

Supplementary Material

DFT Exploration of [3+2] Cycloaddition Reaction of 1*H*-Phosphorinium-3-olate and 1-Methylphosphorinium-3-olate with Methyl Methacrylate

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Table S1: Relative electronic energies^a (ΔE , in kcal·mol⁻¹) computed using various methods in the gas phase for the most favorable TS and CA involved in the 32CA.

Gas phase			
	B3LYP/6-31G(d)	B3LYP/6-311G(d,p)	B3LYP/6-311++G(d,p)
TS6x-H	8.4	10.8	12.6
CA6x-H	-42.4	-37.7	-34.9
	M06-2X/6-31G(d)	M06-2X/6-311G(d,p)	M06-2X/6-311++G(d,p)
TS6x-H	2.8	3.9	5.3
CA6x-H	-61.8	-58.3	-55.7
	MPWB1K/6-31G(d)	MPWB1K/6-311G(d,p)	MPWB1K/6-311++G(d,p)
TS6x-H	6.1	7.4	8.6
CA6x-H	-61.4	-58.3	-56.0
	B3LYP-G3/6-31G(d)// B3LYP/6-31G(d)	B3LYP-G3/6-311G(d,p)// B3LYP/6-311G(d,p)	B3LYP-G3/6-311++G(d,p)// B3LYP/6-311++G(d,p)
TS6x-H	-2.6	-0.3	1.3
CA6x-H	-56.8	-52.1	-49.4

Table S2: Total electronic energies (E, in a.u.) and relative electronic energies^a including ZPE (ΔE , in kcal mol⁻¹) computed at the B3LYP/6-31G(d) computational level, in the gas phase and solvents for the TSs and CAs involved in the 32CA reactions of **1a** and **1b** with **MMA**.

	Gas phase		THF		EtOH	
	E	ΔE	E	ΔE	E	ΔE
1a	-609.948959	-	-609.962117	-	-609.964723	-
1b	-649.250043	-	-649.265294	-	-649.268134	-
MMA	-345.667602	-	-345.671750	-	-345.672521	-
TS6n-H	-955.597419	12.0	-955.610746	14.5	-955.613526	14.9
TS6x-H	-955.603209	8.4	-955.614090	12.4	-955.616111	13.3
TS7n-H	-955.593764	14.3	-955.606072	17.4	-955.608768	17.9
TS7x-H	-955.599628	10.6	-955.611168	14.2	-955.613456	14.9
CA6n-H	-955.684248	-42.5	-955.693524	-37.4	-955.695270	-36.4
CA6x-H	-955.684425	-42.6	-955.693399	-37.4	-955.695016	-36.3
CA7n-H	-955.683305	-41.9	-955.692256	-36.6	-955.693972	-35.6
CA7x-H	-955.683988	-42.3	-955.692665	-36.9	-955.694252	-35.8
TS6n-Me	-994.892140	16.0	-994.906373	19.6	-994.909374	19.2
TS6x-Me	-994.899186	11.6	-994.910130	17.9	-994.912170	16.9
TS7n-Me	-994.887568	18.9	-994.900876	23.2	-994.903674	22.7
TS7x-Me	-994.894184	14.7	-994.906267	20.0	-994.908820	19.3
CA6n-Me	-994.972159	-34.2	-994.982374	-27.4	-994.984322	-28.4
CA6x-Me	-994.974533	-35.7	-994.984058	-28.3	-994.985824	-29.5
CA7n-Me	-994.971539	-33.8	-994.981733	-27.0	-994.983649	-28.0
CA7x-Me	-994.974338	-35.6	-994.983654	-28.1	-994.985391	-29.2

^a Relative to **1a** + **MMA** or **1b** + **MMA**.

Table S3: Wiberg bond order of the TSs involved in the 32CA reactions of **1a** and **1b** with **MA**.

Wiberg Bond Order						
	Gas phase		THF		EtOH	
	C3–C4	C1–C5	C3–C4	C1–C5	C3–C4	C1–C5
TS6n-H	0.14	0.33	0.14	0.35	0.14	0.05
TS6x-H	0.15	0.33	0.15	0.35	0.15	0.35
TS6n-Me	0.14	0.37	0.14	0.41	0.14	0.41
TS6x-Me	0.16	0.40	0.16	0.42	0.15	0.43
	C1–C4	C3–C5	C1–C4	C3–C5	C1–C4	C3–C5
TS7n-H	0.22	0.30	0.21	0.32	0.21	0.33
TS7x-H	0.19	0.31	0.19	0.33	0.19	0.33
TS7n-Me	0.22	0.34	0.21	0.37	0.21	0.37
TS7x-Me	0.20	0.37	0.19	0.40	0.18	0.41

Table S4: Dipole moment and global electron density transfer of the TSs involved in the 32CA reactions of **1a** and **1b** with **MA**.

	Gas phase		THF		EtOH	
	GEDT (e)	Dipole Moment (debye)	GEDT (e)	Dipole Moment (debye)	GEDT (e)	Dipole Moment (debye)
TS6n-H	0.04	5.774	0.05	7.841	0.05	8.334
TS6x-H	0.05	4.598	0.05	5.913	0.05	6.182
TS6n-Me	0.08	6.536	0.09	8.837	0.09	9.366
TS6x-Me	0.08	4.635	0.09	5.997	0.09	6.269
TS7n-H	0.01	4.832	0.02	6.938	0.03	7.453
TS7x-H	0.04	3.712	0.04	5.152	0.04	5.484
TS7n-Me	0.04	5.790	0.06	8.126	0.06	8.662
TS7x-Me	0.08	4.281	0.09	6.023	0.09	6.446

Cartesian coordinates of the B3LYP/6-31G(d) optimised geometries associated with the stationary points for 32CA reaction of **1a** and **1b** with **MMA**.

Gas Phase:

1a:

6	-0.378605000	-1.217955000	0.000000000
6	-1.344474000	-0.106020000	-0.000001000
6	-0.787032000	1.253649000	0.000000000
6	0.537272000	1.630291000	0.000000000
6	1.664194000	0.762563000	0.000000000
1	2.250847000	-1.867386000	0.000001000
1	-0.750483000	-2.235674000	0.000001000
1	-1.543987000	2.032846000	0.000000000
1	0.755748000	2.696721000	0.000001000
1	2.684367000	1.121754000	0.000000000
8	-2.561836000	-0.322093000	0.000000000
15	1.263338000	-0.873779000	0.000000000

1b:

6	-0.223420000	-1.140756000	-0.017906000
6	-1.579577000	-0.570663000	0.004611000
6	-1.678308000	0.894546000	0.021017000

6	-0.649891000	1.808921000	0.019563000
6	0.741745000	1.515162000	0.006781000
1	-0.119623000	-2.219927000	-0.037977000
1	-2.699850000	1.263952000	0.038633000
1	-0.917025000	2.864495000	0.031301000
1	1.498571000	2.288891000	-0.004260000
8	-2.579024000	-1.300804000	0.025263000
15	1.113284000	-0.127422000	-0.083900000
6	2.829529000	-0.729012000	0.083318000
1	3.510365000	0.010078000	-0.347310000
1	3.083543000	-0.889193000	1.134426000
1	2.936489000	-1.669722000	-0.462720000

MMA:

6	-1.363296000	1.580528000	0.000035000
1	-0.546782000	2.293607000	0.000141000
1	-2.373963000	1.980423000	0.000102000
6	-1.144836000	0.259535000	-0.000012000
6	0.241517000	-0.299144000	0.000018000
8	0.484179000	-1.491011000	0.000081000
8	1.207341000	0.649071000	-0.000058000

6	2.552255000	0.149509000	-0.000013000
1	2.737894000	-0.458384000	-0.889789000
1	3.192081000	1.032677000	0.001193000
1	2.737146000	-0.460376000	0.888537000
6	-2.240301000	-0.773947000	-0.000051000
1	-2.162821000	-1.426362000	-0.877098000
1	-2.162618000	-1.426657000	0.876750000
1	-3.225123000	-0.298280000	0.000123000

TS6n-H: (Imaginary frequency = $342.10i$ cm⁻¹)

6	-0.590705000	-0.718920000	1.752043000
6	-1.134787000	-1.582815000	0.812288000
6	-1.888875000	-1.208318000	-0.383638000
1	-1.609434000	2.602112000	0.331611000
1	-0.974327000	-2.650752000	0.923491000
6	-2.044430000	0.248834000	-0.633036000
1	-2.741617000	0.476444000	-1.437588000
6	-0.738402000	0.675960000	1.742381000
1	-0.292376000	1.275731000	2.529940000
6	-0.201690000	0.598197000	-1.746826000
1	-0.661846000	1.406411000	-2.308903000

6	0.886963000	0.893806000	-0.945878000
8	-2.283746000	-2.042686000	-1.204566000
1	0.024158000	-1.158372000	2.536200000
6	1.686902000	-0.241092000	-0.462713000
8	1.403329000	-1.418416000	-0.628937000
8	2.809085000	0.156703000	0.198638000
6	3.644056000	-0.907276000	0.670614000
1	4.506823000	-0.422649000	1.129925000
1	3.113792000	-1.519868000	1.405917000
1	3.959141000	-1.549723000	-0.156339000
1	-0.296731000	-0.397452000	-2.168901000
15	-2.041086000	1.328511000	0.768957000
6	1.340428000	2.308212000	-0.692465000
1	2.163272000	2.580717000	-1.368932000
1	0.525839000	3.017968000	-0.873607000
1	1.713513000	2.447440000	0.325140000

TS6x-H: (Imaginary frequency = $336.93i$ cm⁻¹)

6	1.321739000	-0.463485000	1.908573000
6	2.308642000	0.293140000	1.292118000
6	2.573394000	0.374186000	-0.142060000

1	-0.305510000	-2.058956000	-1.060731000
1	2.946054000	0.926897000	1.903250000
6	1.702955000	-0.449170000	-1.023068000
1	2.063487000	-0.517948000	-2.047694000
6	0.464034000	-1.361536000	1.253360000
1	-0.270448000	-1.924057000	1.821316000
6	0.140146000	0.982179000	-1.457814000
1	-0.172702000	0.416596000	-2.328748000
6	-0.762076000	1.122250000	-0.417941000
8	3.400851000	1.160161000	-0.621300000
1	1.193781000	-0.335409000	2.982830000
6	-1.940073000	0.240129000	-0.453495000
8	-2.097248000	-0.682614000	-1.248356000
8	-2.870662000	0.551534000	0.483035000
6	-4.045502000	-0.269137000	0.477507000
1	-4.543927000	-0.225150000	-0.494610000
1	-3.792135000	-1.310909000	0.695298000
1	-4.690076000	0.137379000	1.257833000
1	0.899628000	1.743864000	-1.617745000
15	0.906205000	-1.878054000	-0.354229000
6	-0.572625000	2.159997000	0.650628000

1	-0.709862000	3.171864000	0.246227000
1	-1.271650000	2.028304000	1.477519000
1	0.452970000	2.114368000	1.044809000

