

Electronic Supplementary Information of

In Search of Stable Singlet Metalla-*N*-Heterocyclic Carbenes (MNHCs): A

Contribution From Theory

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Table S1 Calculated Mullikens Spin Density Values at different position of the carbene framework in the triplet states of all MNHCs and their parent carbenes. (**TM** = Transition Metal)

Molecule	Cc	C₂	TM	N₁	N₂
I	1.789			0.033	0.033
I'	1.620			-0.021	-0.021
II'	1.730			-0.050	-0.051
III	1.669			-0.005	-0.007
IV	1.783			-0.049	-0.092
1a	1.067	0.977	0.054	0.070	-0.170
1b	1.013	0.930	0.045	0.073	-0.173
1c	1.050	0.833	0.094	0.062	-0.167
1'a	1.105	0.969	-0.030	0.058	-0.191
1'b	1.065	0.866	-0.029	0.079	-0.201
1'c	1.144	0.862	-0.047	0.053	-0.194
2a	1.045	0.994	0.094	0.092	-0.178
2b	1.011	1.011	0.157	0.099	-0.193
2c	1.029	0.851	0.120	0.093	-0.166
2'a	1.121	0.949	-0.000	0.083	-0.188
2'b	1.091	0.834	-0.018	0.098	-0.202
2'c	1.150	0.788	0.008	0.093	-0.210
3a	1.035	1.019	0.229	0.109	-0.205
3b	0.943	0.949	0.284	0.107	-0.187
3c	1.001	0.918	0.243	0.102	-0.179
3'a	1.101	0.896	0.157	0.111	-0.211
3'b	1.095	0.843	0.100	0.109	-0.226
3'c	1.101	0.896	0.156	0.111	-0.210
4'a	1.463	-0.020	0.098	-0.028	-0.102
4'b	1.465	0.004	-0.040	-0.009	-0.097
5a	1.549		0.046	-0.019	-0.019
5b	1.527		-0.034	-0.019	-0.019
6a	1.779		-0.009	-0.0553	-0.011
6b	1.820		-0.019	-0.056	-0.012

N₁= Amino group attached with TM center and C₂ = Carbon atom of the carbene backbone for the five membered MNHCs (**1a-4'b**).

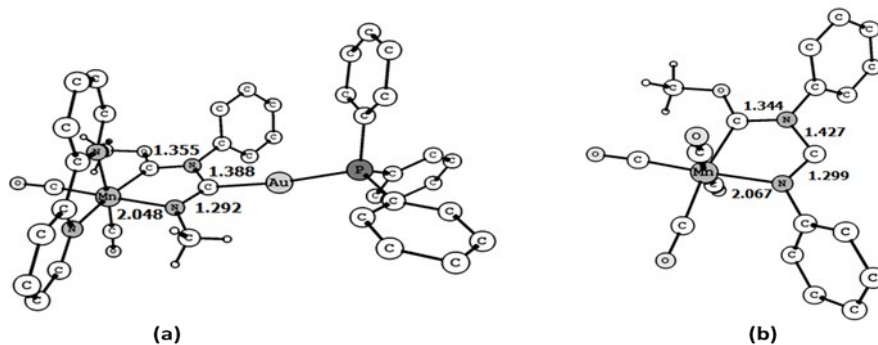


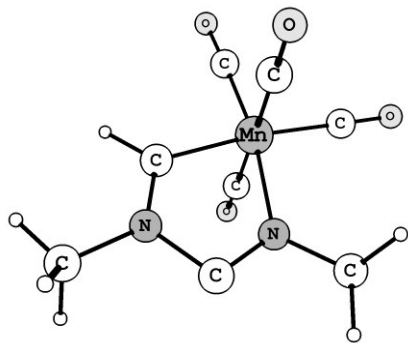
Fig. S1 Figure showing the structure along with key geometrical parameters for the experimentally trapped (a)⁴² and computationally designed MNHC (b = 1'c). (Hydrogen atoms of the phenyl and bipy groups are omitted for the sake of clarity).

Table S2 PBE1PBE/6-311++G** Calculated ΔE_{S-T} (in kcal mol⁻¹) values for some experimentally known carbenes.

