}$	4	2	0.214 180 662 690 648 319D+3
1	1	1	0	0	1	$C_{1,1,1,0,0,1}$	4	3	-0.436 091 233 884 895 075D+2
0	0	1	1	1	2	$C_{0,0,1,1,1,2}$	5	4	-0.103 744 891 016 244 992D+3
0	0	2	1	1	1	$C_{0,0,2,1,1,1}$	5	5	-0.743 460 791 978 010 093D+3
0	1	1	0	1	2	$C_{0,1,1,0,1,2}$	5	6	-0.518 441 804 114 952 788D+3
0	1	1	1	1	1	$C_{0,1,1,1,1,1}$	5	7	-0.264 613 150 587 689 120D+3
0	1	2	0	1	1	$C_{0,1,2,0,1,1}$	5	8	-0.141 581 206 229 683 312D+4
1	1	1	0	0	2	$C_{1,1,1,0,0,2}$	5	9	0.521 862 406 482 583 552D+2
1	1	1	0	1	1	$C_{1,1,1,0,1,1}$	5	10	-0.357 289 290 150 529 382D+3
1	1	2	0	0	1	$C_{1,1,2,0,0,1}$	5	11	0.165 153 771 309 824 378D+3
0	0	1	1	1	3	$C_{0,0,1,1,1,3}$	6	12	-0.187 103 383 414 424 047D+4
0	0	1	1	2	2	$C_{0,0,1,1,2,2}$	6	13	0.267 368 398 204 560 492D+3
0	0	2	1	1	2	$C_{0,0,2,1,1,2}$	6	14	0.286 350 256 315 648 539D+4
0	0	3	1	1	1	$C_{0,0,3,1,1,1}$	6	15	0.642 346 836 013 249 231D+3
0	1	1	0	1	3	$C_{0,1,1,0,1,3}$	6	16	0.130 573 059 179 311 917D+4
0	1	1	0	2	2	$C_{0,1,1,0,2,2}$	6	17	0.338 379 103 550 885 645D+3
0	1	1	1	1	2	$C_{0,1,1,1,1,2}$	6	18	0.304 458 443 087 224 282D+3
0	1	2	0	1	2	$C_{0,1,2,0,1,2}$	6	19	0.112 741 673 655 101 681D+4
0	1	2	1	1	1	$C_{0,1,2,1,1,1}$	6	20	0.445 522 257 692 820 915D+3
0	1	3	0	1	1	$C_{0,1,3,0,1,1}$	6	21	0.634 097 854 411 330 445D+4
0	2	2	0	1	1	$C_{0,2,2,0,1,1}$	6	22	-0.747 383 680 165 876 285D+3
1	1	1	0	0	3	$C_{1,1,1,0,0,3}$	6	23	0.409 390 475 689 841 594D+3
1	1	1	0	1	2	$C_{1,1,1,0,1,2}$	6	24	0.944 026 632 976 589 099D+3
1	1	1	1	1	1	$C_{1,1,1,1,1,1}$	6	25	0.647 875 120 838 008 797D+3
1	1	2	0	0	2	$C_{1,1,2,0,0,2}$	6	26	-0.138 889 271 593 558 931D+3
1	1	2	0	1	1	$C_{1,1,2,0,1,1}$	6	27	0.231 265 418 711 596 931D+4
1	1	3	0	0	1	$C_{1,1,3,0,0,1}$	6	28	-0.148 989 124 680 232 726D+4
1	2	2	0	0	1	$C_{1,2,2,0,0,1}$	6	29	0.129 498 632 234 143 338D+4
0	0	1	1	1	4	$C_{0,0,1,1,1,4}$	7	30	0.349 551 009 020 385 345D+4
0	0	1	1	2	3	$C_{0,0,1,1,2,3}$	7	31	0.229 368 133 129 966 145D+4
0	0	1	2	2	2	$C_{0,0,1,2,2,2}$	7	32	-0.257 056 252 735 831 322D+3
0	0	2	1	1	3	$C_{0,0,2,1,1,3}$	7	33	0.136 078 793 138 659 353D+4
0	0	2	1	2	2	$C_{0,0,2,1,2,2}$	7	34	-0.450 769 744 093 081 772D+4
0	0	3	1	1	2	$C_{0,0,3,1,1,2}$	7	35	-0.448 303 496 846 114 467D+4
0	0	4	1	1	1	$C_{0,0,4,1,1,1}$	7	36	0.164 063 807 763 876 707D+4
0	1	1	0	1	4	$C_{0,1,1,0,1,4}$	7	37	-0.204 064 018 154 141 036D+4

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
0	1	1	0	2	3	$C_{0,1,1,0,2,3}$	7	38	−0.306 286 275 798 424 276D+4
0	1	1	1	1	3	$C_{0,1,1,1,1,3}$	7	39	−0.140 446 935 254 759 069D+4
0	1	1	1	2	2	$C_{0,1,1,1,2,2}$	7	40	0.538 738 368 896 812 176D+3
0	1	2	0	1	3	$C_{0,1,2,0,1,3}$	7	41	0.142 092 200 444 375 658D+4
0	1	2	0	2	2	$C_{0,1,2,0,2,2}$	7	42	0.643 412 050 421 171 557D+3
0	1	2	1	1	2	$C_{0,1,2,1,1,2}$	7	43	0.884 305 304 829 234 842D+3
0	1	3	0	1	2	$C_{0,1,3,0,1,2}$	7	44	−0.632 972 865 866 772 281D+4
0	1	3	1	1	1	$C_{0,1,3,1,1,1}$	7	45	−0.254 847 136 114 357 272D+4
0	1	4	0	1	1	$C_{0,1,4,0,1,1}$	7	46	−0.138 674 610 796 128 727D+5
0	2	2	0	1	2	$C_{0,2,2,0,1,2}$	7	47	0.210 199 729 164 228 302D+4
0	2	2	1	1	1	$C_{0,2,2,1,1,1}$	7	48	0.252 732 301 836 195 484D+4
0	2	3	0	1	1	$C_{0,2,3,0,1,1}$	7	49	0.851 226 485 576 037 931D+3
1	1	1	0	0	4	$C_{1,1,1,0,0,4}$	7	50	−0.658 213 592 423 678 620D+3
1	1	1	0	1	3	$C_{1,1,1,0,1,3}$	7	51	0.333 716 168 676 036 276D+2
1	1	1	0	2	2	$C_{1,1,1,0,2,2}$	7	52	0.426 271 857 059 777 233D+3
1	1	1	1	1	2	$C_{1,1,1,1,1,2}$	7	53	−0.111 663 513 033 272 875D+4