TS7n-H: (Imaginary frequency = $386.59i$ cm⁻¹)

6	0.275217000	-1.566531000	-0.606635000
6	0.870382000	-1.828555000	0.716926000
6	1.757451000	-1.022395000	1.378454000
1	2.388574000	1.569902000	-1.314320000
1	0.477713000	-2.708500000	1.218565000
6	2.297369000	0.197742000	0.844132000
1	3.091678000	0.680285000	1.409776000
6	0.812384000	-0.423461000	-1.338328000
1	0.418655000	-0.278101000	-2.341359000
6	0.583654000	1.611499000	1.231848000
1	1.242163000	2.474054000	1.188020000
6	-0.386914000	1.443464000	0.257572000
6	-1.500392000	0.509066000	0.581756000
8	-1.576662000	-0.139215000	1.611914000
8	-2.424807000	0.458046000	-0.398097000
6	-3.460723000	-0.525460000	-0.214650000

1	-4.010398000	-0.335097000	0.710802000
1	-4.115560000	-0.417074000	-1.080017000
1	-3.015387000	-1.521442000	-0.189654000
1	0.415375000	1.174973000	2.208745000
8	-0.683371000	-2.233575000	-1.023354000
1	2.017852000	-1.280928000	2.403574000
15	2.394863000	0.208499000	-0.926585000
6	-0.524994000	2.406584000	-0.897503000
1	-1.138839000	3.268517000	-0.598815000
1	0.451261000	2.802186000	-1.199505000
1	-1.007912000	1.949978000	-1.762175000

TS7x-H: (Imaginary frequency = $385.76i$ cm⁻¹)

6	-1.451340000	1.339950000	-0.743695000
6	-2.548602000	0.917724000	0.149115000
6	-2.705965000	-0.328288000	0.686981000
1	0.089152000	-2.127526000	-1.158153000
1	-3.216560000	1.720518000	0.450942000
6	-1.838113000	-1.445193000	0.400629000
1	-2.138234000	-2.415992000	0.789455000
6	-0.630762000	0.281297000	-1.313464000

1	0.094945000	0.590539000	-2.061699000
6	-0.103194000	-1.034548000	1.698191000
1	0.259264000	-2.048359000	1.571005000
6	0.660279000	0.007993000	1.190011000
6	1.790645000	-0.381054000	0.319153000
8	1.992295000	-1.512253000	-0.109460000
8	2.619089000	0.655875000	0.055390000
6	3.753711000	0.348147000	-0.765406000
1	4.317108000	1.278392000	-0.844753000
1	4.363390000	-0.434254000	-0.305265000
1	3.434811000	0.009847000	-1.755536000
1	-0.727799000	-0.851197000	2.566494000
8	-1.205204000	2.541484000	-0.930501000
1	-3.489640000	-0.476814000	1.428787000
15	-1.116656000	-1.391030000	-1.216928000
6	0.556923000	1.422356000	1.699137000
1	0.473545000	2.157512000	0.892493000
1	-0.313305000	1.531294000	2.352953000
1	1.452228000	1.680343000	2.279849000

TS6n-Me: (Imaginary frequency = $388.75i$ cm^{-1})

6	-0.328822000	-0.972610000	1.801516000
6	-0.425574000	-1.949576000	0.823664000
6	-1.145442000	-1.832498000	-0.442498000
1	0.074458000	-2.901250000	0.970544000
6	-1.740306000	-0.495069000	-0.756737000
1	-2.422380000	-0.541129000	-1.605289000
6	-0.964379000	0.281326000	1.757027000
1	-0.846584000	0.976142000	2.583768000
6	-0.153246000	0.400026000	-1.736518000
1	-0.758462000	1.080500000	-2.331627000
6	0.848903000	0.967496000	-0.948542000
8	-1.176076000	-2.742679000	-1.275328000
1	0.302679000	-1.187289000	2.662437000
6	1.861697000	0.061364000	-0.410267000
8	1.857655000	-1.156580000	-0.542609000
8	2.840252000	0.717910000	0.278533000
6	3.872842000	-0.119168000	0.809337000
1	4.580337000	0.556283000	1.292985000
1	3.464731000	-0.827781000	1.536290000
1	4.365741000	-0.683617000	0.012438000
1	0.046098000	-0.566810000	-2.193843000

15	-2.277438000	0.468694000	0.627013000
6	1.017851000	2.455121000	-0.762845000
1	1.988551000	2.780188000	-1.158922000
1	0.240573000	3.011304000	-1.297046000
1	1.004737000	2.756954000	0.289933000
6	-2.544345000	2.235845000	0.176726000
1	-1.676682000	2.661769000	-0.329890000
1	-3.420452000	2.305480000	-0.474361000
1	-2.751497000	2.806099000	1.087444000

TS6x-Me: (Imaginary frequency = $386.03i \text{ cm}^{-1}$)

6	-1.284230000	-0.227038000	2.057228000
6	-2.001164000	-1.114166000	1.263026000
6	-2.290233000	-0.957458000	-0.158957000
1	-2.397707000	-2.023413000	1.706626000
6	-1.737866000	0.258679000	-0.843059000
1	-2.248299000	0.463055000	-1.783859000
6	-0.796106000	1.021544000	1.639910000
1	-0.249391000	1.652227000	2.334328000
6	-0.055056000	-0.469553000	-1.665493000
1	0.241277000	0.412752000	-2.225470000

6	0.877680000	-0.990493000	-0.765651000
8	-2.858524000	-1.834144000	-0.821608000
1	-1.080704000	-0.529895000	3.083488000
6	2.041191000	-0.157624000	-0.418685000
8	2.248532000	0.984057000	-0.816043000
8	2.926151000	-0.803104000	0.385466000
6	4.093715000	-0.052281000	0.737185000
1	4.655761000	0.232800000	-0.156524000
1	3.821084000	0.855337000	1.283807000
1	4.688309000	-0.714107000	1.368378000
1	-0.669368000	-1.188550000	-2.206811000
15	-1.450553000	1.683406000	0.172628000
6	0.677684000	-2.340063000	-0.164173000
1	0.250854000	-3.040384000	-0.890490000
1	1.599069000	-2.752740000	0.248949000
1	-0.063469000	-2.278417000	0.658379000
6	-0.342478000	2.920368000	-0.624602000
1	-0.184958000	3.747881000	0.073984000
1	0.615338000	2.470680000	-0.896268000
1	-0.847593000	3.315710000	-1.510827000

TS7n-Me: (Imaginary frequency = $432.31i \text{ cm}^{-1}$)

6	-0.137052000	-1.501032000	-0.880807000
6	0.087597000	-2.109623000	0.444591000
6	0.961204000	-1.658762000	1.388186000
1	-0.581344000	-2.931282000	0.683047000
6	1.845742000	-0.524111000	1.206012000
1	2.596296000	-0.370570000	1.980428000
6	0.801196000	-0.451771000	-1.281483000
1	0.680432000	-0.080533000	-2.296935000
6	0.516096000	1.134014000	1.550247000
1	1.303015000	1.868796000	1.701595000
6	-0.379177000	1.317610000	0.497187000
6	-1.670320000	0.587043000	0.596059000
8	-1.971744000	-0.178073000	1.498127000
8	-2.488607000	0.870040000	-0.439307000
6	-3.696584000	0.091762000	-0.500150000
1	-4.276176000	0.206162000	0.419473000
1	-4.249178000	0.483154000	-1.355153000
1	-3.442471000	-0.958570000	-0.655775000
1	0.139344000	0.655650000	2.447138000
8	-1.110484000	-1.821993000	-1.577895000

1	0.946031000	-2.127774000	2.370376000
15	2.347063000	-0.332939000	-0.481750000
6	-0.296759000	2.483095000	-0.464955000
1	-1.015661000	3.258755000	-0.165010000
1	0.695182000	2.942119000	-0.458986000
1	-0.550240000	2.204567000	-1.489263000
6	3.153856000	1.301242000	-0.768463000
1	4.169579000	1.268494000	-0.363506000
1	3.223939000	1.471258000	-1.847200000
1	2.607189000	2.127264000	-0.309923000

TS7x-Me: (Imaginary frequency = $434.85i$ cm⁻¹)

6	1.102034000	-1.377581000	-1.134667000
6	2.140133000	-1.610051000	-0.107548000
6	2.535149000	-0.708719000	0.830587000
1	2.537460000	-2.621464000	-0.089629000
6	2.003930000	0.645052000	0.930128000
1	2.522845000	1.308700000	1.621036000
6	0.676289000	0.003753000	-1.345384000
1	0.014892000	0.174723000	-2.191133000
6	0.174852000	0.374046000	1.905152000

1	-0.055264000	1.428874000	2.020074000
6	-0.720444000	-0.406317000	1.169443000
6	-1.809084000	0.289265000	0.448468000
8	-1.954073000	1.501559000	0.346606000
8	-2.708371000	-0.585013000	-0.064785000
6	-3.810228000	0.003366000	-0.765815000
1	-4.428442000	-0.833431000	-1.092775000
1	-4.377561000	0.668866000	-0.109180000
1	-3.457803000	0.576746000	-1.628188000
1	0.658044000	-0.086676000	2.762542000
8	0.584550000	-2.326370000	-1.741644000
1	3.236369000	-1.028173000	1.600190000
15	1.589790000	1.305791000	-0.656241000
6	-0.800819000	-1.902464000	1.324971000
1	-0.786066000	-2.423448000	0.360769000
1	0.028579000	-2.273501000	1.933355000
1	-1.740229000	-2.183445000	1.819789000
6	0.684632000	2.906132000	-0.558248000
1	-0.256053000	2.795852000	-0.015472000
1	1.338868000	3.638204000	-0.074939000
1	0.481992000	3.251020000	-1.576767000

CA6n-H:

6	0.283899000	-0.710902000	-1.494114000
6	1.090310000	-1.604246000	-0.890065000
6	1.980656000	-1.239950000	0.240856000
1	1.692439000	2.545995000	-0.153337000
1	1.149352000	-2.635963000	-1.225350000
6	1.923228000	0.215879000	0.711819000
1	2.782150000	0.383062000	1.365966000
6	0.153550000	0.729667000	-1.043501000
1	-0.399127000	1.308055000	-1.786248000
6	0.581458000	0.524347000	1.427077000
1	0.727732000	1.400316000	2.067482000
6	-0.526516000	0.829023000	0.372674000
8	2.718709000	-2.059125000	0.764681000
1	-0.326181000	-1.025750000	-2.337767000
6	-1.686002000	-0.171815000	0.497307000
8	-1.905439000	-0.892032000	1.445542000
8	-2.496005000	-0.113854000	-0.586846000
6	-3.645649000	-0.977583000	-0.543720000
1	-3.335964000	-2.022932000	-0.466088000