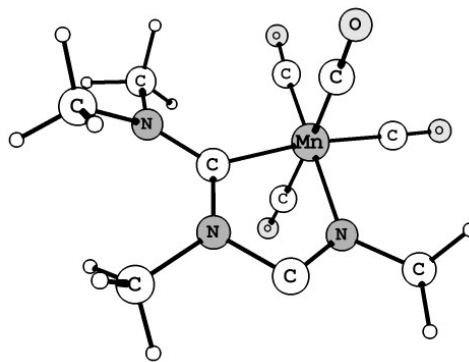
Sl. No.	Molecule	ΔE_{S-T}
1	CAAC	38.5
2	BICAAC	38.1
3	6-membered CAAC	30.8
4	DAC	40.4
5	5-membered DAC	34.0
6	aNHC	48.3

Table S3 Comparison of ΔE_{S-T} values for some representative MNHCs with different functionals.

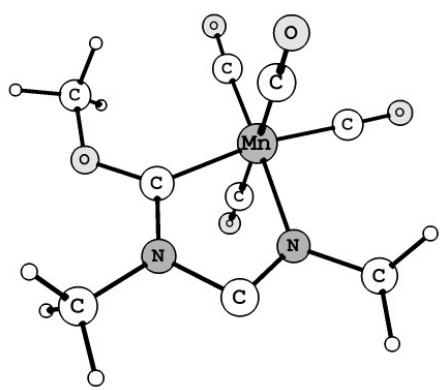
Molecules	ΔE_{S-T} (kcal mol ⁻¹)			
	PBE1PBE	M06	WB97XD	TPSSH
1c	43.3	46.1	46.7	43.4
2c	45.8	48.5	49.3	45.7
3c	48.0	50.1	51.4	47.9
6a	36.0	38.2	41.0	35.1



