

Supplementary Information for Overcoming the Out-of-plane Bending Issue in an Aromatic Hydrocarbon: The Anharmonic Vibrational Frequencies of c-(CH)C₃H₂⁺

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Table S1: Fermi and Coriolis resonances for c-(CH)C₃H₂⁺

Coriolis	Fermi 1	Fermi Polyad
A-type ν_{10}/ν_8	$2\nu_5 = \nu_1$	$2\nu_5 = \nu_{15} + \nu_3 = \nu_2$
B-type ν_{11}/ν_8		$2\nu_7 = 2\nu_8 = \nu_7 + \nu_6 = \nu_4$
C-type ν_{12}/ν_9		$\nu_{12} + \nu_6 = \nu_{12} + \nu_7 = 2\nu_7 = 2\nu_8 = 2\nu_9 = \nu_5$
B-type ν_{12}/ν_{10}		$\nu_{14} + \nu_{10} = \nu_{15} + \nu_8 = \nu_6$
		$\nu_{15} + \nu_8 = \nu_{15} + \nu_9 = \nu_7$
		$2\nu_{13} = 2\nu_{14} = \nu_{14} + \nu_{11} = \nu_{15} + \nu_{12} = \nu_{14} + \nu_{13} = \nu_8$
		$\nu_{15} + \nu_{12} = \nu_{14} + \nu_{13} = 2\nu_{14} = \nu_9$

Table S2: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺

15	15	0	0	0.122252888505	3	1	0	0	-0.007474323084	6	6	6	0	0.002673872249
14	14	0	0	0.165280650564	2	1	0	0	-0.160362248724	15	15	5	0	1.121061752673
14	13	0	0	-0.564523346111	1	1	0	0	6.066255268228	14	14	5	0	0.798932776744
13	13	0	0	2.479023811431	15	14	11	0	-0.008910454010	14	13	5	0	-3.549161923571
14	12	0	0	0.005492791865	15	13	11	0	-0.196937501344	13	13	5	0	154.671939619310
13	12	0	0	-0.450313524753	15	12	11	0	0.191272297085	14	12	5	0	0.021207834103
12	12	0	0	0.697827512473	15	14	10	0	-0.033931293137	13	12	5	0	-1.792902099983
11	11	0	0	0.953265997830	15	13	10	0	0.118989461814	12	12	5	0	1.842813873516
11	10	0	0	-0.025541501085	15	12	10	0	-0.021305377091	11	11	5	0	-0.481815572815
10	10	0	0	0.517403101537	15	14	9	0	-0.006005147546	11	10	5	0	0.043017797033
11	9	0	0	-0.980882598796	15	13	9	0	-0.397463477690	10	10	5	0	1.045755143507
10	9	0	0	0.026038122388	15	12	9	0	-0.227543126281	11	9	5	0	0.998719804963
9	9	0	0	1.092199027448	15	14	8	0	-0.047271606231	10	9	5	0	-0.046970353934
11	8	0	0	0.000722328798	15	13	8	0	0.152994188332	9	9	5	0	-1.508268627747
10	8	0	0	-0.025236626499	15	12	8	0	-0.002183479338	11	8	5	0	-0.005773236530
9	8	0	0	-0.010861779714	15	14	7	0	-0.082997548301	10	8	5	0	-0.392287662541
8	8	0	0	5.823366669416	15	13	7	0	0.277878425677	9	8	5	0	-0.005233341226
11	7	0	0	0.098389981110	15	12	7	0	0.001733900371	8	8	5	0	-0.309143260699
10	7	0	0	0.178969764192	15	15	6	0	0.047224127966	11	7	5	0	-0.384402927247
9	7	0	0	0.199060308983	14	14	6	0	-0.046189951832	10	7	5	0	-2.341967858473
8	7	0	0	0.057213893297	14	13	6	0	0.164544163573	9	7	5	0	-0.160195190566
7	7	0	0	2.221584986770	13	13	6	0	1.784367989446	8	7	5	0	0.877322476133
6	6	0	0	0.563467825350	14	12	6	0	-0.015040065785	7	7	5	0	-24.526135686524
6	5	0	0	0.805193138436	13	12	6	0	0.182555483299	6	6	5	0	0.500040003936
5	5	0	0	45.128622402294	12	12	6	0	-0.152193718615	6	5	5	0	2.538759273404
6	4	0	0	-0.019427958406	11	11	6	0	0.088131645546	5	5	5	0	561.021691812892
5	4	0	0	0.193562953679	11	10	6	0	-0.030940277041	15	15	4	0	-0.057452661336
4	4	0	0	5.829365741285	10	10	6	0	0.012101926865	14	14	4	0	-0.058930319359
6	3	0	0	0.171030147119	11	9	6	0	-0.154797502660	14	13	4	0	0.197504509742
5	3	0	0	-13.903977763997	10	9	6	0	0.014593577595	13	13	4	0	-0.094144566849
4	3	0	0	-0.082991934790	9	9	6	0	0.175310500109	14	12	4	0	-0.002091227520
3	3	0	0	7.364834643513	11	8	6	0	0.006107558126	13	12	4	0	0.062692098334
6	2	0	0	-0.266317224571	10	8	6	0	-0.142926303873	12	12	4	0	-0.051415498204
5	2	0	0	1.987091648964	9	8	6	0	0.008220994534	11	11	4	0	-0.048964070471
4	2	0	0	-0.016987435127	8	8	6	0	-0.012256167994	11	10	4	0	0.008014078594
3	2	0	0	0.342807080518	11	7	6	0	0.086177233079	10	10	4	0	-0.135247092822
2	2	0	0	13.760855687904	10	7	6	0	-0.649465849463	11	9	4	0	0.052334833508
6	1	0	0	-0.010635400339	9	7	6	0	0.014952552326	10	9	4	0	0.009928721069
5	1	0	0	0.018875834339	8	7	6	0	-0.045320179636	9	9	4	0	-0.035036376814
4	1	0	0	0.007745987883	7	7	6	0	-0.214814284201	11	8	4	0	-0.004494048581