1	-4.278569000	-0.730231000	0.312337000
1	-4.178101000	-0.802000000	-1.478912000
1	0.275541000	-0.299540000	2.078315000
15	1.945432000	1.313773000	-0.834101000
6	-1.144659000	2.230614000	0.588694000
1	-1.934314000	2.429627000	-0.142056000
1	-1.577371000	2.305688000	1.592540000
1	-0.378831000	3.006976000	0.495446000

CA6x-H:

6	1.289692000	1.214441000	1.278702000
6	2.480630000	1.025858000	0.679164000
6	2.725752000	-0.085421000	-0.275630000
1	-0.424281000	-2.072996000	0.514696000
1	3.330731000	1.669854000	0.887444000
6	1.521009000	-0.971737000	-0.593180000
1	1.881491000	-1.840550000	-1.148335000
6	0.075545000	0.344381000	1.037462000
1	-0.678856000	0.530396000	1.802222000
6	0.450109000	-0.168208000	-1.385568000
1	-0.118734000	-0.846308000	-2.025473000

6	-0.523185000	0.546126000	-0.400626000
8	3.820779000	-0.262040000	-0.785710000
1	1.178560000	2.036597000	1.983980000
6	-1.920340000	-0.098464000	-0.481648000
8	-2.323055000	-0.802805000	-1.382038000
8	-2.696840000	0.269299000	0.562608000
6	-4.045869000	-0.230376000	0.536698000
1	-4.518560000	0.160021000	1.438246000
1	-4.566935000	0.123070000	-0.356652000
1	-4.049368000	-1.323299000	0.541497000
1	0.935114000	0.561885000	-2.043942000
15	0.729758000	-1.436380000	1.068103000
6	-0.722262000	2.037959000	-0.761919000
1	-1.159817000	2.132431000	-1.762135000
1	-1.389055000	2.533246000	-0.049162000
1	0.239783000	2.558376000	-0.763542000

CA7n-H:

6	-0.287741000	1.483859000	-0.561329000
6	-0.956041000	1.877174000	0.701787000
6	-1.774974000	1.047432000	1.374534000

1	-2.341190000	-1.665936000	-1.210401000
1	-0.756712000	2.887318000	1.047727000
6	-2.073750000	-0.366456000	0.931739000
1	-2.942703000	-0.756073000	1.468598000
6	-0.496816000	0.032819000	-1.025296000
1	-0.091069000	-0.048321000	-2.035272000
6	-0.840295000	-1.290521000	1.106308000
1	-1.173148000	-2.333113000	1.061683000
6	0.172490000	-1.011585000	-0.045266000
6	1.487983000	-0.434950000	0.509793000
8	1.733823000	-0.212542000	1.676291000
8	2.358955000	-0.190507000	-0.489443000
6	3.591408000	0.441936000	-0.103748000
1	4.168130000	0.538788000	-1.023573000
1	3.389597000	1.426094000	0.326046000
1	4.125282000	-0.170464000	0.627244000
1	-0.361347000	-1.135855000	2.076784000
8	0.403263000	2.267525000	-1.193968000
1	-2.244984000	1.394829000	2.293219000
15	-2.368928000	-0.262939000	-0.937180000
6	0.512831000	-2.311079000	-0.810418000

1	1.239822000	-2.123476000	-1.604078000
1	0.934006000	-3.057303000	-0.126694000
1	-0.390663000	-2.739985000	-1.255241000

CA7x-H:

6	-1.622276000	1.319224000	-0.324464000
6	-2.762396000	0.586463000	0.275941000
6	-2.720670000	-0.738330000	0.512697000
1	0.325728000	-1.743711000	-1.497800000
1	-3.644238000	1.181035000	0.497907000
6	-1.505715000	-1.591075000	0.226051000
1	-1.763140000	-2.651629000	0.284446000
6	-0.363281000	0.504357000	-0.648625000
1	0.272299000	1.131311000	-1.274094000
6	-0.330229000	-1.240248000	1.177330000
1	0.381443000	-2.068122000	1.208649000
6	0.389705000	0.041124000	0.653487000
6	1.848873000	-0.300249000	0.289736000
8	2.422430000	-1.336597000	0.550482000
8	2.454712000	0.732330000	-0.334636000
6	3.837852000	0.528853000	-0.672228000

1	4.154311000	1.447090000	-1.167301000
1	4.429674000	0.352785000	0.229728000
1	3.946186000	-0.328272000	-1.341710000
1	-0.697619000	-1.085362000	2.198062000
8	-1.677996000	2.518863000	-0.548490000
1	-3.592800000	-1.230567000	0.940891000
15	-0.941902000	-1.082827000	-1.512245000
6	0.450502000	1.159669000	1.723390000
1	1.045096000	0.832149000	2.583995000
1	0.898394000	2.070550000	1.317901000
1	-0.554165000	1.399646000	2.084269000

CA6n-Me:

6	0.094905000	0.811976000	-1.529242000
6	-0.369406000	1.927569000	-0.934126000
6	-1.288295000	1.888361000	0.231501000
1	-0.123631000	2.917213000	-1.308985000
6	-1.695273000	0.498442000	0.730882000
1	-2.555460000	0.629630000	1.392750000
6	-0.197288000	-0.583272000	-1.013454000
1	0.143457000	-1.330055000	-1.733798000

6	-0.518183000	-0.209890000	1.450243000
1	-0.919340000	-1.014503000	2.074843000
6	0.466662000	-0.802681000	0.398851000
8	-1.710967000	2.910207000	0.749167000
1	0.726170000	0.898238000	-2.410643000
6	1.827691000	-0.088079000	0.484420000
8	2.209103000	0.611646000	1.396090000
8	2.602623000	-0.387396000	-0.585679000
6	3.914627000	0.201751000	-0.578771000
1	3.843538000	1.292454000	-0.566688000
1	4.477983000	-0.126890000	0.298318000
1	4.394668000	-0.142759000	-1.495237000
1	0.006392000	0.476693000	2.120630000
15	-2.089322000	-0.540424000	-0.807540000
6	0.768598000	-2.299317000	0.654096000
1	1.504357000	-2.675334000	-0.062883000
1	1.172957000	-2.438822000	1.663268000
1	-0.135137000	-2.905889000	0.566990000
6	-2.620968000	-2.177124000	-0.070203000
1	-3.714298000	-2.149830000	-0.000826000
1	-2.363829000	-2.985498000	-0.764396000

1	-2.222490000	-2.420351000	0.917949000
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CA6x-Me:

6	-1.343015000	0.997751000	-1.535065000
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6	-2.527074000	0.972161000	-0.893644000
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6	-2.765131000	0.131458000	0.306932000
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1	-3.378388000	1.547361000	-1.247639000
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6	-1.566311000	-0.679487000	0.802407000
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1	-1.933728000	-1.393991000	1.543527000
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6	-0.125452000	0.215446000	-1.090296000
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1	0.628597000	0.217346000	-1.877744000
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6	-0.475795000	0.261320000	1.390560000
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1	0.117471000	-0.270622000	2.137490000
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6	0.458758000	0.779162000	0.253950000
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8	-3.852847000	0.098153000	0.861303000
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1	-1.241767000	1.610517000	-2.429552000
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6	1.903778000	0.307576000	0.489882000
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8	2.378626000	0.030009000	1.571385000
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8	2.635385000	0.319283000	-0.646561000
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6	4.026594000	-0.013173000	-0.489346000
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1	4.453909000	0.041202000	-1.490888000
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1	4.516653000	0.699265000	0.178998000
1	4.134732000	-1.019545000	-0.077244000
1	-0.946542000	1.100834000	1.915382000
15	-0.827224000	-1.516714000	-0.731871000
6	0.564911000	2.327435000	0.256672000
1	1.001323000	2.673478000	1.200052000
1	1.197348000	2.681882000	-0.564203000
1	-0.425737000	2.777482000	0.153359000
6	0.583876000	-2.507286000	-0.008168000
1	1.318110000	-2.699270000	-0.798994000
1	1.095143000	-2.071216000	0.852744000
1	0.171088000	-3.477735000	0.290467000

CA7n-Me:

6	0.169948000	1.489578000	-0.744799000
6	-0.085547000	2.136346000	0.567587000
6	-0.934757000	1.618703000	1.475443000
1	0.424752000	3.079892000	0.739224000
6	-1.683842000	0.320330000	1.274799000
1	-2.513323000	0.248043000	1.984391000
6	-0.423963000	0.081790000	-0.920067000

1	-0.238914000	-0.225654000	-1.951341000
6	-0.732497000	-0.897203000	1.391102000
1	-1.326389000	-1.813898000	1.470355000
6	0.166063000	-0.950059000	0.122342000
6	1.622805000	-0.599793000	0.488414000
8	2.063838000	-0.454117000	1.608548000
8	2.381428000	-0.503915000	-0.622183000
6	3.756132000	-0.138920000	-0.414396000
1	4.199408000	-0.100077000	-1.409323000
1	3.819553000	0.838245000	0.070628000
1	4.260939000	-0.882780000	0.207555000
1	-0.112987000	-0.834442000	2.289773000
8	0.803618000	2.048176000	-1.625521000
1	-1.104161000	2.154720000	2.407992000
15	-2.265651000	0.363617000	-0.530965000
6	0.213782000	-2.371328000	-0.491398000
1	0.888976000	-2.400796000	-1.350343000
1	0.571794000	-3.094804000	0.250663000
1	-0.777030000	-2.690590000	-0.822064000
6	-3.100011000	-1.291330000	-0.785735000
1	-4.168572000	-1.150712000	-0.588520000

1	-3.000215000	-1.578716000	-1.838696000
1	-2.738809000	-2.112526000	-0.162321000

CA7x-Me:

6	-1.648870000	1.251968000	-0.737937000
6	-2.766983000	0.835211000	0.143756000
6	-2.731902000	-0.303949000	0.861097000
1	-3.630109000	1.495084000	0.159044000
6	-1.549891000	-1.246422000	0.860966000
1	-1.829371000	-2.204483000	1.308411000
6	-0.402364000	0.355095000	-0.739288000
1	0.233703000	0.691981000	-1.558139000
6	-0.331338000	-0.620091000	1.588942000
1	0.386613000	-1.396001000	1.863373000
6	0.348178000	0.418467000	0.644099000
6	1.840065000	0.081920000	0.473957000
8	2.484115000	-0.647291000	1.200470000
8	2.393792000	0.761787000	-0.551681000
6	3.809152000	0.576538000	-0.728660000
1	4.077889000	1.194355000	-1.585655000
1	4.351439000	0.897176000	0.164432000

1	4.035993000	-0.474706000	-0.923961000
1	-0.648004000	-0.142784000	2.523322000
8	-1.715514000	2.259924000	-1.424768000
1	-3.591554000	-0.572705000	1.473623000
15	-1.071390000	-1.408748000	-0.969869000
6	0.336379000	1.848607000	1.250978000
1	0.941061000	1.876101000	2.164784000
1	0.738045000	2.580032000	0.544436000
1	-0.682228000	2.145444000	1.515654000
6	0.453264000	-2.488841000	-0.944942000
1	0.993833000	-2.339659000	-1.886976000
1	1.144232000	-2.333446000	-0.114055000
1	0.116016000	-3.531552000	-0.930233000