1	1	2	0	0	3	$C_{1,1,2,0,0,3}$	7	54	−0.210 112 459 258 583 704D+4
1	1	2	0	1	2	$C_{1,1,2,0,1,2}$	7	55	−0.856 433 433 830 807 917D+4
1	1	2	1	1	1	$C_{1,1,2,1,1,1}$	7	56	−0.167 749 500 025 721 727D+4
1	1	3	0	0	2	$C_{1,1,3,0,0,2}$	7	57	0.146 816 186 321 149 985D+4
1	1	3	0	1	1	$C_{1,1,3,0,1,1}$	7	58	−0.521 668 434 219 529 718D+4
1	1	4	0	0	1	$C_{1,1,4,0,0,1}$	7	59	0.477 968 139 937 327 669D+4
1	2	2	0	0	2	$C_{1,2,2,0,0,2}$	7	60	−0.156 029 583 917 386 117D+4
1	2	2	0	1	1	$C_{1,2,2,0,1,1}$	7	61	0.387 336 725 633 557 137D+3
1	2	3	0	0	1	$C_{1,2,3,0,0,1}$	7	62	−0.344 186 946 526 578 504D+4
2	2	2	0	0	1	$C_{2,2,2,0,0,1}$	7	63	−0.493 807 940 190 894 385D+3
0	0	1	1	1	5	$C_{0,0,1,1,1,5}$	8	64	−0.178 599 894 999 784 374D+4
0	0	1	1	2	4	$C_{0,0,1,1,2,4}$	8	65	−0.748 194 195 972 353 100D+4
0	0	1	1	3	3	$C_{0,0,1,1,3,3}$	8	66	0.573 935 291 427 520 838D+3
0	0	1	2	2	3	$C_{0,0,1,2,2,3}$	8	67	0.526 822 251 045 120 538D+3
0	0	2	1	1	4	$C_{0,0,2,1,1,4}$	8	68	−0.414 698 879 084 301 643D+4
0	0	2	1	2	3	$C_{0,0,2,1,2,3}$	8	69	0.388 047 706 535 349 698D+4
0	0	2	2	2	2	$C_{0,0,2,2,2,2}$	8	70	0.579 435 849 884 440 927D+3
0	0	3	1	1	3	$C_{0,0,3,1,1,3}$	8	71	−0.440 627 930 237 491 285D+3
0	0	3	1	2	2	$C_{0,0,3,1,2,2}$	8	72	0.681 009 397 451 319 273D+4
0	0	4	1	1	2	$C_{0,0,4,1,1,2}$	8	73	−0.424 962 703 079 246 694D+3
0	0	5	1	1	1	$C_{0,0,5,1,1,1}$	8	74	−0.319 455 641 217 896 118D+4
0	1	1	0	1	5	$C_{0,1,1,0,1,5}$	8	75	0.101 715 117 270 272 140D+4

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
0	1	1	0	2	4	$C_{0,1,1,0,2,4}$	8	76	0.635 452 239 423 415 904D+4
0	1	1	0	3	3	$C_{0,1,1,0,3,3}$	8	77	0.660 172 918 410 906 391D+3
0	1	1	1	1	4	$C_{0,1,1,1,1,4}$	8	78	0.348 259 688 282 954 130D+4
0	1	1	1	2	3	$C_{0,1,1,1,2,3}$	8	79	0.525 918 888 222 238 820D+3
0	1	1	2	2	2	$C_{0,1,1,2,2,2}$	8	80	−0.607 025 587 968 818 058D+3
0	1	2	0	1	4	$C_{0,1,2,0,1,4}$	8	81	−0.124 212 854 828 145 578D+4
0	1	2	0	2	3	$C_{0,1,2,0,2,3}$	8	82	−0.270 572 423 309 373 505D+3
0	1	2	1	1	3	$C_{0,1,2,1,1,3}$	8	83	−0.360 398 682 841 167 010D+4
0	1	2	1	2	2	$C_{0,1,2,1,2,2}$	8	84	−0.809 937 395 251 088 333D+3
0	1	3	0	1	3	$C_{0,1,3,0,1,3}$	8	85	−0.148 355 705 264 567 450D+4
0	1	3	0	2	2	$C_{0,1,3,0,2,2}$	8	86	−0.103 033 083 364 280 628D+4
0	1	3	1	1	2	$C_{0,1,3,1,1,2}$	8	87	0.592 510 737 754 694 765D+4
0	1	4	0	1	2	$C_{0,1,4,0,1,2}$	8	88	0.148 397 164 898 123 592D+5
0	1	4	1	1	1	$C_{0,1,4,1,1,1}$	8	89	0.484 041 688 239 539 417D+4
0	1	5	0	1	1	$C_{0,1,5,0,1,1}$	8	90	0.146 049 992 125 300 978D+5
0	2	2	0	1	3	$C_{0,2,2,0,1,3}$	8	91	−0.223 247 389 357 491 738D+4
0	2	2	0	2	2	$C_{0,2,2,0,2,2}$	8	92	−0.258 312 351 580 138 682D+3
0	2	2	1	1	2	$C_{0,2,2,1,1,2}$	8	93	−0.493 822 457 240 313 179D+4
0	2	3	0	1	2	$C_{0,2,3,0,1,2}$	8	94	−0.507 717 742 166 409 789D+4
0	2	3	1	1	1	$C_{0,2,3,1,1,1}$	8	95	−0.557 696 764 355 942 742D+4
0	2	4	0	1	1	$C_{0,2,4,0,1,1}$	8	96	0.103 169 998 743 552 628D+4
0	3	3	0	1	1	$C_{0,3,3,0,1,1}$	8	97	0.124 416 676 288 342 160D+4
1	1	1	0	0	5	$C_{1,1,1,0,0,5}$	8	98	−0.176 881 614 261 155 562D+3
1	1	1	0	1	4	$C_{1,1,1,0,1,4}$	8	99	−0.169 294 698 595 565 569D+4
1	1	1	0	2	3	$C_{1,1,1,0,2,3}$	8	100	−0.202 155 660 218 359 799D+4
1	1	1	1	1	3	$C_{1,1,1,1,1,3}$	8	101	0.151 796 777 991 061 299D+4
1	1	1	1	2	2	$C_{1,1,1,1,2,2}$	8	102	−0.685 255 630 361 830 072D+3
1	1	2	0	0	4	$C_{1,1,2,0,0,4}$	8	103	0.529 042 940 450 143 124D+4
1	1	2	0	1	3	$C_{1,1,2,0,1,3}$	8	104	0.629 011 576 519 761 365D+4
1	1	2	0	2	2	$C_{1,1,2,0,2,2}$	8	105	0.299 691 289 887 419 452D+4