Table S3: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

10	8	4	0	-0.008197858458	5	4	3	0	0.398786123568	4	2	2	0	0.025864202368
9	8	4	0	-0.002200049986	4	4	3	0	0.183708818283	3	2	2	0	0.158996926673
8	8	4	0	-23.622044573339	6	3	3	0	-0.168427108428	2	2	2	0	-82.700313317017
11	7	4	0	0.015320546138	5	3	3	0	32.901476164588	15	15	1	0	-0.002524257452
10	7	4	0	-0.062802095185	4	3	3	0	-0.182930498544	14	14	1	0	-0.008109538833
9	7	4	0	0.012469874487	3	3	3	0	-25.667131901971	14	13	1	0	0.026006181617
8	7	4	0	0.218560092385	15	15	2	0	0.015187631092	13	13	1	0	-1.143888303554
7	7	4	0	-0.459016881863	14	14	2	0	-0.068827350866	14	12	1	0	-0.001579731120
6	6	4	0	-0.137305061880	14	13	2	0	0.212961016862	13	12	1	0	1.186402482364
6	5	4	0	-0.446139489477	13	13	2	0	-1.441974611656	12	12	1	0	-1.293536399225
5	5	4	0	-0.537431073382	14	12	2	0	0.040023966935	11	11	1	0	-1.395749542144
6	4	4	0	-0.012425215854	13	12	2	0	5.261223148595	11	10	1	0	0.020287333067
5	4	4	0	-0.300857694560	12	12	2	0	-4.568497527677	10	10	1	0	-0.000634936128
4	4	4	0	-23.630047671118	11	11	2	0	0.008969916428	11	9	1	0	1.422950568910
15	15	3	0	-0.353412560291	11	10	2	0	-0.062015963177	10	9	1	0	-0.016971795832
14	14	3	0	-0.126940709961	10	10	2	0	0.060202773878	9	9	1	0	-1.461532586928
14	13	3	0	0.421972184689	11	9	2	0	-0.027789571156	11	8	1	0	-0.000926688112
13	13	3	0	-43.669529940338	10	9	2	0	0.176064423563	10	8	1	0	-0.000441557435
14	12	3	0	-0.031894719802	9	9	2	0	0.038185382708	9	8	1	0	0.005084569607
13	12	3	0	-0.770482973964	11	8	2	0	-0.006618275958	8	8	1	0	-0.000704712796
12	12	3	0	0.735263529112	10	8	2	0	0.024038443894	11	7	1	0	-0.071493312667
11	11	3	0	-0.265625648317	9	8	2	0	-0.007627451108	10	7	1	0	-0.005235298946
11	10	3	0	-0.052559900238	8	8	2	0	-0.036038459745	9	7	1	0	0.038034175425
10	10	3	0	-0.508727319303	11	7	2	0	0.338828278880	8	7	1	0	0.011319998500
11	9	3	0	0.372718968216	10	7	2	0	-0.135836949985	7	7	1	0	0.043335407505
10	9	3	0	0.045229120693	9	7	2	0	-0.788077868386	6	6	1	0	0.000212559156
9	9	3	0	-0.685442770671	8	7	2	0	0.181547828584	6	5	1	0	-0.006156954184
11	8	3	0	0.008856587515	7	7	2	0	-1.085012000134	5	5	1	0	0.010379893247
10	8	3	0	0.000634270678	6	6	2	0	-0.007969792509	6	4	1	0	0.001717930793
9	8	3	0	0.021473437633	6	5	2	0	0.424646487659	5	4	1	0	-0.005534956687
8	8	3	0	0.185151756039	5	5	2	0	0.314829416103	4	4	1	0	-0.002534399851
11	7	3	0	0.025641846043	6	4	2	0	0.048474695624	6	3	1	0	-0.004237130517
10	7	3	0	0.387896550193	5	4	2	0	-0.049277327553	5	3	1	0	0.068887197389
9	7	3	0	-0.206385827279	4	4	2	0	-0.047420710142	4	3	1	0	0.002975452762
8	7	3	0	-0.400227279927	6	3	2	0	0.156001644890	3	3	1	0	0.027064957731
7	7	3	0	-7.754914486427	5	3	2	0	-1.808080266638	6	2	1	0	-0.005151964669
6	6	3	0	-0.332870774515	4	3	2	0	0.073794136009	5	2	1	0	-0.053196191212
6	5	3	0	-0.654002459887	3	3	2	0	-0.718793741576	4	2	1	0	0.002227231420
5	5	3	0	-117.643468641947	6	2	2	0	-0.031583365023	3	2	1	0	-0.049481005080
6	4	3	0	-0.034765715799	5	2	2	0	0.510787712883	2	2	1	0	-0.014536590049