THF Solvent:

1a:

6	-0.373089000	-1.210098000	-0.000002000
6	-1.337564000	-0.111411000	-0.000008000
6	-0.796111000	1.247194000	-0.000001000
6	0.529219000	1.632850000	0.000000000
6	1.654693000	0.770230000	-0.000001000

1	2.252393000	-1.867034000	0.000004000
1	-0.733197000	-2.232488000	0.000000000
1	-1.553805000	2.026431000	0.000001000
1	0.741590000	2.700195000	0.000002000
1	2.673854000	1.133328000	0.000001000
8	-2.566998000	-0.333098000	0.000006000
15	1.272818000	-0.871215000	0.000000000

1b:

6	-0.224315000	-1.132363000	-0.009324000
6	-1.572658000	-0.570042000	0.002476000
6	-1.684059000	0.886883000	0.010712000
6	-0.657153000	1.807703000	0.008727000
6	0.731104000	1.517067000	0.000749000
1	-0.107163000	-2.210657000	-0.019961000
1	-2.706013000	1.257042000	0.018701000
1	-0.928586000	2.861959000	0.014031000
1	1.486822000	2.292162000	-0.004693000
8	-2.582318000	-1.309055000	0.010385000
15	1.121174000	-0.123757000	-0.035323000
6	2.834563000	-0.730213000	0.037528000

1	3.494272000	0.039024000	-0.371008000
1	3.117815000	-0.947882000	1.070172000
1	2.918889000	-1.637068000	-0.565696000

MMA:

6	1.360513000	1.580935000	-0.000250000
1	0.544568000	2.294827000	-0.000373000
1	2.370656000	1.981518000	-0.000312000
6	1.144229000	0.258846000	-0.000037000
6	-0.241569000	-0.300293000	0.000043000
8	-0.482609000	-1.496012000	0.000186000
8	-1.206367000	0.642530000	-0.000062000
6	-2.558519000	0.152494000	-0.000030000
1	-2.747763000	-0.451123000	0.891278000
1	-3.190196000	1.040634000	-0.000490000
1	-2.747537000	-0.451909000	-0.890847000
6	2.245941000	-0.768650000	0.000140000
1	2.175900000	-1.420095000	0.878793000
1	2.175880000	-1.420423000	-0.878267000
1	3.226726000	-0.285557000	0.000040000

TS6n-H: (Imaginary frequency = $967.41i$ cm⁻¹)

6	-0.575583000	-0.645000000	1.779989000
6	-1.091930000	-1.564359000	0.875007000
6	-1.826793000	-1.257958000	-0.343317000
1	-1.708356000	2.582880000	0.223702000
1	-0.908219000	-2.621480000	1.043271000
6	-2.024838000	0.177266000	-0.654591000
1	-2.720858000	0.354963000	-1.472410000
6	-0.772506000	0.741094000	1.714444000
1	-0.347413000	1.387771000	2.475690000
6	-0.226503000	0.574156000	-1.745613000
1	-0.695997000	1.375299000	-2.309324000
6	0.861438000	0.891103000	-0.945226000
8	-2.180451000	-2.142898000	-1.144551000
1	0.047197000	-1.032005000	2.584623000
6	1.686727000	-0.226916000	-0.468383000
8	1.434557000	-1.411898000	-0.656816000
8	2.787591000	0.186395000	0.210401000
6	3.644798000	-0.858163000	0.695271000
1	4.484230000	-0.351390000	1.172033000
1	3.117418000	-1.484612000	1.420140000

1	3.995269000	-1.484985000	-0.128913000
1	-0.286616000	-0.416951000	-2.184350000
15	-2.087092000	1.312569000	0.706472000
6	1.287766000	2.314840000	-0.698825000
1	2.099679000	2.599395000	-1.383705000
1	0.458662000	3.006688000	-0.878810000
1	1.662358000	2.466727000	0.316160000

TS6x-H: (Imaginary frequency = $357.53i$ cm⁻¹)

6	1.248050000	-0.249949000	1.921439000
6	2.282734000	0.411224000	1.272767000
6	2.596931000	0.335408000	-0.146032000
1	-0.270391000	-2.155432000	-0.924644000
1	2.907555000	1.092142000	1.844974000
6	1.727007000	-0.537243000	-0.970016000
1	2.097703000	-0.701122000	-1.980152000
6	0.397603000	-1.197284000	1.327895000
1	-0.366878000	-1.686892000	1.923127000
6	0.175837000	0.843341000	-1.511750000
1	-0.125779000	0.218141000	-2.344932000
6	-0.741847000	1.060349000	-0.495229000

8	3.478399000	1.042110000	-0.671513000
1	1.075869000	-0.001704000	2.967403000
6	-1.934588000	0.196534000	-0.486687000
8	-2.108166000	-0.763669000	-1.234386000
8	-2.856317000	0.574815000	0.429992000
6	-4.047122000	-0.226766000	0.485862000
1	-4.557749000	-0.227162000	-0.480523000
1	-3.805822000	-1.256436000	0.763771000
1	-4.674466000	0.234983000	1.248447000
1	0.919958000	1.606049000	-1.727076000
15	0.906912000	-1.898939000	-0.189879000
6	-0.587449000	2.199960000	0.471893000
1	-0.906998000	3.146340000	0.013410000
1	-1.177107000	2.053945000	1.378188000
1	0.466158000	2.321738000	0.752589000

TS7n-H: (Imaginary frequency = $401.87i \text{ cm}^{-1}$)

6	0.332621000	-1.586018000	-0.591927000
6	0.949737000	-1.824330000	0.721640000
6	1.807188000	-0.979780000	1.374517000
1	2.323071000	1.614881000	-1.351115000

1	0.606562000	-2.721845000	1.229200000
6	2.288812000	0.262106000	0.831363000
1	3.066872000	0.778474000	1.388463000
6	0.821063000	-0.436250000	-1.336312000
1	0.416472000	-0.303909000	-2.336869000
6	0.561389000	1.583788000	1.245871000
1	1.193938000	2.465642000	1.218025000
6	-0.411403000	1.418039000	0.269143000
6	-1.519634000	0.477787000	0.572305000
8	-1.609507000	-0.189577000	1.592676000
8	-2.445513000	0.443840000	-0.409478000
6	-3.510367000	-0.507188000	-0.227188000
1	-4.065316000	-0.294301000	0.690003000
1	-4.155604000	-0.389809000	-1.098160000
1	-3.098561000	-1.517184000	-0.187187000
1	0.401171000	1.136891000	2.219445000
8	-0.607622000	-2.299462000	-0.998101000
1	2.090676000	-1.224200000	2.396438000
15	2.379119000	0.265370000	-0.940160000
6	-0.551131000	2.396862000	-0.872111000
1	-1.196498000	3.234357000	-0.570716000

1	0.419361000	2.826601000	-1.140673000
1	-0.997440000	1.945339000	-1.759032000

TS7x-H: (Imaginary frequency = $399.71i$ cm⁻¹)

6	-1.402914000	1.377793000	-0.713079000
6	-2.492113000	0.965143000	0.187607000
6	-2.679276000	-0.291300000	0.692240000
1	0.024233000	-2.118607000	-1.266162000
1	-3.133531000	1.774269000	0.527715000
6	-1.850225000	-1.424847000	0.359491000
1	-2.178445000	-2.396964000	0.719971000
6	-0.620033000	0.320153000	-1.320890000
1	0.110706000	0.623162000	-2.066830000
6	-0.128790000	-1.140471000	1.643659000
1	0.220402000	-2.149213000	1.454503000
6	0.652339000	-0.077520000	1.204635000
6	1.782174000	-0.413213000	0.312620000
8	2.001918000	-1.525623000	-0.158033000
8	2.588752000	0.647490000	0.081778000
6	3.723282000	0.400263000	-0.764368000
1	4.262660000	1.346218000	-0.812827000

1	4.358615000	-0.381181000	-0.339564000
1	3.399274000	0.095870000	-1.763279000
1	-0.741425000	-1.006676000	2.529428000
8	-1.136123000	2.586390000	-0.881995000
1	-3.452208000	-0.437946000	1.444348000
15	-1.154346000	-1.341279000	-1.269215000
6	0.550797000	1.303713000	1.797037000
1	0.480621000	2.085209000	1.033611000
1	-0.324520000	1.377658000	2.448241000
1	1.440987000	1.523044000	2.401370000

TS6n-Me: (Imaginary frequency = $403.61i$ cm⁻¹)

6	0.296650000	0.913618000	1.817740000
6	0.364538000	1.929126000	0.876021000
6	1.064587000	1.864954000	-0.396578000
1	-0.160582000	2.860161000	1.065371000
6	1.700736000	0.562615000	-0.754838000
1	2.375120000	0.652224000	-1.605882000
6	0.982073000	-0.312371000	1.735348000
1	0.889924000	-1.037277000	2.538883000
6	0.182649000	-0.382538000	-1.712724000

1	0.810852000	-1.052196000	-2.295369000
6	-0.809451000	-0.975650000	-0.923912000
8	1.050589000	2.802988000	-1.212684000
1	-0.340576000	1.076370000	2.685271000
6	-1.868502000	-0.101668000	-0.424984000
8	-1.923697000	1.112142000	-0.606095000
8	-2.817017000	-0.774730000	0.282631000
6	-3.895312000	0.024947000	0.787441000
1	-4.562720000	-0.669877000	1.298406000
1	-3.524411000	0.778846000	1.487520000
1	-4.422158000	0.527223000	-0.028669000
1	-0.061728000	0.559007000	-2.199893000
15	2.296770000	-0.415782000	0.599175000
6	-0.923512000	-2.466097000	-0.720120000
1	-1.876223000	-2.832247000	-1.124610000
1	-0.120280000	-2.997928000	-1.238528000
1	-0.908269000	-2.755761000	0.335709000
6	2.679810000	-2.144653000	0.106055000
1	1.839687000	-2.619270000	-0.403402000
1	3.551460000	-2.133823000	-0.553743000
1	2.933748000	-2.715607000	1.003795000

TS6x-Me: (Imaginary frequency = 391.63i cm⁻¹)

6	-1.208953000	-0.274930000	2.046776000
6	-1.967492000	-1.137037000	1.261435000
6	-2.305483000	-0.942032000	-0.139894000
1	-2.355700000	-2.049761000	1.705418000
6	-1.746715000	0.268346000	-0.820128000
1	-2.269837000	0.496630000	-1.748319000
6	-0.731986000	0.981577000	1.641123000
1	-0.162070000	1.595108000	2.332196000
6	-0.087843000	-0.430720000	-1.660769000
1	0.198306000	0.464155000	-2.205611000
6	0.862028000	-0.971886000	-0.786118000
8	-2.932765000	-1.792011000	-0.797856000
1	-0.966244000	-0.603661000	3.055841000
6	2.033234000	-0.153016000	-0.437408000
8	2.257096000	0.985504000	-0.841874000
8	2.906048000	-0.805562000	0.371456000
6	4.087089000	-0.074587000	0.732329000
1	4.663759000	0.192671000	-0.157166000
1	3.825856000	0.837760000	1.275594000