1	1	2	1	1	2	$C_{1,1,2,1,1,2}$	8	106	0.226 876 656 802 115 485D+4
1	1	3	0	0	3	$C_{1,1,3,0,0,3}$	8	107	−0.279 525 706 388 795 243D+3
1	1	3	0	1	2	$C_{1,1,3,0,1,2}$	8	108	0.131 180 960 512 418 551D+5
1	1	3	1	1	1	$C_{1,1,3,1,1,1}$	8	109	−0.103 704 137 596 096 143D+4
1	1	4	0	0	2	$C_{1,1,4,0,0,2}$	8	110	−0.338 085 048 236 855 073D+4
1	1	4	0	1	1	$C_{1,1,4,0,1,1}$	8	111	0.482 254 865 643 055 564D+4
1	1	5	0	0	1	$C_{1,1,5,0,0,1}$	8	112	−0.585 743 350 559 108 148D+4
1	2	2	0	0	3	$C_{1,2,2,0,0,3}$	8	113	−0.135 594 551 729 759 019D+4

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
1	2	2	0	1	2	$C_{1,2,2,0,1,2}$	8	114	0.160 774 283 547 072 059D+4
1	2	2	1	1	1	$C_{1,2,2,1,1,1}$	8	115	0.126 070 880 745 027 534D+4
1	2	3	0	0	2	$C_{1,2,3,0,0,2}$	8	116	0.722 333 849 308 639 128D+4
1	2	3	0	1	1	$C_{1,2,3,0,1,1}$	8	117	0.222 256 628 298 503 665D+4
1	2	4	0	0	1	$C_{1,2,4,0,0,1}$	8	118	−0.420 038 069 503 599 309D+4
1	3	3	0	0	1	$C_{1,3,3,0,0,1}$	8	119	0.433 379 742 714 602 344D+4
2	2	2	0	0	2	$C_{2,2,2,0,0,2}$	8	120	0.117 261 377 103 660 629D+4
2	2	2	0	1	1	$C_{2,2,2,0,1,1}$	8	121	−0.102 055 959 615 379 311D+4
2	2	3	0	0	1	$C_{2,2,3,0,0,1}$	8	122	0.919 533 810 914 026 731D+3
0	0	1	1	1	6	$C_{0,0,1,1,1,6}$	9	123	0.364 053 208 694 356 059D+2
0	0	1	1	2	5	$C_{0,0,1,1,2,5}$	9	124	0.502 044 249 787 059 653D+4
0	0	1	1	3	4	$C_{0,0,1,1,3,4}$	9	125	0.821 230 629 387 445 447D+3
0	0	1	2	2	4	$C_{0,0,1,2,2,4}$	9	126	0.811 226 192 796 838 291D+3
0	0	1	2	3	3	$C_{0,0,1,2,3,3}$	9	127	−0.944 759 524 050 981 554D+3
0	0	2	1	1	5	$C_{0,0,2,1,1,5}$	9	128	−0.176 399 998 553 245 069D+3
0	0	2	1	2	4	$C_{0,0,2,1,2,4}$	9	129	0.553 607 611 227 659 163D+4
0	0	2	1	3	3	$C_{0,0,2,1,3,3}$	9	130	−0.285 248 336 177 935 835D+4
0	0	2	2	2	3	$C_{0,0,2,2,2,3}$	9	131	−0.776 819 983 058 004 595D+3
0	0	3	1	1	4	$C_{0,0,3,1,1,4}$	9	132	0.497 536 387 430 003 560D+4
0	0	3	1	2	3	$C_{0,0,3,1,2,3}$	9	133	−0.668 566 447 973 528 284D+4
0	0	3	2	2	2	$C_{0,0,3,2,2,2}$	9	134	−0.203 523 752 106 627 285D+3
0	0	4	1	1	3	$C_{0,0,4,1,1,3}$	9	135	−0.560 005 970 271 174 533D+3
0	0	4	1	2	2	$C_{0,0,4,1,2,2}$	9	136	−0.366 589 910 383 998 040D+4
0	0	5	1	1	2	$C_{0,0,5,1,1,2}$	9	137	0.555 196 490 485 129 470D+4
0	0	6	1	1	1	$C_{0,0,6,1,1,1}$	9	138	0.151 079 920 668 023 738D+4
0	1	1	0	1	6	$C_{0,1,1,0,1,6}$	9	139	−0.352 488 092 754 733 884D+3
0	1	1	0	2	5	$C_{0,1,1,0,2,5}$	9	140	−0.346 997 636 887 561 066D+4
0	1	1	0	3	4	$C_{0,1,1,0,3,4}$	9	141	−0.216 326 719 100 262 426D+4
0	1	1	1	1	5	$C_{0,1,1,1,1,5}$	9	142	−0.165 367 014 152 304 546D+4
0	1	1	1	2	4	$C_{0,1,1,1,2,4}$	9	143	−0.248 250 701 948 707 501D+4
0	1	1	1	3	3	$C_{0,1,1,1,3,3}$	9	144	0.121 243 424 378 772 843D+3
0	1	1	2	2	3	$C_{0,1,1,2,2,3}$	9	145	0.897 139 234 668 334 439D+3
0	1	2	0	1	5	$C_{0,1,2,0,1,5}$	9	146	0.126 427 091 066 017 806D+4
0	1	2	0	2	4	$C_{0,1,2,0,2,4}$	9	147	−0.411 235 663 281 238 612D+4
0	1	2	0	3	3	$C_{0,1,2,0,3,3}$	9	148	0.715 623 409 965 689 461D+3
0	1	2	1	1	4	$C_{0,1,2,1,1,4}$	9	149	0.235 544 008 406 353 527D+3
0	1	2	1	2	3	$C_{0,1,2,1,2,3}$	9	150	−0.419 408 236 821 691 048D+3
0	1	2	2	2	2	$C_{0,1,2,2,2,2}$	9	151	−0.997 156 511 816 473 198D+3

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
0	1	3	0	1	4	$C_{0,1,3,0,1,4}$	9	152	0.228 162 116 087 948 880D+4
0	1	3	0	2	3	$C_{0,1,3,0,2,3}$	9	153	0.409 770 415 545 479 136D+4
0	1	3	1	1	3	$C_{0,1,3,1,1,3}$	9	154	−0.144 363 346 604 669 368D+4
0	1	3	1	2	2	$C_{0,1,3,1,2,2}$	9	155	0.559 401 051 062 765 532D+3