Table S4: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

6	1	1	0	0.002173176575	14	12	11	10	-0.087632254427	11	10	9	9	0.074491447127
5	1	1	0	0.052926480373	13	12	11	10	0.116843005893	10	10	9	9	-0.077320534833
4	1	1	0	-0.002067095576	12	12	11	10	-0.082109975779	11	9	9	9	0.274309626169
3	1	1	0	-0.008666287862	11	11	11	10	0.014711207981	10	9	9	9	-0.121063263632
2	1	1	0	0.213674760603	15	15	10	10	-0.000490831584	9	9	9	9	0.013976538184
1	1	1	0	-34.489892630633	14	14	10	10	-0.056482573215	15	15	11	8	0.004387334952
15	15	15	15	0.201997800560	14	13	10	10	0.232515861672	14	14	11	8	0.003317656683
15	15	14	14	0.041046017391	13	13	10	10	2.778256833087	14	13	11	8	0.027139839992
14	14	14	14	-0.006893855655	14	12	10	10	-0.011043432488	13	13	11	8	-0.153669544989
15	15	14	13	-0.141429957659	13	12	10	10	-0.114261203376	14	12	11	8	-0.095806905027
14	14	14	13	0.030250243482	12	12	10	10	0.188399454175	13	12	11	8	0.084144403505
15	15	13	13	4.101029094938	11	11	10	10	-0.003987752448	12	12	11	8	0.072846995472
14	14	13	13	2.376924828214	11	10	10	10	-0.083979119240	11	11	11	8	0.000398737982
14	13	13	13	-26.796972950773	10	10	10	10	0.271014718986	15	15	10	8	0.015757989725
13	13	13	13	1460.076453749885	15	15	11	9	0.101700114333	14	14	10	8	0.010435077210
15	15	14	12	-0.015959672775	14	14	11	9	-0.025517164776	14	13	10	8	-0.049156898943
14	14	14	12	-0.017236398368	14	13	11	9	0.146925720107	13	13	10	8	-1.183612149616
15	15	13	12	-0.181574034465	13	13	11	9	2.046009795982	14	12	10	8	-0.006103739113
14	14	13	12	-0.034197155371	14	12	11	9	0.085452347598	13	12	10	8	-0.287747701101
14	13	13	12	0.254712253812	13	12	11	9	-3.149529382919	12	12	10	8	-0.080191756413
13	13	13	12	-28.886427179603	12	12	11	9	-2.533926004411	11	11	10	8	-0.055869331107
15	15	12	12	0.211738381953	11	11	11	9	0.212558811456	11	10	10	8	-0.023339748160
14	14	12	12	0.077750357364	15	15	10	9	0.009411249916	10	10	10	8	-0.099796129706
14	13	12	12	-0.060806198760	14	14	10	9	0.017604506000	15	15	9	8	0.013598928056
13	13	12	12	15.500042137863	14	13	10	9	0.063762274676	14	14	9	8	0.007838908831
14	12	12	12	-0.106476277037	13	13	10	9	-0.707036755784	14	13	9	8	0.137770111437
13	12	12	12	-7.184340547219	14	12	10	9	0.015586333810	13	13	9	8	-1.229898196310
12	12	12	12	5.829524084501	13	12	10	9	-0.014823366427	14	12	9	8	0.007629673894
15	15	11	11	-0.079081090985	12	12	10	9	-0.176495876575	13	12	9	8	-0.327422005348
14	14	11	11	0.016156965860	11	11	10	9	-0.141072802437	12	12	9	8	0.023209132305
14	13	11	11	-0.050832391020	11	10	10	9	0.061941262619	11	11	9	8	0.016068860046
13	13	11	11	-2.877961505828	10	10	10	9	-0.027129096745	11	10	9	8	0.160441142426
14	12	11	11	-0.000540245051	15	15	9	9	-0.094669660781	10	10	9	8	-0.020486500615
13	12	11	11	1.279927933474	14	14	9	9	0.025693063470	11	9	9	8	0.053527120242
12	12	11	11	8.208606597115	14	13	9	9	-2.681484497221	10	9	9	8	-0.192365035472
11	11	11	11	0.218118511126	13	13	9	9	24.158045234738	9	9	9	8	-0.004711061399
15	15	11	10	0.001600861953	14	12	9	9	-0.193858345891	15	15	8	8	0.018132038023
14	14	11	10	-0.003521164553	13	12	9	9	5.236974074268	14	14	8	8	-0.041224211000
14	13	11	10	0.106379453132	12	12	9	9	-3.379087339774	14	13	8	8	0.168941851792
13	13	11	10	-0.193333666301	11	11	9	9	-0.043551806473	13	13	8	8	-1.261863948968