1	4.662359000	-0.745424000	1.370873000
1	-0.688902000	-1.142779000	-2.225820000
15	-1.432236000	1.678909000	0.211844000
6	0.676995000	-2.344326000	-0.231087000
1	0.282192000	-3.029260000	-0.990244000
1	1.597745000	-2.754786000	0.185074000
1	-0.080195000	-2.325586000	0.578116000
6	-0.368241000	2.940861000	-0.597880000
1	-0.202007000	3.758068000	0.109947000
1	0.585898000	2.508344000	-0.904764000
1	-0.906470000	3.337933000	-1.462887000

TS7n-Me: (Imaginary frequency = $444.90i \text{ cm}^{-1}$)

6	-0.075527000	-1.542175000	-0.868507000
6	0.117350000	-2.105081000	0.477945000
6	0.950556000	-1.605788000	1.433285000
1	-0.533147000	-2.940302000	0.722280000
6	1.810728000	-0.450674000	1.244149000
1	2.537818000	-0.263502000	2.032550000
6	0.857059000	-0.500509000	-1.280910000
1	0.764894000	-0.156747000	-2.308863000

6	0.487683000	1.152337000	1.522428000
1	1.259398000	1.905638000	1.658644000
6	-0.410887000	1.309509000	0.462186000
6	-1.697789000	0.585794000	0.570567000
8	-2.019793000	-0.151702000	1.493061000
8	-2.513402000	0.838177000	-0.478473000
6	-3.749824000	0.105265000	-0.493342000
1	-4.336296000	0.314969000	0.404825000
1	-4.280068000	0.446519000	-1.382849000
1	-3.543785000	-0.965219000	-0.558489000
1	0.105986000	0.713062000	2.437595000
8	-1.021994000	-1.915425000	-1.590558000
1	0.922107000	-2.047631000	2.427283000
15	2.365453000	-0.303913000	-0.432199000
6	-0.313758000	2.443568000	-0.535316000
1	-1.036033000	3.229401000	-0.271833000
1	0.677920000	2.900781000	-0.525887000
1	-0.545569000	2.134161000	-1.556127000
6	3.174915000	1.313139000	-0.771685000
1	4.183907000	1.291475000	-0.351288000
1	3.255184000	1.441214000	-1.855018000

1	2.624373000	2.154164000	-0.346875000
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TS7x-Me: (Imaginary frequency = $440.66i$ cm⁻¹)

6	1.036829000	-1.385746000	-1.148080000
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6	2.060654000	-1.667072000	-0.124832000
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6	2.490977000	-0.787139000	0.819163000
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1	2.420601000	-2.692549000	-0.107848000
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6	2.009589000	0.584644000	0.927629000
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1	2.554274000	1.223509000	1.620908000
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6	0.671382000	0.006299000	-1.358528000
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1	0.016078000	0.214101000	-2.201070000
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6	0.209468000	0.393361000	1.901228000
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1	0.008402000	1.455679000	2.000208000
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6	-0.718204000	-0.377241000	1.191276000
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6	-1.795050000	0.323993000	0.462538000
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8	-1.937344000	1.539123000	0.368753000
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8	-2.689819000	-0.543805000	-0.070363000
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6	-3.785809000	0.048427000	-0.783363000
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1	-4.395206000	-0.786975000	-1.128687000
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1	-4.368121000	0.700556000	-0.127001000
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1	-3.422121000	0.630861000	-1.634401000
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1	0.678480000	-0.062229000	2.769348000
8	0.484078000	-2.317706000	-1.767471000
1	3.176206000	-1.137762000	1.588551000
15	1.626013000	1.272845000	-0.656607000
6	-0.825943000	-1.868319000	1.376715000
1	-0.827646000	-2.407983000	0.422528000
1	0.000535000	-2.242825000	1.986142000
1	-1.765932000	-2.123416000	1.884740000
6	0.778744000	2.901286000	-0.562837000
1	-0.156060000	2.825742000	-0.005520000
1	1.462835000	3.611277000	-0.089657000
1	0.576345000	3.243485000	-1.581931000

CA6n-H:

6	0.280272000	-0.711027000	-1.491656000
6	1.089667000	-1.604044000	-0.887758000
6	1.981414000	-1.236026000	0.235875000
1	1.696087000	2.548036000	-0.160571000
1	1.144322000	-2.635428000	-1.224821000
6	1.926454000	0.216066000	0.707616000
1	2.785809000	0.390523000	1.358972000

6	0.149417000	0.729074000	-1.043828000
1	-0.403633000	1.307238000	-1.785557000
6	0.585524000	0.524491000	1.426249000
1	0.735983000	1.400447000	2.064565000
6	-0.526090000	0.827747000	0.375911000
8	2.725285000	-2.057428000	0.759718000
1	-0.330466000	-1.029816000	-2.332899000
6	-1.685336000	-0.174250000	0.499042000
8	-1.896506000	-0.903163000	1.446928000
8	-2.496392000	-0.111551000	-0.576109000
6	-3.651392000	-0.974233000	-0.547709000
1	-3.343001000	-2.020567000	-0.486884000
1	-4.285820000	-0.732369000	0.308138000
1	-4.179227000	-0.784116000	-1.481810000
1	0.284559000	-0.299003000	2.079956000
15	1.938568000	1.315141000	-0.836706000
6	-1.143160000	2.229885000	0.593777000
1	-1.929904000	2.431517000	-0.138863000
1	-1.577371000	2.302992000	1.596885000
1	-0.375578000	3.004473000	0.504076000

CA6x-H:

6	-1.286835000	1.221923000	-1.268929000
6	-2.479896000	1.030361000	-0.671714000
6	-2.725066000	-0.085795000	0.270877000
1	0.417272000	-2.079495000	-0.525936000
1	-3.325395000	1.680886000	-0.878094000
6	-1.523574000	-0.970830000	0.591059000
1	-1.879467000	-1.843945000	1.142125000
6	-0.074092000	0.349358000	-1.034938000
1	0.677458000	0.538443000	-1.800941000
6	-0.451929000	-0.169061000	1.385847000
1	0.110527000	-0.852567000	2.025038000
6	0.524884000	0.544663000	0.404551000
8	-3.827455000	-0.273720000	0.772497000
1	-1.173684000	2.050319000	-1.965484000
6	1.921846000	-0.102168000	0.481545000
8	2.321572000	-0.811470000	1.383608000
8	2.694831000	0.265686000	-0.557320000
6	4.048858000	-0.230575000	-0.545995000
1	4.511751000	0.168741000	-1.447829000
1	4.574460000	0.121368000	0.344645000

1	4.053462000	-1.322873000	-0.562853000
1	-0.934856000	0.560900000	2.045144000
15	-0.729887000	-1.428176000	-1.070426000
6	0.726404000	2.035716000	0.769468000
1	1.167857000	2.126766000	1.768041000
1	1.389255000	2.532592000	0.054703000
1	-0.235522000	2.555994000	0.776931000

CA7n-H:

6	-0.322801000	1.523076000	-0.481610000
6	-0.926561000	1.814199000	0.838012000
6	-1.727420000	0.936252000	1.474121000
1	-2.364185000	-1.586917000	-1.287629000
1	-0.719998000	2.796748000	1.252894000
6	-2.051107000	-0.438592000	0.938677000
1	-2.909562000	-0.860105000	1.466451000
6	-0.511540000	0.099766000	-1.019862000
1	-0.133353000	0.076384000	-2.043163000
6	-0.820326000	-1.376614000	1.017837000
1	-1.157589000	-2.409655000	0.886884000
6	0.178573000	-0.998293000	-0.117010000

6	1.502639000	-0.474715000	0.468071000
8	1.811531000	-0.468602000	1.643354000
8	2.316521000	-0.033215000	-0.508257000
6	3.591142000	0.489764000	-0.085567000
1	4.097984000	0.793400000	-1.000899000
1	3.448083000	1.347518000	0.575685000
1	4.165180000	-0.280273000	0.435128000
1	-0.331981000	-1.311646000	1.993421000
8	0.286518000	2.378354000	-1.112925000
1	-2.165107000	1.215506000	2.430736000
15	-2.381603000	-0.211400000	-0.910750000
6	0.528276000	-2.236959000	-0.977273000
1	1.246797000	-1.984288000	-1.760964000
1	0.960776000	-3.025380000	-0.351190000
1	-0.374809000	-2.639879000	-1.445852000

CA7x-H:

6	-1.613627000	1.325417000	-0.314217000
6	-2.752222000	0.601728000	0.290171000
6	-2.719872000	-0.726678000	0.516170000
1	0.305786000	-1.736924000	-1.528795000

1	-3.628673000	1.198262000	0.527462000
6	-1.517693000	-1.589421000	0.211868000
1	-1.786174000	-2.646888000	0.259636000
6	-0.360918000	0.507905000	-0.644020000
1	0.280135000	1.131372000	-1.267115000
6	-0.333606000	-1.260570000	1.160176000
1	0.369653000	-2.095626000	1.170791000
6	0.390665000	0.025174000	0.653578000
6	1.850600000	-0.308247000	0.283365000
8	2.423325000	-1.352055000	0.527212000
8	2.454766000	0.732124000	-0.319374000
6	3.841927000	0.545445000	-0.665368000
1	4.150062000	1.476209000	-1.140474000
1	4.435291000	0.357025000	0.232411000
1	3.951751000	-0.293826000	-1.355999000
1	-0.692230000	-1.122530000	2.185860000
8	-1.665082000	2.528602000	-0.544593000
1	-3.591451000	-1.213404000	0.950151000
15	-0.954488000	-1.066776000	-1.519115000
6	0.452010000	1.127377000	1.740537000
1	1.046199000	0.786015000	2.595472000

1	0.901858000	2.044398000	1.351031000
1	-0.552549000	1.359410000	2.106778000

CA6n-Me:

6	0.098521000	0.806342000	-1.528374000
6	-0.365955000	1.924646000	-0.934689000
6	-1.287057000	1.885600000	0.224451000
1	-0.114942000	2.911593000	-1.313447000
6	-1.696261000	0.502421000	0.728742000
1	-2.558470000	0.629630000	1.388451000
6	-0.194704000	-0.586473000	-1.011591000
1	0.144383000	-1.335900000	-1.728959000
6	-0.521096000	-0.207160000	1.451346000
1	-0.927820000	-1.010079000	2.073231000
6	0.466659000	-0.800991000	0.404348000
8	-1.714616000	2.913829000	0.738132000
1	0.730691000	0.893535000	-2.408709000
6	1.827062000	-0.083712000	0.484992000
8	2.200970000	0.633923000	1.390539000
8	2.603122000	-0.393750000	-0.573185000
6	3.920676000	0.191211000	-0.582472000