0	1	4	0	1	3	$C_{0,1,4,0,1,3}$	9	156	−0.391 056 895 582 332 936D+4
0	1	4	0	2	2	$C_{0,1,4,0,2,2}$	9	157	−0.616 739 090 801 017 937D+3
0	1	4	1	1	2	$C_{0,1,4,1,1,2}$	9	158	−0.775 518 476 935 933 631D+4
0	1	5	0	1	2	$C_{0,1,5,0,1,2}$	9	159	−0.123 023 883 392 756 488D+5
0	1	5	1	1	1	$C_{0,1,5,1,1,1}$	9	160	−0.531 623 174 810 055 298D+4
0	1	6	0	1	1	$C_{0,1,6,0,1,1}$	9	161	−0.722 335 856 846 141 178D+4
0	2	2	0	1	4	$C_{0,2,2,0,1,4}$	9	162	0.125 052 337 933 603 303D+4
0	2	2	0	2	3	$C_{0,2,2,0,2,3}$	9	163	0.822 697 742 133 246 493D+3
0	2	2	1	1	3	$C_{0,2,2,1,1,3}$	9	164	0.588 259 897 184 372 949D+4
0	2	2	1	2	2	$C_{0,2,2,1,2,2}$	9	165	0.152 522 196 111 752 851D+4
0	2	3	0	1	3	$C_{0,2,3,0,1,3}$	9	166	0.297 735 850 317 416 134D+4
0	2	3	0	2	2	$C_{0,2,3,0,2,2}$	9	167	−0.552 330 894 463 124 309D+3
0	2	3	1	1	2	$C_{0,2,3,1,1,2}$	9	168	0.408 426 018 192 705 124D+4
0	2	4	0	1	2	$C_{0,2,4,0,1,2}$	9	169	0.517 376 351 883 177 904D+4
0	2	4	1	1	1	$C_{0,2,4,1,1,1}$	9	170	0.258 851 255 643 551 804D+4
0	2	5	0	1	1	$C_{0,2,5,0,1,1}$	9	171	−0.173 822 212 825 872 452D+4
0	3	3	0	1	2	$C_{0,3,3,0,1,2}$	9	172	−0.459 538 700 805 852 386D+3
0	3	3	1	1	1	$C_{0,3,3,1,1,1}$	9	173	0.222 169 096 498 816 543D+4
0	3	4	0	1	1	$C_{0,3,4,0,1,1}$	9	174	−0.262 573 905 892 170 160D+4
1	1	1	0	0	6	$C_{1,1,1,0,0,6}$	9	175	0.400 555 938 432 751 816D+3
1	1	1	0	1	5	$C_{1,1,1,0,1,5}$	9	176	0.211 672 279 634 288 680D+4
1	1	1	0	2	4	$C_{1,1,1,0,2,4}$	9	177	0.108 706 474 982 437 840D+4
1	1	1	0	3	3	$C_{1,1,1,0,3,3}$	9	178	0.151 876 070 987 314 483D+4
1	1	1	1	1	4	$C_{1,1,1,1,1,4}$	9	179	−0.208 062 672 337 354 525D+4
1	1	1	1	2	3	$C_{1,1,1,1,2,3}$	9	180	0.256 757 455 961 845 437D+3
1	1	1	2	2	2	$C_{1,1,1,2,2,2}$	9	181	0.120 677 249 154 803 371D+4
1	1	2	0	0	5	$C_{1,1,2,0,0,5}$	9	182	−0.201 792 846 482 169 739D+4
1	1	2	0	1	4	$C_{1,1,2,0,1,4}$	9	183	−0.267 843 255 103 006 504D+4
1	1	2	0	2	3	$C_{1,1,2,0,2,3}$	9	184	−0.240 584 646 474 326 155D+4
1	1	2	1	1	3	$C_{1,1,2,1,1,3}$	9	185	0.461 295 718 002 992 544D+3
1	1	2	1	2	2	$C_{1,1,2,1,2,2}$	9	186	0.297 006 416 752 606 924D+3
1	1	3	0	0	4	$C_{1,1,3,0,0,4}$	9	187	−0.575 370 476 696 713 740D+4
1	1	3	0	1	3	$C_{1,1,3,0,1,3}$	9	188	−0.538 234 328 994 636 053D+4
1	1	3	0	2	2	$C_{1,1,3,0,2,2}$	9	189	−0.205 469 294 475 607 830D+4

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
1	1	3	1	1	2	$C_{1,1,3,1,1,2}$	9	190	−0.107 595 087 280 309 917D+4
1	1	4	0	0	3	$C_{1,1,4,0,0,3}$	9	191	0.537 693 186 901 114 859D+4
1	1	4	0	1	2	$C_{1,1,4,0,1,2}$	9	192	−0.984 121 373 064 496 765D+4
1	1	4	1	1	1	$C_{1,1,4,1,1,1}$	9	193	0.556 912 597 572 649 247D+4
1	1	5	0	0	2	$C_{1,1,5,0,0,2}$	9	194	0.332 902 963 535 171 807D+3
1	1	5	0	1	1	$C_{1,1,5,0,1,1}$	9	195	−0.163 515 079 445 708 034D+4
1	1	6	0	0	1	$C_{1,1,6,0,0,1}$	9	196	0.470 341 768 185 410 001D+4
1	2	2	0	0	4	$C_{1,2,2,0,0,4}$	9	197	0.584 877 202 892 319 474D+3
1	2	2	0	1	3	$C_{1,2,2,0,1,3}$	9	198	−0.109 867 660 046 949 595D+4
1	2	2	0	2	2	$C_{1,2,2,0,2,2}$	9	199	−0.119 725 039 732 674 236D+4
1	2	2	1	1	2	$C_{1,2,2,1,1,2}$	9	200	−0.179 145 158 137 144 767D+4
1	2	3	0	0	3	$C_{1,2,3,0,0,3}$	9	201	0.165 157 781 522 466 485D+4
1	2	3	0	1	2	$C_{1,2,3,0,1,2}$	9	202	−0.325 585 128 070 253 995D+4
1	2	3	1	1	1	$C_{1,2,3,1,1,1}$	9	203	−0.176 750 090 139 178 315D+4
1	2	4	0	0	2	$C_{1,2,4,0,0,2}$	9	204	0.376 079 514 471 645 211D+3
1	2	4	0	1	1	$C_{1,2,4,0,1,1}$	9	205	−0.177 505 881 627 533 495D+4