Table S5: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

14	12	8	8	0.007188515512	10	10	9	7	0.235712591457	9	7	7	7	-1.357708272942
13	12	8	8	0.017484438287	11	9	9	7	-1.126896225631	8	7	7	7	-0.851288964551
12	12	8	8	0.143554090785	10	9	9	7	0.234629792103	7	7	7	7	91.750629085818
11	11	8	8	0.046732466508	9	9	9	7	2.282973935400	15	14	11	6	-0.005313522889
11	10	8	8	-0.003515680229	15	15	8	7	0.001558725415	15	13	11	6	0.008719627305
10	10	8	8	0.023823474096	14	14	8	7	0.006381598102	15	12	11	6	-0.019728156773
11	9	8	8	0.043361749253	14	13	8	7	0.037167411390	15	14	10	6	-0.073844343748
10	9	8	8	0.028222115389	13	13	8	7	2.282496819849	15	13	10	6	0.248836364233
9	9	8	8	0.006168648337	14	12	8	7	-0.020055142802	15	12	10	6	0.030845681592
11	8	8	8	0.060088550351	13	12	8	7	0.002179906815	15	14	9	6	0.026758356292
10	8	8	8	-0.078234869463	12	12	8	7	0.043587181908	15	13	9	6	-0.292434500770
9	8	8	8	-0.017077078291	11	11	8	7	0.017359038699	15	12	9	6	-0.030736686255
8	8	8	8	86.043974817369	11	10	8	7	-0.008719627315	15	14	8	6	0.004468808994
15	15	11	7	0.026195860339	10	10	8	7	-0.046025944427	15	13	8	6	-0.013842408359
14	14	11	7	0.049585668760	11	9	8	7	-0.164800956075	15	12	8	6	0.019183180083
14	13	11	7	-0.095043937635	10	9	8	7	-0.109431322682	15	14	7	6	-0.030355202554
13	13	11	7	-2.344338743549	9	9	8	7	-0.019867062518	15	13	7	6	0.175155513500
14	12	11	7	-0.089812161251	11	8	8	7	-0.005619228151	15	12	7	6	-0.077277696999
13	12	11	7	0.980086109203	10	8	8	7	-0.149637475844	15	15	6	6	-0.178012819978
12	12	11	7	-0.168501076462	9	8	8	7	0.054008973342	14	14	6	6	-0.045014190973
11	11	11	7	-0.421378088687	8	8	8	7	-0.599608812784	14	13	6	6	0.173930624664
15	15	10	7	-0.091100143622	15	15	7	7	-0.662783867880	13	13	6	6	1.395474232003
14	14	10	7	-0.163026378126	14	14	7	7	-0.269798765059	14	12	6	6	-0.010033532367
14	13	10	7	0.543777757868	14	13	7	7	0.872298697994	13	12	6	6	0.037063515412
13	13	10	7	-8.667884834461	13	13	7	7	-73.173687604691	12	12	6	6	0.114722543343
14	12	10	7	0.001525934779	14	12	7	7	0.027481466336	11	11	6	6	-0.025960138095
13	12	10	7	0.260280875081	13	12	7	7	-0.972272530277	11	10	6	6	-0.081057368962
12	12	10	7	-0.136117054503	12	12	7	7	0.606951246448	10	10	6	6	0.086779723527
11	11	10	7	0.124427117788	11	11	7	7	-1.422316738135	11	9	6	6	0.258571683591
11	10	10	7	-0.168810406866	11	10	7	7	0.223127555670	10	9	6	6	-0.089986272492
10	10	10	7	0.351565124561	10	10	7	7	0.361994435757	9	9	6	6	-0.062621628394
15	15	9	7	-0.006289659946	11	9	7	7	1.988442304887	11	8	6	6	0.030096853445
14	14	9	7	0.016336554120	10	9	7	7	-0.157237649995	10	8	6	6	-0.132281293124
14	13	9	7	0.398595963226	9	9	7	7	-1.430357026598	9	8	6	6	0.028412242063
13	13	9	7	-0.662895628521	11	8	7	7	-0.076059956333	8	8	6	6	0.011269555461
14	12	9	7	0.024087970432	10	8	7	7	0.640694742537	11	7	6	6	-0.015099756624
13	12	9	7	-1.018016487986	9	8	7	7	0.138210716390	10	7	6	6	0.176912687838
12	12	9	7	0.636522609499	8	8	7	7	0.078863118690	9	7	6	6	0.247004601890
11	11	9	7	0.554649728931	11	7	7	7	0.008023921494	8	7	6	6	0.142683770934
11	10	9	7	-0.180932266596	10	7	7	7	1.229076708901	7	7	6	6	0.397636710598

Table S6: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

6	6	6	6	0.087976126408	14	14	5	5	1.210375420442	14	14	6	4	0.031340984883
15	14	11	5	-0.002370648675	14	13	5	5	-14.761971302285	14	13	6	4	-0.128723498685
15	13	11	5	0.844604899928	13	13	5	5	2259.248775498512	13	13	6	4	-1.012755967197
15	12	11	5	-0.647214336787	14	12	5	5	0.012027124681	14	12	6	4	-0.000544976705
15	14	10	5	-0.528736400765	13	12	5	5	-1.338056587074	13	12	6	4	-0.205783204916
15	13	10	5	2.005623275724	12	12	5	5	1.676416323284	12	12	6	4	0.010153206271
15	12	10	5	0.045669048006	11	11	5	5	-1.129765882111	11	11	6	4	0.047162916877
15	14	9	5	0.075370278526	11	10	5	5	-0.276028235342	11	10	6	4	-0.040110285675
15	13	9	5	-8.679517020390	10	10	5	5	0.671664683681	10	10	6	4	-0.069363012403
15	12	9	5	0.802096716817	11	9	5	5	2.286687249751	11	9	6	4	0.029210750134
15	14	8	5	-0.368703990868	10	9	5	5	0.014998040089	10	9	6	4	-0.324370135825
15	13	8	5	1.487241432395	9	9	5	5	-1.904610727755	9	9	6	4	0.028851699172
15	12	8	5	-0.022671030994	11	8	5	5	0.082205346322	11	8	6	4	0.088504217121
15	14	7	5	-0.278755585436	10	8	5	5	-1.858348957371	10	8	6	4	-0.139950018333
15	13	7	5	1.512419356226	9	8	5	5	0.053245740599	9	8	6	4	0.105507490401
15	12	7	5	-0.142238920426	8	8	5	5	-2.649557544481	8	8	6	4	0.119377289422
15	15	6	5	-1.155642150762	11	7	5	5	0.480523858909	11	7	6	4	-0.049701875505
14	14	6	5	-0.653658231960	10	7	5	5	-8.502464820284	10	7	6	4	0.136462167542
14	13	6	5	2.467436523718	9	7	5	5	0.820128263568	9	7	6	4	-0.204039278770
13	13	6	5	3.387848922518	8	7	5	5	5.493674898335	8	7	6	4	0.017875236107
14	12	6	5	0.041091243714	7	7	5	5	-434.781368199085	7	7	6	4	0.259921832234
13	12	6	5	-0.347477158622	6	6	5	5	0.624610301105	6	6	6	4	-0.078098751254
12	12	6	5	0.399826074436	6	5	5	5	3.618765446857	15	15	5	4	-0.374720441391
11	11	6	5	0.209303735205	5	5	5	5	5710.329988726040	14	14	5	4	-0.389726645849
11	10	6	5	0.099403750942	15	14	11	4	0.003406104417	14	13	5	4	1.595146820172
10	10	6	5	0.302286667103	15	13	11	4	-0.016240305859	13	13	5	4	-6.758997736410
11	9	6	5	-0.089376184211	15	12	11	4	-0.001852920803	14	12	5	4	0.005776753075
10	9	6	5	0.032262620855	15	14	10	4	0.029047258464	13	12	5	4	0.146053757193
9	9	6	5	0.491264335435	15	13	10	4	-0.066051176844	12	12	5	4	0.095598172074
11	8	6	5	0.044034117640	15	12	10	4	-0.009264604013	11	11	5	4	-0.029374967078
10	8	6	5	-0.583343067106	15	14	9	4	0.014196643208	11	10	5	4	-0.020055142743
9	8	6	5	0.063217297851	15	13	9	4	0.264858679418	10	10	5	4	-0.584339609041
8	8	6	5	-0.078761681956	15	12	9	4	-0.034442527861	11	9	5	4	-0.038366360268
11	7	6	5	0.251125266762	15	14	8	4	-0.018556456861	10	9	5	4	0.078476645815
10	7	6	5	0.419850055946	15	13	8	4	0.096678867760	9	9	5	4	-0.092631898245
9	7	6	5	0.123382726150	15	12	8	4	-0.024850937822	11	8	5	4	0.074988794846
8	7	6	5	1.155350618630	15	14	7	4	-0.005994743773	10	8	5	4	-0.102019639496
7	7	6	5	-4.653236709836	15	13	7	4	0.023869979752	9	8	5	4	-0.194883670267
6	6	6	5	0.068909755821	15	12	7	4	0.048066945525	8	8	5	4	1.282849674627
15	15	5	5	1.238044000816	15	15	6	4	0.002483262498	11	7	5	4	-0.066705148921