1	3.852169000	1.281614000	-0.592022000
1	4.485637000	-0.128977000	0.296089000
1	4.393472000	-0.171005000	-1.494908000
1	-0.000212000	0.478782000	2.124946000
15	-2.085245000	-0.545174000	-0.805423000
6	0.767146000	-2.297352000	0.664209000
1	1.500355000	-2.676849000	-0.052971000
1	1.171489000	-2.434176000	1.673478000
1	-0.138271000	-2.901146000	0.579545000
6	-2.625594000	-2.175771000	-0.074798000
1	-3.718916000	-2.145752000	-0.010830000
1	-2.362048000	-2.981993000	-0.768491000
1	-2.231021000	-2.416254000	0.915064000

CA6x-Me:

6	1.345828000	-0.991457000	-1.535437000
6	2.531124000	-0.962888000	-0.893519000
6	2.764678000	-0.122455000	0.303051000
1	3.380918000	-1.538009000	-1.251246000
6	1.563743000	0.671775000	0.809442000
1	1.920374000	1.385657000	1.556181000

6	0.125722000	-0.214604000	-1.091852000
1	-0.624199000	-0.214338000	-1.882480000
6	0.477640000	-0.281611000	1.387670000
1	-0.111032000	0.243677000	2.142428000
6	-0.458801000	-0.788520000	0.247831000
8	3.861680000	-0.070965000	0.848780000
1	1.247022000	-1.605246000	-2.428741000
6	-1.904570000	-0.320110000	0.488390000
8	-2.381301000	-0.082760000	1.581961000
8	-2.626263000	-0.286824000	-0.646380000
6	-4.022499000	0.044699000	-0.498287000
1	-4.432991000	0.026823000	-1.507302000
1	-4.522310000	-0.692455000	0.134199000
1	-4.131514000	1.037356000	-0.055732000
1	0.951142000	-1.126009000	1.901248000
15	0.817237000	1.515848000	-0.717617000
6	-0.565751000	-2.337118000	0.235752000
1	-1.004249000	-2.691620000	1.174707000
1	-1.195854000	-2.682818000	-0.590224000
1	0.424752000	-2.786922000	0.131029000
6	-0.589711000	2.503049000	0.007860000

1	-1.321813000	2.701433000	-0.782744000
1	-1.100936000	2.056225000	0.863119000
1	-0.175212000	3.468348000	0.319514000

CA7n-Me:

6	0.143503000	1.526232000	-0.689037000
6	-0.069641000	2.098057000	0.662372000
6	-0.907199000	1.536509000	1.557777000
1	0.443729000	3.031374000	0.876619000
6	-1.667800000	0.255628000	1.304858000
1	-2.487971000	0.152438000	2.019991000
6	-0.430143000	0.122920000	-0.915217000
1	-0.266211000	-0.143362000	-1.961265000
6	-0.719091000	-0.967568000	1.349075000
1	-1.313961000	-1.885436000	1.381559000
6	0.173427000	-0.950276000	0.075030000
6	1.632894000	-0.627746000	0.450863000
8	2.098992000	-0.639549000	1.573114000
8	2.370138000	-0.379025000	-0.647298000
6	3.764040000	-0.088319000	-0.425554000
1	4.180915000	0.104391000	-1.413467000

1	3.871553000	0.790736000	0.214046000
1	4.260964000	-0.941661000	0.042207000
1	-0.098200000	-0.957708000	2.248534000
8	0.718025000	2.152940000	-1.570804000
1	-1.057480000	2.024966000	2.518913000
15	-2.269526000	0.378278000	-0.489164000
6	0.224927000	-2.341555000	-0.607076000
1	0.891802000	-2.326150000	-1.473283000
1	0.592215000	-3.096535000	0.097298000
1	-0.767649000	-2.648228000	-0.943587000
6	-3.107555000	-1.254233000	-0.824021000
1	-4.174022000	-1.120726000	-0.612686000
1	-3.010872000	-1.487707000	-1.890224000
1	-2.743336000	-2.103375000	-0.241705000

CA7x-Me:

6	1.654004000	-1.241115000	-0.742557000
6	2.767521000	-0.828553000	0.139951000
6	2.729435000	0.310653000	0.859912000
1	3.633709000	-1.484267000	0.158352000
6	1.547367000	1.250682000	0.861961000

1	1.824760000	2.208467000	1.309125000
6	0.402234000	-0.357259000	-0.736501000
1	-0.235983000	-0.690846000	-1.554621000
6	0.332567000	0.618899000	1.591817000
1	-0.383781000	1.395781000	1.866511000
6	-0.345351000	-0.422428000	0.648609000
6	-1.840654000	-0.097075000	0.481717000
8	-2.493370000	0.592761000	1.242135000
8	-2.381760000	-0.736571000	-0.569937000
6	-3.802146000	-0.566415000	-0.753754000
1	-4.051779000	-1.152965000	-1.637225000
1	-4.344885000	-0.935153000	0.119597000
1	-4.040806000	0.487822000	-0.911829000
1	0.653178000	0.144438000	2.525668000
8	1.730130000	-2.240719000	-1.449084000
1	3.587156000	0.578422000	1.474514000
15	1.058928000	1.411702000	-0.963912000
6	-0.327208000	-1.851548000	1.258416000
1	-0.924074000	-1.877210000	2.176785000
1	-0.736674000	-2.585309000	0.558261000
1	0.693600000	-2.146275000	1.516856000

6	-0.467698000	2.481676000	-0.944068000
1	-1.010933000	2.324068000	-1.882730000
1	-1.152130000	2.322902000	-0.108455000
1	-0.135696000	3.525715000	-0.930056000

EtOH Solvent:

1a:

6	-0.371709000	-1.208717000	-0.000001000
6	-1.336102000	-0.112765000	-0.000007000
6	-0.798273000	1.245699000	-0.000001000
6	0.527145000	1.633563000	0.000000000
6	1.652416000	0.772145000	0.000000000
1	2.253354000	-1.866527000	0.000003000
1	-0.728782000	-2.232340000	0.000000000
1	-1.556252000	2.024857000	0.000001000
1	0.738000000	2.701123000	0.000002000
1	2.671355000	1.136028000	0.000001000
8	-2.567994000	-0.335640000	0.000006000
15	1.275028000	-0.870504000	0.000000000

1b:

6	-0.224513000	-1.130705000	-0.008895000
6	-1.571355000	-0.569714000	0.002315000
6	-1.685092000	0.885654000	0.010212000
6	-0.658219000	1.807593000	0.008136000
6	0.729193000	1.517173000	0.000294000
1	-0.104964000	-2.208801000	-0.018843000
1	-2.707035000	1.256357000	0.017840000
1	-0.930077000	2.861708000	0.013242000
1	1.484780000	2.292457000	-0.004930000
8	-2.582882000	-1.310651000	0.009517000
15	1.122883000	-0.123155000	-0.032622000
6	2.834821000	-0.730545000	0.034940000
1	3.493817000	0.043105000	-0.365918000
1	3.116018000	-0.957085000	1.066146000
1	2.918267000	-1.631937000	-0.576365000

MMA:

6	1.360030000	1.581030000	-0.000255000
1	0.544125000	2.294998000	-0.000380000
1	2.370045000	1.981798000	-0.000318000
6	1.144102000	0.258758000	-0.000036000

6	-0.241541000	-0.300417000	0.000043000
8	-0.482208000	-1.496868000	0.000177000
8	-1.206246000	0.641358000	-0.000055000
6	-2.559595000	0.152957000	-0.000029000
1	-2.749543000	-0.449793000	0.891639000
1	-3.189905000	1.041910000	-0.000473000
1	-2.749321000	-0.450546000	-0.891229000
6	2.246845000	-0.767762000	0.000143000
1	2.178137000	-1.418948000	0.879158000
1	2.178111000	-1.419290000	-0.878615000
1	3.226940000	-0.283447000	0.000037000

TS6n-H: (Imaginary frequency = 374.20i cm⁻¹)

6	-0.580889000	-0.629984000	1.790327000
6	-1.081628000	-1.561936000	0.888617000
6	-1.803218000	-1.271586000	-0.339580000
1	-1.739258000	2.574540000	0.202681000
1	-0.890353000	-2.615885000	1.069033000
6	-2.016365000	0.157857000	-0.663527000
1	-2.710135000	0.321613000	-1.486129000
6	-0.793641000	0.752788000	1.712697000

1	-0.379825000	1.410991000	2.470210000
6	-0.230136000	0.570950000	-1.745591000
1	-0.701197000	1.370189000	-2.310652000
6	0.856624000	0.893588000	-0.944197000
8	-2.133760000	-2.167338000	-1.141980000
1	0.039721000	-1.003809000	2.602697000
6	1.686675000	-0.219870000	-0.466634000
8	1.440228000	-1.406929000	-0.656381000
8	2.784049000	0.197322000	0.213454000
6	3.644711000	-0.842410000	0.703834000
1	4.479235000	-0.330595000	1.183505000
1	3.117160000	-1.469549000	1.427818000
1	4.002736000	-1.468051000	-0.118034000
1	-0.280274000	-0.418901000	-2.188611000
15	-2.105179000	1.302836000	0.689361000
6	1.274736000	2.319574000	-0.697672000
1	2.084920000	2.608416000	-1.382900000
1	0.441767000	3.006426000	-0.877892000
1	1.647835000	2.473823000	0.317485000

TS6x-H: (Imaginary frequency = $361.48i$ cm⁻¹)

6	1.236886000	-0.243957000	1.921161000
6	2.275327000	0.414708000	1.274959000
6	2.595028000	0.333848000	-0.141170000
1	-0.265095000	-2.163211000	-0.924985000
1	2.896695000	1.097562000	1.848716000
6	1.727610000	-0.538593000	-0.966585000
1	2.101218000	-0.705403000	-1.975191000
6	0.390539000	-1.194157000	1.327135000
1	-0.377076000	-1.681668000	1.919992000
6	0.181028000	0.835817000	-1.514851000
1	-0.120113000	0.208559000	-2.346655000
6	-0.738538000	1.058298000	-0.500476000
8	3.481448000	1.038230000	-0.665342000
1	1.058763000	0.009026000	2.964851000
6	-1.933452000	0.197302000	-0.490356000
8	-2.111340000	-0.760637000	-1.240378000
8	-2.851189000	0.575609000	0.429486000
6	-4.042340000	-0.225904000	0.492192000
1	-4.559967000	-0.223509000	-0.470435000
1	-3.798952000	-1.255788000	0.767004000
1	-4.664020000	0.234605000	1.260004000

1	0.923493000	1.599241000	-1.733458000
15	0.907639000	-1.901079000	-0.185850000
6	-0.584241000	2.202348000	0.461291000
1	-0.904733000	3.146252000	-0.001709000
1	-1.172641000	2.060253000	1.369005000
1	0.469418000	2.326390000	0.740693000

TS7n-H: (Imaginary frequency = $405.55i$ cm⁻¹)