1	2	5	0	0	1	$C_{1,2,5,0,0,1}$	9	206	0.289 020 706 415 587 347D+4
1	3	3	0	0	2	$C_{1,3,3,0,0,2}$	9	207	−0.834 984 000 837 911 481D+4
1	3	3	0	1	1	$C_{1,3,3,0,1,1}$	9	208	−0.181 634 439 464 478 282D+4
1	3	4	0	0	1	$C_{1,3,4,0,0,1}$	9	209	0.497 384 856 820 251 343D+3
2	2	2	0	0	3	$C_{2,2,2,0,0,3}$	9	210	−0.575 136 836 778 991 665D+3
2	2	2	0	1	2	$C_{2,2,2,0,1,2}$	9	211	0.981 426 596 917 182 110D+3
2	2	2	1	1	1	$C_{2,2,2,1,1,1}$	9	212	−0.348 176 241 034 609 859D+3
2	2	3	0	0	2	$C_{2,2,3,0,0,2}$	9	213	−0.228 622 721 517 762 739D+4
2	2	3	0	1	1	$C_{2,2,3,0,1,1}$	9	214	0.807 838 280 760 042 039D+3
2	2	4	0	0	1	$C_{2,2,4,0,0,1}$	9	215	−0.216 976 111 691 570 300D0
2	3	3	0	0	1	$C_{2,3,3,0,0,1}$	9	216	0.313 167 693 666 316 183D+2
0	0	1	1	1	7	$C_{0,0,1,1,1,7}$	10	217	0.176 181 974 826 722 261D+2
0	0	1	1	2	6	$C_{0,0,1,1,2,6}$	10	218	−0.557 146 931 799 665 708D+3
0	0	1	1	3	5	$C_{0,0,1,1,3,5}$	10	219	−0.855 566 766 878 714 134D+3
0	0	1	1	4	4	$C_{0,0,1,1,4,4}$	10	220	−0.163 346 232 590 809 457D+2
0	0	1	2	2	5	$C_{0,0,1,2,2,5}$	10	221	−0.664 623 936 216 559 628D+3
0	0	1	2	3	4	$C_{0,0,1,2,3,4}$	10	222	0.678 496 782 208 945 092D+3
0	0	1	3	3	3	$C_{0,0,1,3,3,3}$	10	223	−0.438 411 791 334 663 690D+2
0	0	2	1	1	6	$C_{0,0,2,1,1,6}$	10	224	0.123 272 540 656 704 018D+4
0	0	2	1	2	5	$C_{0,0,2,1,2,5}$	10	225	−0.378 293 385 443 651 459D+4
0	0	2	1	3	4	$C_{0,0,2,1,3,4}$	10	226	0.122 223 721 076 916 650D+4
0	0	2	2	2	4	$C_{0,0,2,2,2,4}$	10	227	0.233 613 869 921 638 582D+3

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
0	0	2	2	3	3	$C_{0,0,2,2,3,3}$	10	228	−0.613 352 204 096 933 860D+3
0	0	3	1	1	5	$C_{0,0,3,1,1,5}$	10	229	−0.661 693 767 164 672 522D+3
0	0	3	1	2	4	$C_{0,0,3,1,2,4}$	10	230	0.842 852 769 204 336 312D+2
0	0	3	1	3	3	$C_{0,0,3,1,3,3}$	10	231	0.103 840 527 102 258 466D+4
0	0	3	2	2	3	$C_{0,0,3,2,2,3}$	10	232	0.762 678 017 482 378 664D+3
0	0	4	1	1	4	$C_{0,0,4,1,1,4}$	10	233	−0.244 353 649 162 371 130D+4
0	0	4	1	2	3	$C_{0,0,4,1,2,3}$	10	234	0.239 021 598 002 721 248D+4
0	0	4	2	2	2	$C_{0,0,4,2,2,2}$	10	235	−0.286 163 156 002 884 136D+3
0	0	5	1	1	3	$C_{0,0,5,1,1,3}$	10	236	0.764 482 885 193 994 434D+3
0	0	5	1	2	2	$C_{0,0,5,1,2,2}$	10	237	0.392 637 866 807 965 850D+3
0	0	6	1	1	2	$C_{0,0,6,1,1,2}$	10	238	−0.311 502 387 910 785 137D+4
0	0	7	1	1	1	$C_{0,0,7,1,1,1}$	10	239	−0.598 464 397 948 408 120D+2
0	1	1	0	1	7	$C_{0,1,1,0,1,7}$	10	240	0.271 088 303 932 029 760D+3
0	1	1	0	2	6	$C_{0,1,1,0,2,6}$	10	241	0.153 262 045 044 436 547D+3
0	1	1	0	3	5	$C_{0,1,1,0,3,5}$	10	242	0.122 545 440 859 903 351D+4
0	1	1	0	4	4	$C_{0,1,1,0,4,4}$	10	243	0.884 385 283 766 968 087D+2
0	1	1	1	1	6	$C_{0,1,1,1,1,6}$	10	244	−0.531 512 899 742 355 785D+3
0	1	1	1	2	5	$C_{0,1,1,1,2,5}$	10	245	0.182 083 275 957 712 362D+4
0	1	1	1	3	4	$C_{0,1,1,1,3,4}$	10	246	−0.717 853 814 503 531 680D+3
0	1	1	2	2	4	$C_{0,1,1,2,2,4}$	10	247	−0.732 589 595 282 053 324D+3
0	1	1	2	3	3	$C_{0,1,1,2,3,3}$	10	248	0.778 876 620 115 383 162D+3
0	1	2	0	1	6	$C_{0,1,2,0,1,6}$	10	249	−0.633 495 732 370 809 037D+3
0	1	2	0	2	5	$C_{0,1,2,0,2,5}$	10	250	0.230 060 557 067 348 782D+4
0	1	2	0	3	4	$C_{0,1,2,0,3,4}$	10	251	0.551 529 191 639 552 892D+2
0	1	2	1	1	5	$C_{0,1,2,1,1,5}$	10	252	0.167 319 035 681 091 304D+4
0	1	2	1	2	4	$C_{0,1,2,1,2,4}$	10	253	0.137 758 492 762 024 594D+4
0	1	2	1	3	3	$C_{0,1,2,1,3,3}$	10	254	0.310 603 058 503 707 928D+3
0	1	2	2	2	3	$C_{0,1,2,2,2,3}$	10	255	0.926 676 425 033 069 563D+3
0	1	3	0	1	5	$C_{0,1,3,0,1,5}$	10	256	−0.702 446 498 080 517 131D+3