Table S7: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

10	7	5	4	1.253882406583	15	12	10	3	-0.035859467306	11	11	5	3	0.050900057816
9	7	5	4	0.330473874895	15	14	9	3	0.008419890117	11	10	5	3	0.088504216252
8	7	5	4	0.845803848685	15	13	9	3	1.622613646318	10	10	5	3	0.492906033482
7	7	5	4	-3.368516612566	15	12	9	3	0.096460877075	11	9	5	3	-0.018311247793
6	6	5	4	-0.357776596071	15	14	8	3	0.114390610719	10	9	5	3	-0.097659824513
6	5	5	4	-1.138398081960	15	13	8	3	-0.366224346841	9	9	5	3	0.660164079684
5	5	5	4	1.013812219782	15	12	8	3	0.070955967192	11	8	5	3	0.064089260759
15	15	4	4	-0.002378524251	15	14	7	3	0.198480516551	10	8	5	3	0.388459395567
14	14	4	4	-0.041304401602	15	13	7	3	-0.663127656620	9	8	5	3	-0.014823366371
14	13	4	4	0.131378843598	15	12	7	3	-0.019292175414	8	8	5	3	0.839947759822
13	13	4	4	-1.130898573368	15	15	6	3	0.366235043080	11	7	5	3	-0.421593977145
14	12	4	4	0.000935758763	14	14	6	3	0.107763208610	10	7	5	3	1.038071637007
13	12	4	4	0.039714281868	14	13	6	3	-0.370257165087	9	7	5	3	-0.269000495055
12	12	4	4	0.099068260465	13	13	6	3	-0.712827890957	8	7	5	3	-1.362441765077
11	11	4	4	-0.006049469716	14	12	6	3	0.003378855508	7	7	5	3	112.077105277779
11	10	4	4	0.051271695084	13	12	6	3	0.124254691218	6	6	5	3	0.167396566504
10	10	4	4	0.025253258209	12	12	6	3	-0.051686430044	6	5	5	3	-1.202493471059
11	9	4	4	0.092410473411	11	11	6	3	-0.178863424576	5	5	5	3	-845.600942286610
10	9	4	4	0.177462136086	11	10	6	3	0.028774770842	15	15	4	3	0.072786552609
9	9	4	4	-0.082095224411	10	10	6	3	-0.078587994590	14	14	4	3	0.067636142951
11	8	4	4	0.062185081992	11	9	6	3	0.020491161348	14	13	4	3	-0.121093823647
10	8	4	4	-0.011462137025	10	9	6	3	-0.135154224243	13	13	4	3	1.934473420597
9	8	4	4	-0.041554047472	9	9	6	3	-0.078508638272	14	12	4	3	0.015477338454
8	8	4	4	85.774992995489	11	8	6	3	-0.280336017478	13	12	4	3	-0.071936924786
11	7	4	4	-0.114782536187	10	8	6	3	0.063217299040	12	12	4	3	0.129994985859
10	7	4	4	-0.141876887639	9	8	6	3	-0.155209365631	11	11	4	3	-0.077348038412
9	7	4	4	-0.052462279740	8	8	6	3	-0.163881614324	11	10	4	3	0.015259347899
8	7	4	4	-0.471945319132	11	7	6	3	-0.160441143009	10	10	4	3	0.317175456292
7	7	4	4	-0.153318435260	10	7	6	3	0.651356154026	11	9	4	3	-0.090248141106
6	6	4	4	-0.023493563114	9	7	6	3	0.101583648602	10	9	4	3	-0.238917788231
6	5	4	4	-0.159847792659	8	7	6	3	0.091120102756	9	9	4	3	-0.126177952122
5	5	4	4	-2.631494448249	7	7	6	3	-1.475075960520	11	8	4	3	-0.189215912533
6	4	4	4	0.024723140928	6	6	6	3	0.102723245953	10	8	4	3	-0.094171974851
5	4	4	4	1.277214657396	15	15	5	3	0.636009375994	9	8	4	3	0.096351881771
4	4	4	4	85.970318264839	14	14	5	3	0.218768191751	8	8	4	3	-0.605757444755
15	14	11	3	0.009646087706	14	13	5	3	0.019946142763	11	7	4	3	0.010463552629
15	13	11	3	0.097223844472	13	13	5	3	-435.619849414027	10	7	4	3	-0.095915900630
15	12	11	3	-0.051009819736	14	12	5	3	0.004032827710	9	7	4	3	-0.108995341651
15	14	10	3	0.164146984033	13	12	5	3	2.968161133321	8	7	4	3	-0.439033234967
15	13	10	3	-0.531243293612	12	12	5	3	-2.695197935841	7	7	4	3	1.156479222070