6	0.345945000	-1.589523000	-0.590498000
6	0.960909000	-1.822440000	0.724172000
6	1.809295000	-0.970043000	1.378550000
1	2.318540000	1.620213000	-1.356106000
1	0.625070000	-2.722673000	1.232212000
6	2.281963000	0.275556000	0.834644000
1	3.054422000	0.798391000	1.393232000
6	0.830970000	-0.441907000	-1.337459000
1	0.429524000	-0.313360000	-2.339787000
6	0.556001000	1.580814000	1.244846000
1	1.183622000	2.466084000	1.217464000
6	-0.416801000	1.412891000	0.267313000
6	-1.524271000	0.472973000	0.568687000

8	-1.617836000	-0.194874000	1.589330000
8	-2.450117000	0.438863000	-0.413787000
6	-3.522305000	-0.502624000	-0.226877000
1	-4.076123000	-0.281047000	0.688887000
1	-4.166920000	-0.385021000	-1.098192000
1	-3.119711000	-1.516293000	-0.181363000
1	0.395235000	1.137004000	2.219815000
8	-0.590950000	-2.310312000	-0.997350000
1	2.092543000	-1.210306000	2.401417000
15	2.381043000	0.274508000	-0.936615000
6	-0.554623000	2.390085000	-0.875463000
1	-1.203963000	3.225662000	-0.577294000
1	0.415550000	2.822828000	-1.139454000
1	-0.994711000	1.936795000	-1.764652000

TS7x-H: (Imaginary frequency = $401.03i$ cm⁻¹)

6	-1.386961000	1.387302000	-0.706451000
6	-2.476329000	0.979056000	0.194765000
6	-2.673363000	-0.278995000	0.691750000
1	0.006567000	-2.117899000	-1.291469000
1	-3.110114000	1.790870000	0.542845000

6	-1.854808000	-1.417522000	0.349423000
1	-2.191514000	-2.388988000	0.703370000
6	-0.615724000	0.328536000	-1.323959000
1	0.116703000	0.628810000	-2.069426000
6	-0.137412000	-1.164797000	1.630813000
1	0.207528000	-2.172090000	1.426720000
6	0.649371000	-0.098426000	1.209321000
6	1.778131000	-0.421969000	0.312093000
8	2.002195000	-1.529746000	-0.167713000
8	2.579258000	0.644485000	0.087025000
6	3.712666000	0.409620000	-0.764951000
1	4.247359000	1.358477000	-0.807563000
1	4.353607000	-0.371370000	-0.347965000
1	3.386682000	0.112044000	-1.765225000
1	-0.748187000	-1.042619000	2.519554000
8	-1.111249000	2.596596000	-0.869392000
1	-3.444698000	-0.423923000	1.445525000
15	-1.163672000	-1.328939000	-1.281182000
6	0.549890000	1.273985000	1.821873000
1	0.489594000	2.067198000	1.069718000
1	-0.329457000	1.342240000	2.468090000

1 1.436610000 1.479906000 2.436128000

TS6n-Me: (Imaginary frequency = 406.00i cm⁻¹)

6 0.293396000 0.901681000 1.820958000

6 0.357875000 1.924958000 0.887070000

6 1.053145000 1.869955000 -0.386832000

1 -0.169801000 2.852833000 1.085703000

6 1.693332000 0.573073000 -0.755042000

1 2.366638000 0.670240000 -1.606038000

6 0.986077000 -0.319742000 1.730573000

1 0.897183000 -1.050941000 2.528628000

6 0.187286000 -0.374442000 -1.708505000

1 0.817812000 -1.042198000 -2.290725000

6 -0.803794000 -0.972921000 -0.920456000

8 1.031949000 2.813548000 -1.199482000

1 -0.344533000 1.054920000 2.689591000

6 -1.871169000 -0.106636000 -0.426992000

8 -1.937323000 1.106789000 -0.613060000

8 -2.815166000 -0.784534000 0.280617000

6 -3.901485000 0.006145000 0.783624000

1 -4.561394000 -0.693690000 1.297202000

1	-3.537593000	0.765314000	1.481598000
1	-4.434502000	0.499600000	-0.033918000
1	-0.064572000	0.562580000	-2.200810000
15	2.299566000	-0.409580000	0.592692000
6	-0.907217000	-2.463949000	-0.715415000
1	-1.855427000	-2.837871000	-1.123550000
1	-0.097943000	-2.989665000	-1.230127000
1	-0.892888000	-2.752494000	0.340667000
6	2.702891000	-2.131228000	0.094050000
1	1.869630000	-2.613882000	-0.419003000
1	3.575721000	-2.107546000	-0.563604000
1	2.960482000	-2.701294000	0.991215000

TS6x-Me: (Imaginary frequency = $392.40i \text{ cm}^{-1}$)

6	-1.195629000	-0.280472000	2.045431000
6	-1.960644000	-1.139521000	1.262660000
6	-2.305963000	-0.939889000	-0.135206000
1	-2.347114000	-2.052533000	1.707722000
6	-1.746552000	0.268729000	-0.816847000
1	-2.272945000	0.500265000	-1.742370000
6	-0.721174000	0.977186000	1.640346000

1	-0.147673000	1.588799000	2.330138000
6	-0.094641000	-0.425777000	-1.660279000
1	0.190202000	0.470406000	-2.203653000
6	0.858721000	-0.970411000	-0.790278000
8	-2.942003000	-1.786880000	-0.791356000
1	-0.946495000	-0.612051000	3.051898000
6	2.030959000	-0.153790000	-0.441755000
8	2.258504000	0.983142000	-0.849982000
8	2.900489000	-0.805562000	0.370846000
6	4.082414000	-0.076355000	0.734454000
1	4.664060000	0.185298000	-0.153441000
1	3.821145000	0.838265000	1.273688000
1	4.652878000	-0.746439000	1.377913000
1	-0.693306000	-1.136929000	-2.229168000
15	-1.428067000	1.678426000	0.216417000
6	0.675921000	-2.346062000	-0.242016000
1	0.284339000	-3.028111000	-1.005604000
1	1.596959000	-2.757049000	0.172955000
1	-0.081985000	-2.333477000	0.566535000
6	-0.372483000	2.946199000	-0.593882000
1	-0.204018000	3.759504000	0.117797000

1	0.580544000	2.517367000	-0.908827000
1	-0.917062000	3.345666000	-1.453657000

TS7n-Me: (Imaginary frequency = $447.18i$ cm⁻¹)

6	-0.064300000	-1.545833000	-0.868795000
6	0.129202000	-2.108472000	0.476767000
6	0.956405000	-1.603203000	1.434049000
1	-0.514624000	-2.949484000	0.719690000
6	1.807675000	-0.440562000	1.246477000
1	2.532061000	-0.248842000	2.036046000
6	0.865707000	-0.504387000	-1.282777000
1	0.775820000	-0.161946000	-2.311376000
6	0.482550000	1.145227000	1.523611000
1	1.249625000	1.902823000	1.661738000
6	-0.417520000	1.303752000	0.463383000
6	-1.703003000	0.579826000	0.567842000
8	-2.028016000	-0.161597000	1.487064000
8	-2.519058000	0.835854000	-0.481102000
6	-3.760966000	0.112479000	-0.493728000
1	-4.343417000	0.323837000	0.406595000
1	-4.292167000	0.459919000	-1.380223000

1	-3.564448000	-0.959787000	-0.562435000
1	0.100862000	0.706813000	2.439317000
8	-1.010452000	-1.923838000	-1.592027000
1	0.930411000	-2.045383000	2.427904000
15	2.368287000	-0.293477000	-0.428128000
6	-0.318391000	2.439330000	-0.532218000
1	-1.044482000	3.222647000	-0.271770000
1	0.671677000	2.899356000	-0.515953000
1	-0.542144000	2.131267000	-1.555325000
6	3.175154000	1.322559000	-0.772510000
1	4.183934000	1.302245000	-0.351882000
1	3.253793000	1.447700000	-1.856187000
1	2.623918000	2.163341000	-0.348291000

TS7x-Me: (Imaginary frequency = $441.13i \text{ cm}^{-1}$)

6	1.014176000	-1.387630000	-1.151984000
6	2.037224000	-1.683176000	-0.133334000
6	2.480426000	-0.810033000	0.811248000
1	2.386013000	-2.712594000	-0.118447000
6	2.013914000	0.566686000	0.924204000
1	2.567533000	1.197977000	1.617152000

6	0.665977000	0.007684000	-1.360804000
1	0.011195000	0.225841000	-2.201200000
6	0.221883000	0.396776000	1.900977000
1	0.029769000	1.461056000	1.996540000
6	-0.715583000	-0.369832000	1.198529000
6	-1.788702000	0.333959000	0.468035000
8	-1.931545000	1.549690000	0.379507000
8	-2.680692000	-0.531711000	-0.074557000
6	-3.775892000	0.064021000	-0.786964000
1	-4.384298000	-0.769611000	-1.138179000
1	-4.360406000	0.711437000	-0.128038000
1	-3.410750000	0.651158000	-1.634102000
1	0.688560000	-0.058428000	2.770559000
8	0.448152000	-2.313492000	-1.772309000
1	3.163298000	-1.169745000	1.578284000
15	1.635156000	1.263051000	-0.658165000
6	-0.832709000	-1.859153000	1.392172000
1	-0.842917000	-2.403554000	0.440751000
1	-0.006060000	-2.236304000	1.999534000
1	-1.771777000	-2.105169000	1.906503000
6	0.803834000	2.899002000	-0.562699000

1	-0.128371000	2.832577000	-0.000104000
1	1.496398000	3.602630000	-0.092791000
1	0.599876000	3.241247000	-1.581382000

CA6n-H:

6	0.278293000	-0.706298000	-1.493999000
6	1.086144000	-1.602084000	-0.891409000
6	1.977190000	-1.237648000	0.233077000
1	1.701330000	2.547727000	-0.157619000
1	1.138499000	-2.632779000	-1.231118000
6	1.926889000	0.213348000	0.706901000
1	2.786896000	0.385913000	1.357878000
6	0.149550000	0.732663000	-1.042943000
1	-0.402650000	1.313631000	-1.782863000
6	0.587285000	0.524508000	1.426932000
1	0.740595000	1.400736000	2.063944000
6	-0.525062000	0.828551000	0.378012000
8	2.718782000	-2.062525000	0.757002000
1	-0.332433000	-1.022589000	-2.336107000
6	-1.682699000	-0.175761000	0.498682000
8	-1.887920000	-0.913510000	1.442007000

8	-2.497576000	-0.106316000	-0.571473000
6	-3.651863000	-0.970905000	-0.547671000
1	-3.341591000	-2.017232000	-0.498337000
1	-4.283925000	-0.736949000	0.312045000
1	-4.182360000	-0.772585000	-1.478334000
1	0.286045000	-0.297967000	2.081771000
15	1.939162000	1.315599000	-0.834991000
6	-1.142794000	2.230011000	0.598382000
1	-1.929951000	2.432210000	-0.133484000
1	-1.576192000	2.301500000	1.601936000
1	-0.375589000	3.004895000	0.509067000