0	1	3	0	2	4	$C_{0,1,3,0,2,4}$	10	257	−0.668 567 767 611 833 119D+3
0	1	3	0	3	3	$C_{0,1,3,0,3,3}$	10	258	−0.843 011 260 165 655 926D+3
0	1	3	1	1	4	$C_{0,1,3,1,1,4}$	10	259	−0.102 763 261 274 247 475D+4
0	1	3	1	2	3	$C_{0,1,3,1,2,3}$	10	260	−0.184 952 975 206 445 331D+4
0	1	3	2	2	2	$C_{0,1,3,2,2,2}$	10	261	0.592 290 737 432 174 183D+3
0	1	4	0	1	4	$C_{0,1,4,0,1,4}$	10	262	−0.175 363 609 566 727 320D+3
0	1	4	0	2	3	$C_{0,1,4,0,2,3}$	10	263	−0.561 675 441 630 379 737D+3
0	1	4	1	1	3	$C_{0,1,4,1,1,3}$	10	264	0.297 716 417 090 736 377D+4
0	1	4	1	2	2	$C_{0,1,4,1,2,2}$	10	265	0.111 317 593 647 682 725D+4

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #
0	1	5	0	1	3	$C_{0,1,5,0,1,3}$	10	266
0	1	5	0	2	2	$C_{0,1,5,0,2,2}$	10	267
0	1	5	1	1	2	$C_{0,1,5,1,1,2}$	10	268
0	1	6	0	1	2	$C_{0,1,6,0,1,2}$	10	269
0	1	6	1	1	1	$C_{0,1,6,1,1,1}$	10	270
0	1	7	0	1	1	$C_{0,1,7,0,1,1}$	10	271
0	2	2	0	1	5	$C_{0,2,2,0,1,5}$	10	272
0	2	2	0	2	4	$C_{0,2,2,0,2,4}$	10	273
0	2	2	0	3	3	$C_{0,2,2,0,3,3}$	10	274
0	2	2	1	1	4	$C_{0,2,2,1,1,4}$	10	275
0	2	2	1	2	3	$C_{0,2,2,1,2,3}$	10	276
0	2	2	2	2	2	$C_{0,2,2,2,2,2}$	10	277
0	2	3	0	1	4	$C_{0,2,3,0,1,4}$	10	278
0	2	3	0	2	3	$C_{0,2,3,0,2,3}$	10	279
0	2	3	1	1	3	$C_{0,2,3,1,1,3}$	10	280
0	2	3	1	2	2	$C_{0,2,3,1,2,2}$	10	281
0	2	4	0	1	3	$C_{0,2,4,0,1,3}$	10	282
0	2	4	0	2	2	$C_{0,2,4,0,2,2}$	10	283
0	2	4	1	1	2	$C_{0,2,4,1,1,2}$	10	284
0	2	5	0	1	2	$C_{0,2,5,0,1,2}$	10	285
0	2	5	1	1	1	$C_{0,2,5,1,1,1}$	10	286
0	2	6	0	1	1	$C_{0,2,6,0,1,1}$	10	287
0	3	3	0	1	3	$C_{0,3,3,0,1,3}$	10	288
0	3	3	0	2	2	$C_{0,3,3,0,2,2}$	10	289
0	3	3	1	1	2	$C_{0,3,3,1,1,2}$	10	290
0	3	4	0	1	2	$C_{0,3,4,0,1,2}$	10	291
0	3	4	1	1	1	$C_{0,3,4,1,1,1}$	10	292
0	3	5	0	1	1	$C_{0,3,5,0,1,1}$	10	293
0	4	4	0	1	1	$C_{0,4,4,0,1,1}$	10	294
1	1	1	0	0	7	$C_{1,1,1,0,0,7}$	10	295
1	1	1	0	1	6	$C_{1,1,1,0,1,6}$	10	296
1	1	1	0	2	5	$C_{1,1,1,0,2,5}$	10	297
1	1	1	0	3	4	$C_{1,1,1,0,3,4}$	10	298
1	1	1	1	1	5	$C_{1,1,1,1,1,5}$	10	299
1	1	1	1	2	4	$C_{1,1,1,1,2,4}$	10	300
1	1	1	1	3	3	$C_{1,1,1,1,3,3}$	10	301
1	1	1	2	2	3	$C_{1,1,1,2,2,3}$	10	302
1	1	2	0	0	6	$C_{1,1,2,0,0,6}$	10	303

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Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
1	1	2	0	1	5	$C_{1,1,2,0,1,5}$	10	304	−0.260 264 046 277 982 459D+3
1	1	2	0	2	4	$C_{1,1,2,0,2,4}$	10	305	0.320 525 961 655 604 590D+3
1	1	2	0	3	3	$C_{1,1,2,0,3,3}$	10	306	−0.764 283 537 790 093 760D+3
1	1	2	1	1	4	$C_{1,1,2,1,1,4}$	10	307	−0.638 286 566 677 846 167D+3
1	1	2	1	2	3	$C_{1,1,2,1,2,3}$	10	308	0.483 750 524 809 519 334D+3
1	1	2	2	2	2	$C_{1,1,2,2,2,2}$	10	309	0.704 591 977 451 272 896D+3
1	1	3	0	0	5	$C_{1,1,3,0,0,5}$	10	310	0.253 117 896 145 782 652D+4
1	1	3	0	1	4	$C_{1,1,3,0,1,4}$	10	311	0.206 006 203 869 364 754D+4
1	1	3	0	2	3	$C_{1,1,3,0,2,3}$	10	312	0.317 062 988 583 267 179D+4
1	1	3	1	1	3	$C_{1,1,3,1,1,3}$	10	313	−0.136 338 697 697 866 564D+4
1	1	3	1	2	2	$C_{1,1,3,1,2,2}$	10	314	−0.371 193 411 646 215 168D+2
1	1	4	0	0	4	$C_{1,1,4,0,0,4}$	10	315	0.870 931 391 666 504 453D+2
1	1	4	0	1	3	$C_{1,1,4,0,1,3}$	10	316	0.546 088 648 102 431 307D+3
1	1	4	0	2	2	$C_{1,1,4,0,2,2}$	10	317	−0.164 655 470 364 500 638D+4
1	1	4	1	1	2	$C_{1,1,4,1,1,2}$	10	318	−0.716 351 831 510 506 941D+3
1	1	5	0	0	3	$C_{1,1,5,0,0,3}$	10	319	−0.157 109 516 825 187 916D+4
1	1	5	0	1	2	$C_{1,1,5,0,1,2}$	10	320	0.514 522 474 194 177 357D+4
1	1	5	1	1	1	$C_{1,1,5,1,1,1}$	10	321	−0.656 134 889 876 439 502D+4