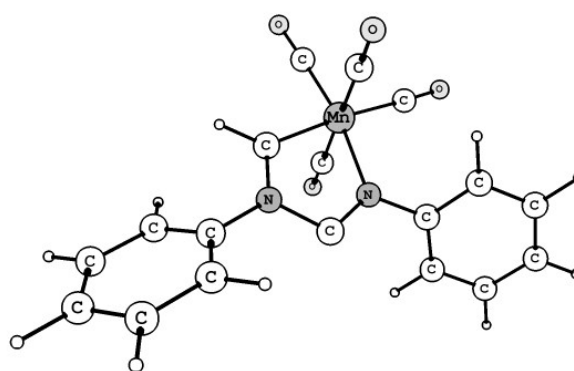
1a



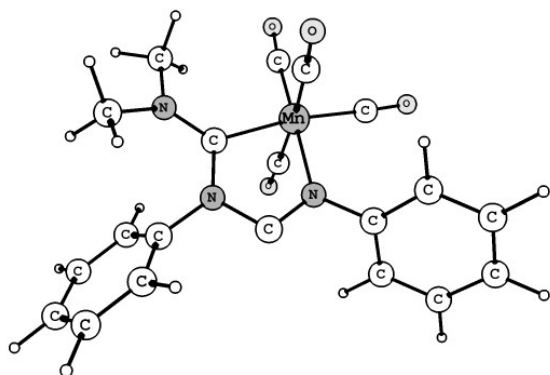
1b



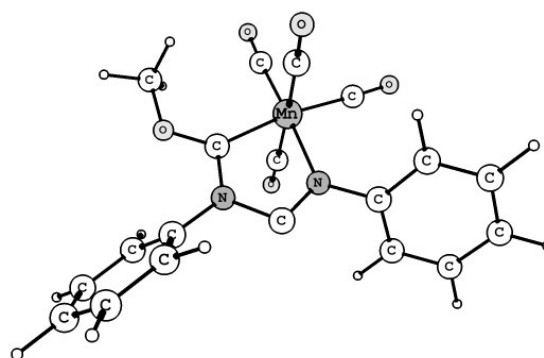
1c



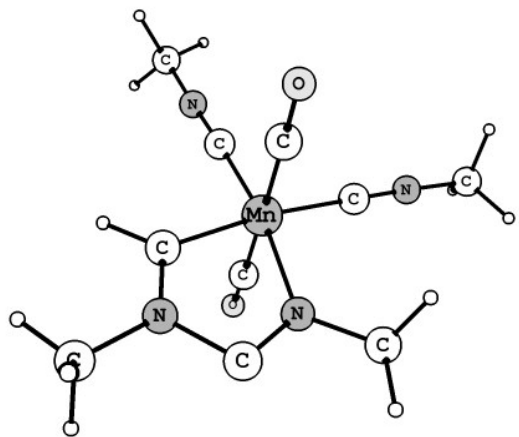
1'a



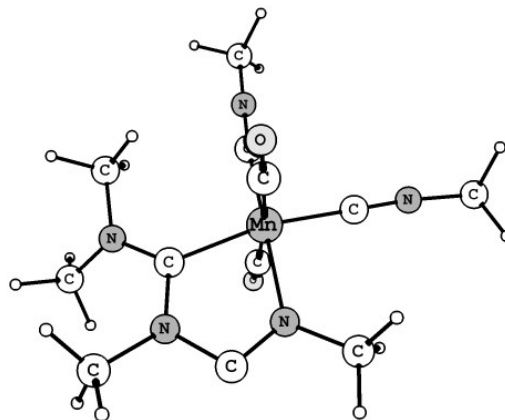
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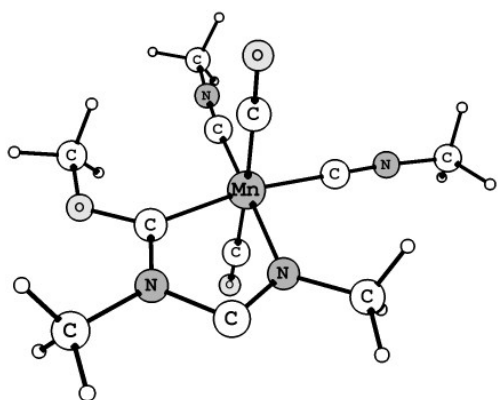
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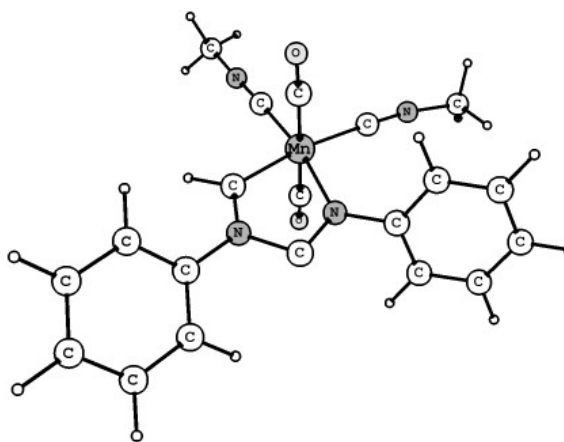
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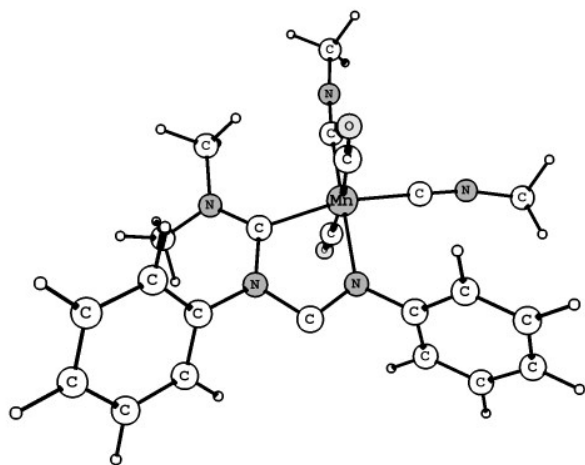
2b



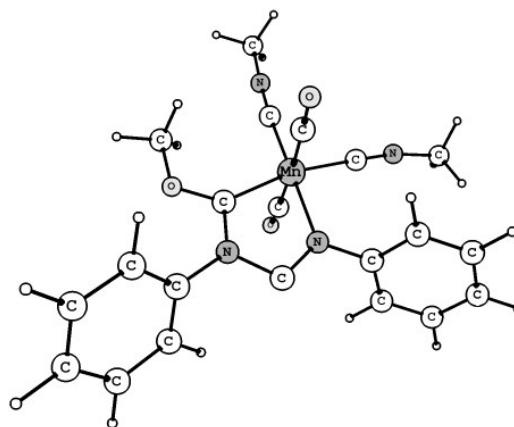
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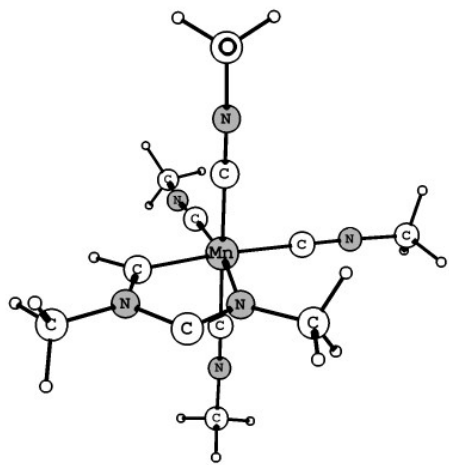
2'a