CA6x-H:

6	-1.286066000	1.224077000	-1.266388000
6	-2.479471000	1.031917000	-0.669470000
6	-2.724883000	-0.085660000	0.270073000
1	0.415413000	-2.081115000	-0.529274000
1	-3.323970000	1.684051000	-0.874853000
6	-1.524112000	-0.970699000	0.590576000
1	-1.879467000	-1.844638000	1.140663000
6	-0.073845000	0.350548000	-1.034299000

1	0.677199000	0.540187000	-1.800492000
6	-0.452033000	-0.169927000	1.385991000
1	0.109305000	-0.854987000	2.024428000
6	0.525290000	0.544052000	0.405478000
8	-3.828915000	-0.276402000	0.769192000
1	-1.172320000	2.053981000	-1.960838000
6	1.922188000	-0.103123000	0.481366000
8	2.321523000	-0.813657000	1.383474000
8	2.694464000	0.265225000	-0.556322000
6	4.049156000	-0.230494000	-0.547982000
1	4.509796000	0.169450000	-1.450538000
1	4.576230000	0.122158000	0.341437000
1	4.053848000	-1.322707000	-0.565934000
1	-0.934358000	0.559726000	2.045923000
15	-0.730319000	-1.426184000	-1.071250000
6	0.727406000	2.034848000	0.771505000
1	1.170149000	2.124852000	1.769576000
1	1.389110000	2.532193000	0.056131000
1	-0.234497000	2.555055000	0.780665000

CA7n-H:

6	-0.326109000	1.524515000	-0.477674000
6	-0.925741000	1.810350000	0.844289000
6	-1.725550000	0.929669000	1.478744000
1	-2.365629000	-1.583376000	-1.292465000
1	-0.719431000	2.791428000	1.262888000
6	-2.050239000	-0.442898000	0.938991000
1	-2.907839000	-0.866505000	1.466089000
6	-0.512356000	0.102996000	-1.019456000
1	-0.136118000	0.081647000	-2.043520000
6	-0.819032000	-1.380767000	1.013320000
1	-1.156278000	-2.413028000	0.877727000
6	0.179407000	-0.997086000	-0.120075000
6	1.503468000	-0.474892000	0.465831000
8	1.815572000	-0.477937000	1.640716000
8	2.314790000	-0.023965000	-0.507995000
6	3.593367000	0.490475000	-0.084841000
1	4.098625000	0.799747000	-0.999102000
1	3.456045000	1.343125000	0.584191000
1	4.166012000	-0.286638000	0.426567000
1	-0.331225000	-1.320464000	1.989417000
8	0.277774000	2.384479000	-1.109589000

1	-2.161472000	1.205440000	2.437081000
15	-2.382018000	-0.210465000	-0.909068000
6	0.530120000	-2.232586000	-0.984830000
1	1.247640000	-1.976578000	-1.768360000
1	0.963803000	-3.022403000	-0.361480000
1	-0.372968000	-2.634699000	-1.453860000

CA7x-H:

6	-1.611368000	1.326569000	-0.313902000
6	-2.749798000	0.605926000	0.292401000
6	-2.719735000	-0.722848000	0.518422000
1	0.300573000	-1.738104000	-1.533317000
1	-3.624738000	1.203607000	0.532414000
6	-1.520621000	-1.588442000	0.211272000
1	-1.791718000	-2.645083000	0.258593000
6	-0.360356000	0.507514000	-0.644066000
1	0.281951000	1.129026000	-1.267848000
6	-0.334345000	-1.263247000	1.158126000
1	0.367023000	-2.099862000	1.164998000
6	0.390906000	0.022603000	0.653357000
6	1.850743000	-0.309941000	0.281801000

8	2.422123000	-1.356452000	0.519152000
8	2.456016000	0.732934000	-0.313939000
6	3.843212000	0.547663000	-0.662719000
1	4.151765000	1.481731000	-1.130806000
1	4.436929000	0.352363000	0.233260000
1	3.951088000	-0.285865000	-1.360460000
1	-0.690829000	-1.127455000	2.184717000
8	-1.661352000	2.530262000	-0.546668000
1	-3.591054000	-1.207428000	0.954999000
15	-0.957825000	-1.065602000	-1.519136000
6	0.452262000	1.122972000	1.742246000
1	1.046250000	0.780004000	2.596564000
1	0.902763000	2.040630000	1.354864000
1	-0.552315000	1.353909000	2.109090000

CA6n-Me:

6	0.100501000	0.802291000	-1.529799000
6	-0.361609000	1.922664000	-0.937296000
6	-1.281487000	1.886669000	0.221993000
1	-0.107859000	2.908231000	-1.317968000
6	-1.695605000	0.506220000	0.727673000

1	-2.558044000	0.635505000	1.386670000
6	-0.195469000	-0.588718000	-1.010840000
1	0.141709000	-1.340449000	-1.726457000
6	-0.522978000	-0.206129000	1.451848000
1	-0.933047000	-1.008097000	2.072481000
6	0.464970000	-0.801655000	0.406303000
8	-1.704603000	2.917618000	0.736426000
1	0.732682000	0.887399000	-2.410269000
6	1.825424000	-0.084184000	0.485054000
8	2.197053000	0.640757000	1.386729000
8	2.602578000	-0.400341000	-0.568877000
6	3.920820000	0.184141000	-0.582827000
1	3.852421000	1.274406000	-0.599070000
1	4.486433000	-0.132317000	0.296591000
1	4.392193000	-0.183337000	-1.493707000
1	-0.002052000	0.478491000	2.126739000
15	-2.085530000	-0.543600000	-0.804804000
6	0.764044000	-2.297919000	0.668252000
1	1.495868000	-2.679428000	-0.049125000
1	1.168953000	-2.433497000	1.677423000
1	-0.142345000	-2.900380000	0.585412000

6	-2.631009000	-2.171464000	-0.074790000
1	-3.724164000	-2.137910000	-0.010396000
1	-2.369079000	-2.977833000	-0.768778000
1	-2.236558000	-2.412551000	0.914857000

CA6x-Me:

6	1.346353000	-0.990882000	-1.535063000
6	2.531997000	-0.961270000	-0.893230000
6	2.764672000	-0.120381000	0.302193000
1	3.381454000	-1.536638000	-1.251405000
6	1.563141000	0.670304000	0.810912000
1	1.917794000	1.384155000	1.558611000
6	0.125816000	-0.214864000	-1.091940000
1	-0.623362000	-0.214350000	-1.883117000
6	0.477846000	-0.285216000	1.387433000
1	-0.110142000	0.239352000	2.143171000
6	-0.458747000	-0.790486000	0.246988000
8	3.863651000	-0.064196000	0.845603000
1	1.247710000	-1.605536000	-2.427634000
6	-1.904624000	-0.322589000	0.488087000
8	-2.381966000	-0.092610000	1.583664000

8	-2.624159000	-0.280930000	-0.646256000
6	-4.020990000	0.051211000	-0.500317000
1	-4.428193000	0.039757000	-1.510607000
1	-4.523067000	-0.689798000	0.125726000
1	-4.129752000	1.041618000	-0.052895000
1	0.951752000	-1.130311000	1.899348000
15	0.814974000	1.515341000	-0.714883000
6	-0.565731000	-2.339122000	0.232274000
1	-1.004868000	-2.695129000	1.170338000
1	-1.195156000	-2.683202000	-0.594788000
1	0.424817000	-2.788772000	0.127518000
6	-0.591506000	2.501771000	0.010384000
1	-1.324129000	2.699216000	-0.779832000
1	-1.101611000	2.053601000	0.865574000
1	-0.177433000	3.466932000	0.322816000

CA7n-Me:

6	0.139262000	1.528817000	-0.685156000
6	-0.071116000	2.095867000	0.668008000
6	-0.907813000	1.530942000	1.562678000
1	0.441133000	3.029250000	0.884906000

6	-1.667433000	0.250544000	1.306737000
1	-2.486945000	0.144204000	2.021825000
6	-0.430135000	0.125293000	-0.914708000
1	-0.267909000	-0.139032000	-1.961540000
6	-0.717185000	-0.971667000	1.346656000
1	-1.311099000	-1.890046000	1.376305000
6	0.175275000	-0.949458000	0.072625000
6	1.634586000	-0.627250000	0.448243000
8	2.102842000	-0.648553000	1.569904000
8	2.370502000	-0.368170000	-0.648175000
6	3.766855000	-0.086127000	-0.426658000
1	4.182985000	0.112482000	-1.413669000
1	3.880118000	0.787075000	0.219898000
1	4.260186000	-0.946227000	0.032155000
1	-0.097030000	-0.964094000	2.246589000
8	0.707756000	2.161725000	-1.567778000
1	-1.058087000	2.016743000	2.525094000
15	-2.269975000	0.376014000	-0.486426000
6	0.227945000	-2.338987000	-0.613403000
1	0.894758000	-2.320902000	-1.479617000
1	0.595445000	-3.095440000	0.089120000

1	-0.764489000	-2.644990000	-0.950659000
6	-3.107294000	-1.254413000	-0.826873000
1	-4.173654000	-1.121319000	-0.615071000
1	-3.009387000	-1.485000000	-1.893504000
1	-2.742900000	-2.104300000	-0.245938000

CA7x-Me:

6	1.651499000	-1.242411000	-0.742484000
6	2.764660000	-0.833443000	0.140776000
6	2.728692000	0.306109000	0.860933000
1	3.629249000	-1.491236000	0.161411000
6	1.549762000	1.249585000	0.861524000
1	1.829485000	2.206801000	1.308003000
6	0.401301000	-0.357477000	-0.735990000
1	-0.238221000	-0.688877000	-1.553988000
6	0.332853000	0.621613000	1.591262000
1	-0.381401000	1.401454000	1.862824000
6	-0.346011000	-0.420480000	0.649666000
6	-1.841287000	-0.095384000	0.481594000
8	-2.493870000	0.596515000	1.240887000
8	-2.382143000	-0.737087000	-0.567900000

6	-3.802788000	-0.566993000	-0.754383000
1	-4.051114000	-1.155378000	-1.636873000
1	-4.346570000	-0.934296000	0.118836000
1	-4.040310000	0.486874000	-0.915816000
1	0.651463000	0.149017000	2.526614000
8	1.726822000	-2.241051000	-1.452108000
1	3.585997000	0.570950000	1.477154000
15	1.061136000	1.410297000	-0.963755000
6	-0.328223000	-1.848725000	1.261704000
1	-0.924891000	-1.872803000	2.180155000
1	-0.738643000	-2.583567000	0.563157000
1	0.692468000	-2.143101000	1.520925000
6	-0.462293000	2.483353000	-0.946919000
1	-1.004875000	2.326588000	-1.885999000
1	-1.147373000	2.325125000	-0.111791000
1	-0.127766000	3.526489000	-0.931411000