1	1	6	0	0	2	$C_{1,1,6,0,0,2}$	10	322	−0.964 853 018 594 192 946D+2
1	1	6	0	1	1	$C_{1,1,6,0,1,1}$	10	323	−0.134 413 462 741 016 532D+1
1	1	7	0	0	1	$C_{1,1,7,0,0,1}$	10	324	−0.193 178 594 879 241 336D+4
1	2	2	0	0	5	$C_{1,2,2,0,0,5}$	10	325	−0.353 264 564 496 563 594D+3
1	2	2	0	1	4	$C_{1,2,2,0,1,4}$	10	326	0.879 972 518 508 311 623D+3
1	2	2	0	2	3	$C_{1,2,2,0,2,3}$	10	327	0.825 017 506 198 965 179D+3
1	2	2	1	1	3	$C_{1,2,2,1,1,3}$	10	328	0.210 368 750 801 015 040D+4
1	2	2	1	2	2	$C_{1,2,2,1,2,2}$	10	329	−0.128 616 512 041 561 600D+4
1	2	3	0	0	4	$C_{1,2,3,0,0,4}$	10	330	−0.126 782 836 851 237 590D+3
1	2	3	0	1	3	$C_{1,2,3,0,1,3}$	10	331	−0.926 693 816 692 389 987D+3
1	2	3	0	2	2	$C_{1,2,3,0,2,2}$	10	332	0.944 852 152 568 418 546D+2
1	2	3	1	1	2	$C_{1,2,3,1,1,2}$	10	333	0.828 303 630 785 224 982D+3
1	2	4	0	0	3	$C_{1,2,4,0,0,3}$	10	334	−0.392 162 021 707 623 489D+4
1	2	4	0	1	2	$C_{1,2,4,0,1,2}$	10	335	0.213 475 327 634 303 994D+4
1	2	4	1	1	1	$C_{1,2,4,1,1,1}$	10	336	0.118 138 035 962 192 735D+5
1	2	5	0	0	2	$C_{1,2,5,0,0,2}$	10	337	0.122 498 529 018 426 461D+4
1	2	5	0	1	1	$C_{1,2,5,0,1,1}$	10	338	−0.167 022 520 222 358 412D+4
1	2	6	0	0	1	$C_{1,2,6,0,0,1}$	10	339	0.145 990 744 524 478 987D+4
1	3	3	0	0	3	$C_{1,3,3,0,0,3}$	10	340	0.224 142 786 508 094 105D+4
1	3	3	0	1	2	$C_{1,3,3,0,1,2}$	10	341	0.505 564 510 822 088 096D+3

Continued on next page.

Table S3 – *Continued from previous page.*

i	i	k	l	m	n	$C_{i,j,k,l,m,n}$	Total order	Coefficient #	
1	3	3	1	1	1	$C_{1,3,3,1,1,1}$	10	342	$-0.841\,751\,039\,161\,378\,321\text{D}+4$
1	3	4	0	0	2	$C_{1,3,4,0,0,2}$	10	343	$0.287\,958\,526\,455\,655\,783\text{D}+4$
1	3	4	0	1	1	$C_{1,3,4,0,1,1}$	10	344	$0.210\,456\,806\,130\,477\,980\text{D}+4$
1	3	5	0	0	1	$C_{1,3,5,0,0,1}$	10	345	$-0.618\,826\,457\,232\,975\,099\text{D}+4$
1	4	4	0	0	1	$C_{1,4,4,0,0,1}$	10	346	$0.289\,459\,834\,680\,884\,842\text{D}+4$
2	2	2	0	0	4	$C_{2,2,2,0,0,4}$	10	347	$0.440\,145\,717\,369\,963\,876\text{D}+2$
2	2	2	0	1	3	$C_{2,2,2,0,1,3}$	10	348	$-0.403\,673\,720\,526\,193\,108\text{D}+3$
2	2	2	0	2	2	$C_{2,2,2,0,2,2}$	10	349	$0.201\,511\,353\,625\,358\,964\text{D}+2$
2	2	2	1	1	2	$C_{2,2,2,1,1,2}$	10	350	$0.537\,072\,355\,754\,478\,110\text{D}+2$
2	2	3	0	0	3	$C_{2,2,3,0,0,3}$	10	351	$0.762\,736\,961\,747\,134\,501\text{D}+3$
2	2	3	0	1	2	$C_{2,2,3,0,1,2}$	10	352	$0.300\,371\,788\,514\,155\,867\text{D}+3$
2	2	3	1	1	1	$C_{2,2,3,1,1,1}$	10	353	$0.703\,288\,926\,276\,651\,637\text{D}+3$
2	2	4	0	0	2	$C_{2,2,4,0,0,2}$	10	354	$-0.104\,019\,543\,499\,578\,887\text{D}+3$
2	2	4	0	1	1	$C_{2,2,4,0,1,1}$	10	355	$0.969\,050\,304\,747\,543\,123\text{D}+2$
2	2	5	0	0	1	$C_{2,2,5,0,0,1}$	10	356	$0.312\,254\,438\,092\,611\,110\text{D}+3$
2	3	3	0	0	2	$C_{2,3,3,0,0,2}$	10	357	$0.843\,332\,815\,879\,894\,270\text{D}+3$
2	3	3	0	1	1	$C_{2,3,3,0,1,1}$	10	358	$-0.324\,895\,804\,470\,902\,192\text{D}+3$
2	3	4	0	0	1	$C_{2,3,4,0,0,1}$	10	359	$-0.567\,729\,689\,458\,891\,812\text{D}+3$
3	3	3	0	0	1	$C_{3,3,3,0,0,1}$	10	360	$-0.329\,125\,077\,788\,115\,021\text{D}+2$

Table S4: Structural parameters (distances in a_0 , angles in deg) and harmonic (w_i) frequencies (in cm^{-1}) of stationary points in ground-(state #1) and some excited-state PESs of doublet C_3H near cyclic and linear forms. Energies (in kJ mol^{-1}) refer to $c\text{-C}_3\text{H}$ ground-state minimum. Calculations performed with truncated-space CASSCF wave functions as reference for MRCI+Q.