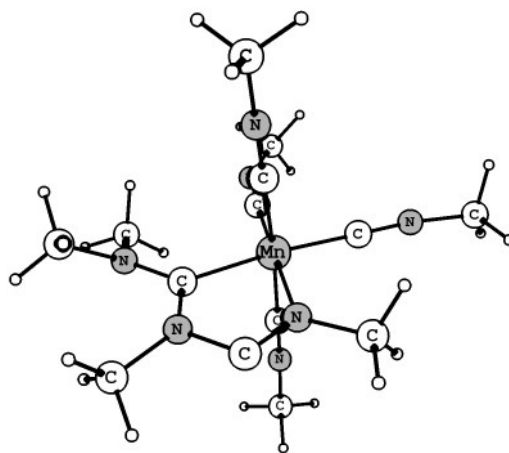
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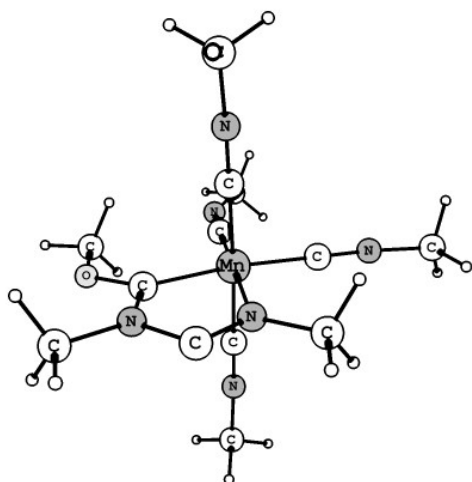
2'c