Table S8: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

6	6	4	3	0.058688063919	15	12	11	2	0.663781628667	14	12	5	2	-0.011444510843
6	5	4	3	0.193573968102	15	14	10	2	-0.000926460401	13	12	5	2	-4.842009042578
5	5	4	3	-0.231161619804	15	13	10	2	0.081746505996	12	12	5	2	4.814392119537
6	4	4	3	-0.248096761227	15	12	10	2	-0.129704456177	11	11	5	2	-2.402568048331
5	4	4	3	1.067032743148	15	14	9	2	0.050056110504	11	10	5	2	0.057113558877
4	4	4	3	-0.593007955268	15	13	9	2	0.661274735823	10	10	5	2	-0.123416015027
15	15	3	3	-0.144649954152	15	12	9	2	-0.794358047574	11	9	5	2	3.317818191415
14	14	3	3	-0.095337496627	15	14	8	2	-0.016540043046	10	9	5	2	-0.032262621116
14	13	3	3	0.383498141167	15	13	8	2	0.046541010745	9	9	5	2	-5.985542236411
13	13	3	3	97.730303797703	15	12	8	2	-0.013515422322	11	8	5	2	-0.012207478172
14	12	3	3	0.005539722037	15	14	7	2	-0.076296738927	10	8	5	2	-0.068885055688
13	12	3	3	1.164057901090	15	13	7	2	0.240334727622	9	8	5	2	0.191831800714
12	12	3	3	-0.998983937806	15	12	7	2	-0.042508183120	8	8	5	2	-0.045573597898
11	11	3	3	-0.061962253074	15	15	6	2	-0.008531833027	11	7	5	2	-0.943463674748
11	10	3	3	-0.033064540621	14	14	6	2	0.037613592030	10	7	5	2	1.268705772703
10	10	3	3	0.170667635247	14	13	6	2	-0.054061690707	9	7	5	2	3.503110269836
11	9	3	3	0.125056743719	13	13	6	2	0.969785749068	8	7	5	2	0.323934154346
10	9	3	3	-0.005301251830	14	12	6	2	-0.050900824420	7	7	5	2	-5.147110436450
9	9	3	3	0.353356810716	13	12	6	2	0.598602413423	6	6	5	2	-0.216380833512
11	8	3	3	-0.031917135888	12	12	6	2	-0.542294549144	6	5	5	2	1.639509365994
10	8	3	3	-0.135001816995	11	11	6	2	0.436287135622	5	5	5	2	-26.070723250539
9	8	3	3	0.037550411410	11	10	6	2	-0.020055142747	15	15	4	2	-0.003591693358
8	8	3	3	-0.348929187787	10	10	6	2	0.082745966828	14	14	4	2	0.002294763529
11	7	3	3	0.153921500068	11	9	6	2	-0.431185570758	14	13	4	2	-0.003923832392
10	7	3	3	-0.493103472973	10	9	6	2	0.153029459250	13	13	4	2	-0.160250476793
9	7	3	3	-0.085527103506	9	9	6	2	0.943928135892	14	12	4	2	0.042835169139
8	7	3	3	0.830348459104	11	8	6	2	0.330037893423	13	12	4	2	-0.157825254325
7	7	3	3	21.811321781558	10	8	6	2	0.059293465660	12	12	4	2	-0.068694389411
6	6	3	3	0.297386008404	9	8	6	2	-0.116407024628	11	11	4	2	-0.123952659833
6	5	3	3	0.495417175336	8	8	6	2	0.022342742203	11	10	4	2	-0.068885055704
5	5	3	3	182.639968379827	11	7	6	2	0.245021527168	10	10	4	2	-0.027164796010
6	4	3	3	0.035205762305	10	7	6	2	-0.607322041953	11	9	4	2	-0.027030844801
5	4	3	3	0.207256000915	9	7	6	2	-0.662255693767	10	9	4	2	-0.199243483959
4	4	3	3	-0.378572849333	8	7	6	2	0.131666372421	9	9	4	2	-0.064183577851
6	3	3	3	-0.422428852320	7	7	6	2	1.867257378994	11	8	4	2	0.034006546495
5	3	3	3	-59.684061774096	6	6	6	2	0.296944742163	10	8	4	2	0.133846279147
4	3	3	3	0.227403931247	15	15	5	2	-0.361256964363	9	8	4	2	0.285567794268
3	3	3	3	77.933642948496	14	14	5	2	-0.107942018669	8	8	4	2	-0.053085871603
15	14	11	2	-0.037412650909	14	13	5	2	0.533423200879	11	7	4	2	-0.108559359933
15	13	11	2	-0.673700204734	13	13	5	2	13.496912587288	10	7	4	2	0.103763564977

Table S9: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺(cont.)