Structure	Property ^a	State #1 (² B ₂ / ² A')	#2 (² A ₁ / ² A')	#3 (² B ₁ / ² A'')	#4 (² A ₂ / ² A'')	#5 (² A ₂ / ² A'')	#6 (² B ₁ / ² A'')	#7 (² A ₁ / ² A')	#8 (² B ₂ / ² A')
<i>c</i> -C ₃ H	<i>R</i> _{HC₁}	2.016	2.019	n.f. ^b	2.001	2.010	2.019	2.008	2.010
	<i>R</i> _{C₁C₂}	2.490	2.581	n.f.	2.737	2.718	2.656	2.559	2.529
	<i>R</i> _{C₂C₃}	2.601	2.938	n.f.	2.538	2.687	2.681	2.822	2.972
	∠HC ₁ C ₂	155.0	145.3	n.f.	153.9	149.9	140.4	168.5	146.2
	∠C ₁ C ₂ C ₃	65.5	55.3	n.f.	64.3	60.5	69.9	65.8	63.1
	<i>d</i> _{HCCC}	180.0	180.0	n.f.	180.0	180.0	124.8	180.0	180.0
	<i>w</i> ₁ (CH stretch)	3419.6	3387.7	n.f.	3500.1	3431.7	3377.3	3302.5	3509.2
	<i>w</i> ₂ (CC sym. stretch)	1679.9	1651.0	n.f.	1550.7	3908.4	5561.0	1398.6	2121.6
	<i>w</i> ₃ (CCH sym. bend)	1197.9	669.6	n.f.	747.7	885.8	1289.1	3947.1	1420.1
	<i>w</i> ₄ (CC asym. stretch)	861.6	2357.6	n.f.	1194.9	2068.9	1645.5	774.2	720.8
	<i>w</i> ₅ (H wag)	952.2	969.5	n.f.	937.0	960.1	588.5	1040.6	897.0
	<i>w</i> ₆ (H out of plane)	902.8	876.6	n.f.	900.9i	261.4	819.2	535.5	115.6i
spg	<i>C_s</i>	<i>C_{2v}</i>	n.f.	<i>C_s</i>	<i>C_s</i>	<i>C₁</i>	<i>C_s</i>	<i>C_s</i>	
	MRCI+Q(7)/AVDZ	0.0	79.9	n.f.	376.5	390.7	437.1	459.2	509.3
	MRCI+Q(7)/AVTZ	0.0	82.0	n.f.	386.6	395.8	446.6	469.6	518.9
	MRCI+Q(7)/CBS(<i>D,T</i>)	0.0	82.4	n.f.	390.5	397.1	449.5	472.9	521.8
Structure	Property ^a	State #1 (² Π/ ² A')	#2 (² Π/ ² A'')	#3 (² Δ/ ² A')	#4 (² Δ/ ² A'')	#5 (² Σ [−] / ² A'')	#6 (² Σ ⁺ / ² A')	#7 (² Π/ ² A'')	#8 (² Π/ ² A')
<i>ℓ</i> -C ₃ H	<i>R</i> _{HC₁}	1.998	1.991	2.017	2.041	1.990	2.005	1.989	1.989
	<i>R</i> _{C₁C₂}	2.352	2.341	2.672	2.610	2.467	2.511	2.513	2.513
	<i>R</i> _{C₂C₃}	2.531	2.536	2.290	2.320	2.367	2.448	2.540	2.540
	∠HC ₁ C ₂	158.0	180.0	129.2	119.8	162.6	137.3	180.0	180.2
	∠C ₁ C ₂ C ₃	174.4	180.0	174.4	169.3	174.4	171.1	180.0	180.0
	<i>d</i> _{HCCC}	180.0	180.0	180.0	180.0	180.0	180.0	180.0	180.0
	<i>w</i> ₁ (CH stretch)	3545.3	3586.6	3393.5	3014.8	3441.7	3432.9	3748.0	3748.0
	<i>w</i> ₂ (CCC asym. stretch)	1883.7	1926.7	2218.5	6320.2	4080.9	2576.8	2706.9	2706.9
	<i>w</i> ₃ (CCC sym. stretch)	1170.9	1173.0	1038.2	1278.7	1362.2	4093.3	1929.7	1929.7
	<i>w</i> ₄ (CCH bend)	331.5	773.0	1057.1	2201.0i	570.0	7293.0	498.1	498.1
	<i>w</i> ₅ (CCC bend)	388.4,275.3	456.0,297.0	475.6,458.3	2269.1,953.0	501.2,494.0	1334.3,1517.3	719.4,697.4	719.4,697.4
	spg	<i>C_s</i>	<i>C_{∞v}</i>	<i>C_s</i>	<i>C_s</i>	<i>C_s</i>	<i>C_s</i>	<i>C_{∞v}</i>	<i>C_{∞v}</i>
	MRCI+Q(7)/AVDZ	−21.0	−19.1	242.6	246.8	273.8	290.1	319.9	319.9
	MRCI+Q(7)/AVTZ	−15.1	−15.0	254.4	259.7	282.4	298.4	333.4	333.4
	MRCI+Q(7)/CBS(<i>D,T</i>)	−12.2	−12.9	259.8	265.4	286.2	301.9	338.9	338.9

^a This work. spg=symmetry point group. Geometries and forces obtained via state-averaged CASSCF(7,10)/AVTZ. MRCI+Q(7) stands for a 7-electron dynamical correlation approach with 6 inner orbitals uncorrelated.
^b n.f.=not found.