9	7	4	2	-0.048393931515	3	3	3	2	0.349451697414	15	12	11	1	-0.254504121994
8	7	4	2	0.044034117901	15	15	2	2	0.062104721792	15	14	10	1	0.002752132369
7	7	4	2	-0.084793607285	14	14	2	2	0.018886953499	15	13	10	1	0.032153625692
6	6	4	2	-0.054316294359	14	13	2	2	-0.186782917875	15	12	10	1	-0.003378855583
6	5	4	2	-0.091119705920	13	13	2	2	-9.497867748576	15	14	9	1	-0.010381806261
5	5	4	2	-0.684054271110	14	12	2	2	0.133386897549	15	13	9	1	-0.250362299022
6	4	4	2	-0.006985325307	13	12	2	2	11.244574883907	15	12	9	1	0.310745718117
5	4	4	2	-0.118961004748	12	12	2	2	-10.398443482874	15	14	8	1	-0.017657245295
4	4	4	2	-0.091258777089	11	11	2	2	0.570788140952	15	13	8	1	-0.065397204797
15	15	3	2	0.046638897038	11	10	2	2	0.050783395938	15	12	8	1	0.064525242065
14	14	3	2	0.021884161939	10	10	2	2	0.070646641659	15	14	7	1	-0.030273456053
14	13	3	2	0.054606673165	11	9	2	2	-0.672754262004	15	13	7	1	0.071718934592
13	13	3	2	-3.160956677921	10	9	2	2	-0.209549802256	15	12	7	1	-0.003923832290
14	12	3	2	-0.076296739015	9	9	2	2	1.197898076757	15	15	6	1	-0.001558874154
13	12	3	2	-1.895646971197	11	8	2	2	0.039444293992	14	14	6	1	0.008581850564
12	12	3	2	1.901949520887	10	8	2	2	-0.093356876692	14	13	6	1	-0.010790538560
11	11	3	2	-0.633866811736	9	8	2	2	0.091960885843	13	13	6	1	0.164824876072
11	10	3	2	-0.156953291356	8	8	2	2	0.165246905187	14	12	6	1	0.025940891225
10	10	3	2	0.016617371016	11	7	2	2	0.210075898806	13	12	6	1	-0.088940198455
11	9	3	2	0.793486095090	10	7	2	2	-0.016314254353	12	12	6	1	0.069393405205
10	9	3	2	0.367096309308	9	7	2	2	-0.915356597785	11	11	6	1	-0.138263406481
9	9	3	2	-0.990261830201	8	7	2	2	-0.233515830103	11	10	6	1	-0.075860757602
11	8	3	2	-0.160877123680	7	7	2	2	2.874895009830	10	10	6	1	0.004262866905
10	8	3	2	0.103763565242	6	6	2	2	0.021568250684	11	9	6	1	0.121202819489
9	8	3	2	-0.107251415706	6	5	2	2	0.905209305430	10	9	6	1	-0.281643961981
8	8	3	2	0.142893447607	5	5	2	2	-5.832425669674	9	9	6	1	-0.276746937010
11	7	3	2	0.241097693996	6	4	2	2	-0.158130904256	11	8	6	1	-0.189215912634
10	7	3	2	-0.183112175240	5	4	2	2	-0.001955548780	10	8	6	1	0.064961223403
9	7	3	2	0.220606568615	4	4	2	2	0.092901103308	9	8	6	1	-0.202731334829
8	7	3	2	0.013079440389	6	3	2	2	0.103715492281	8	8	6	1	0.063477052678
7	7	3	2	1.723999643088	5	3	2	2	-2.346248750619	11	7	6	1	0.031390658240
6	6	3	2	-0.022631086942	4	3	2	2	-0.148958240738	10	7	6	1	-0.204475260191
6	5	3	2	-0.216736495505	3	3	2	2	-0.836696347442	9	7	6	1	0.148233664200
5	5	3	2	3.491226573870	6	2	2	2	-0.814008065805	8	7	6	1	0.065833186240
6	4	3	2	-0.336144005416	5	2	2	2	3.270402052485	7	7	6	1	0.217973005933
5	4	3	2	0.229761527313	4	2	2	2	0.143892111640	6	6	6	1	-0.032996029505
4	4	3	2	0.027099654873	3	2	2	2	0.052295712297	15	15	5	1	-0.000209423843
6	3	3	2	-0.298811547376	2	2	2	2	407.849807848417	14	14	5	1	0.009690815994
5	3	3	2	2.130653335143	15	14	11	1	0.014496380396	14	13	5	1	0.005776752915
4	3	3	2	-0.293294077949	15	13	11	1	0.266929590902	13	13	5	1	-1.664248736313

Table S10: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺ (cont.)

14	12	5	1	0.025395914522	9	7	4	1	-0.059729447045	3	3	3	1	-0.072910940302
13	12	5	1	1.610079181952	8	7	4	1	-0.037930378777	15	15	2	1	-0.016219751072
12	12	5	1	-1.812869944141	7	7	4	1	0.013300455434	14	14	2	1	-0.006176245146
11	11	5	1	0.736152093816	6	6	4	1	0.071449520613	14	13	2	1	0.042399187746
11	10	5	1	-0.048393931507	6	5	4	1	0.165672912345	13	13	2	1	5.038590716757
10	10	5	1	0.147735787898	5	5	4	1	-0.027833993990	14	12	2	1	0.004250818307
11	9	5	1	-1.065974438312	6	4	4	1	-0.027001446150	13	12	2	1	-5.053460005214
10	9	5	1	0.144745813260	5	4	4	1	-0.017677955025	12	12	2	1	4.951781983404
9	9	5	1	1.459326273637	4	4	4	1	-0.032775720197	11	11	2	1	-0.216268692440
11	8	5	1	-0.085016366163	15	15	3	1	-0.001440038160	11	10	2	1	0.125998614567
10	8	5	1	-0.032698602328	14	14	3	1	0.003999001544	10	10	2	1	-0.008186676951
9	8	5	1	0.138642074190	14	13	3	1	-0.011008529360	11	9	2	1	0.197499558442
8	8	5	1	-0.110206650011	13	13	3	1	-0.722720125627	10	9	2	1	0.089812161262
11	7	5	1	0.225838347339	14	12	3	1	0.010572548118	9	9	2	1	-0.149603177587
10	7	5	1	-0.146489738720	13	12	3	1	0.779098699868	11	8	2	1	0.266820595577
9	7	5	1	-0.075424776128	12	12	3	1	-0.913583077005	10	8	2	1	-0.175264508868
8	7	5	1	0.068013093026	11	11	3	1	0.455769482293	9	8	2	1	-0.173084601993
7	7	5	1	-0.046077748966	11	10	3	1	-0.141257962359	8	8	2	1	-0.134066387824
6	6	5	1	0.000001934777	10	10	3	1	-0.069231351626	11	7	2	1	-0.228890216790
6	5	5	1	0.098860774643	11	9	3	1	-0.780406643674	10	7	2	1	-0.057113558819
5	5	5	1	-0.259424296973	10	9	3	1	-0.048393931548	9	7	2	1	0.319138359430
15	15	4	1	-0.001672787354	9	9	3	1	0.604161681932	8	7	2	1	-0.050137856983
14	14	4	1	0.007756819613	11	8	3	1	0.110739266824	7	7	2	1	0.075918091312
14	13	4	1	0.038148369468	10	8	3	1	-0.087196273027	6	6	2	1	-0.015567987982
13	13	4	1	0.030518447409	9	8	3	1	-0.070628981239	6	5	2	1	-0.117279175173
14	12	4	1	-0.006103739112	8	8	3	1	0.105953885110	5	5	2	1	0.147097762886
13	12	4	1	-0.051445801098	11	7	3	1	0.009591590050	6	4	2	1	-0.045778018682
12	12	4	1	0.042338386651	10	7	3	1	0.003487850848	5	4	2	1	-0.094607955306
11	11	4	1	0.002202747980	9	7	3	1	-0.180060303824	4	4	2	1	-0.088031356856
11	10	4	1	0.039674304248	8	7	3	1	0.197499558400	6	3	2	1	-0.069322201394
10	10	4	1	0.116826212419	7	7	3	1	0.030093130796	5	3	2	1	0.106378787206
11	9	4	1	0.043162155170	6	6	3	1	0.104863451630	4	3	2	1	0.068013070142
10	9	4	1	-0.088068235800	6	5	3	1	0.382352498525	3	3	2	1	-0.048221612677
9	9	4	1	0.191973545942	5	5	3	1	-0.120281793705	6	2	2	1	0.094291433091
11	8	4	1	0.105071509042	6	4	3	1	0.091991891538	5	2	2	1	-0.205119834060
10	8	4	1	-0.193139744832	5	4	3	1	-0.002615919974	4	2	2	1	-0.019114358182
9	8	4	1	-0.268128539659	4	4	3	1	-0.071934544479	3	2	2	1	-0.012460518178
8	8	4	1	0.157491383361	6	3	3	1	-0.069877602360	2	2	2	1	-0.400536928781
11	7	4	1	0.231070123591	5	3	3	1	-0.180282823220	15	15	1	1	0.002522991032
10	7	4	1	0.052753745210	4	3	3	1	-0.004260903943	14	14	1	1	0.005977190154

Table S11: CCSD(T)-F12b/cc-pVTZ-F12 force constants for c-(CH)C₃H₂⁺ (cont.)

14	13	1	1	-0.033753458333	8	8	1	1	0.113806119776	4	3	1	1	0.086050622125
13	13	1	1	2.859705581539	11	7	1	1	0.013291349696	3	3	1	1	0.025482258276
14	12	1	1	-0.005115662588	10	7	1	1	-0.069887644656	6	2	1	1	-0.020456799342
13	12	1	1	-2.603518661104	9	7	1	1	0.118512172536	5	2	1	1	0.017004714225
12	12	1	1	2.883766444474	8	7	1	1	-0.033661972235	4	2	1	1	0.087422495964
11	11	1	1	2.875235487984	7	7	1	1	-0.073870049510	3	2	1	1	0.017539601960
11	10	1	1	0.023229373655	6	6	1	1	0.042094986234	2	2	1	1	-0.866628524264
10	10	1	1	0.004646289296	6	5	1	1	-0.091836536815	6	1	1	1	0.075127271494
11	9	1	1	-2.680849551636	5	5	1	1	0.725274846662	5	1	1	1	-0.103656775891
10	9	1	1	0.119982352873	6	4	1	1	-0.093244770393	4	1	1	1	0.042910642534
9	9	1	1	2.799934472786	5	4	1	1	-0.128720961461	3	1	1	1	0.057465277366
11	8	1	1	0.064487063616	4	4	1	1	0.112316903692	2	1	1	1	-1.168282672595
10	8	1	1	-0.128374899932	6	3	1	1	-0.086382876968	1	1	1	1	176.892485113517
9	8	1	1	0.027156615715	5	3	1	1	-0.046493414937					