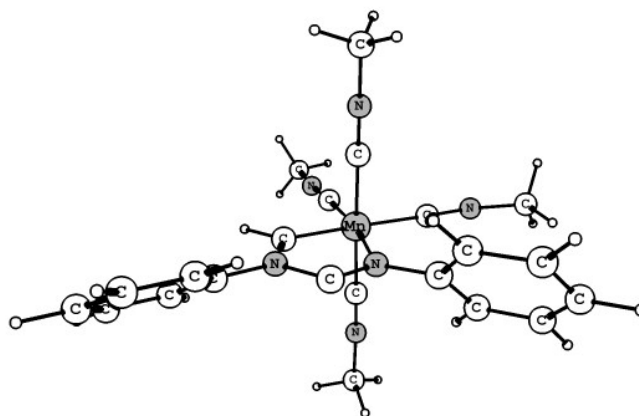
3a



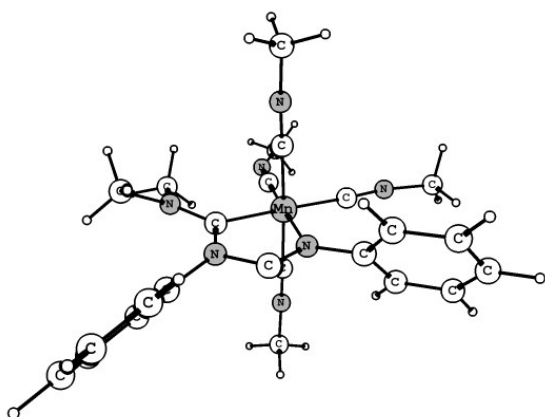
3b



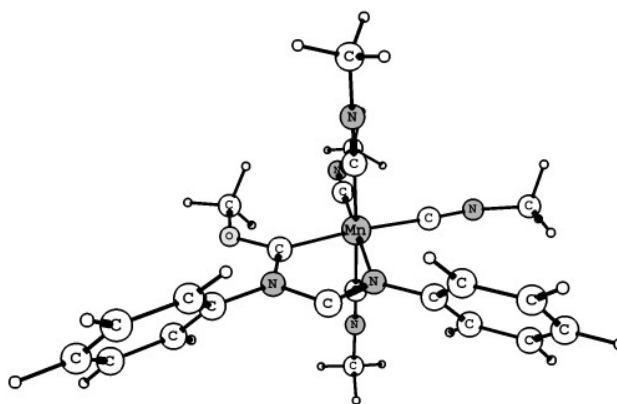
3c



3'a



3'b



3'c

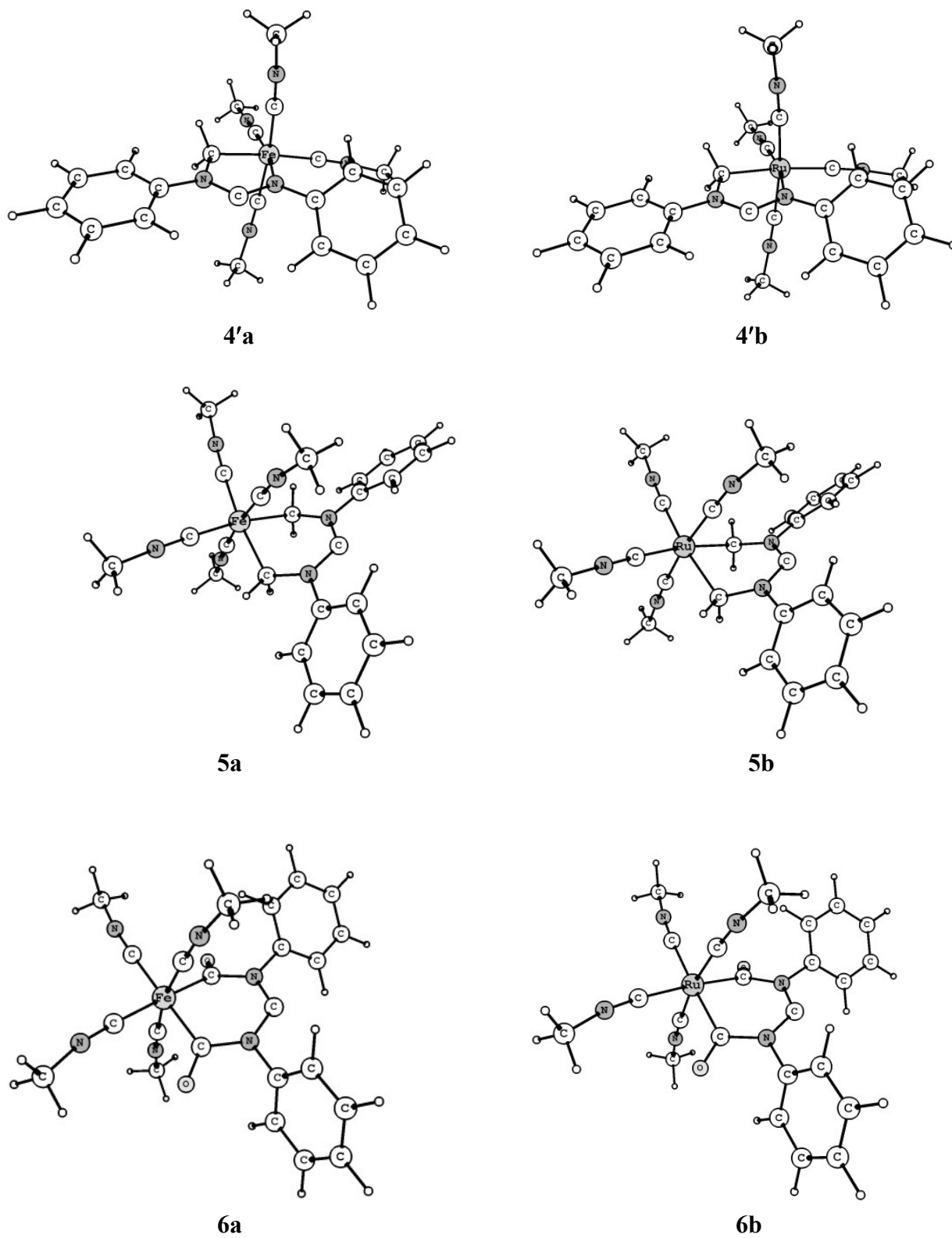


Fig. S2 Singlet state optimized geometries for **1a-6b** (Molecules **4a** and **4b** are excluded as geometry optimizations of their triplet states lead to broken geometries).

Cartesian coordinates for the singlet state optimized geometries of **1a-6b**, along with their total energies (in hartrees) including zero point vibrational correction in gas phase.

1a, TE = -1869.440892

6	-2.172373000	1.051563000	0.000185000
6	-1.210825000	-1.133707000	-0.000209000
1	-1.408825000	-2.211650000	-0.000360000
7	-2.289544000	-0.401172000	-0.000048000
7	-0.913307000	1.335263000	0.000244000
6	-3.648300000	-0.924769000	-0.000117000
1	-4.173562000	-0.558700000	-0.883685000
1	-3.624573000	-2.015078000	-0.000124000
1	-4.173635000	-0.558708000	0.883408000
6	-0.552982000	2.740890000	0.000456000
1	0.049330000	2.974170000	0.884778000
1	0.049383000	2.974419000	-0.883765000
1	-1.453953000	3.358143000	0.000517000
25	0.497174000	-0.168159000	-0.000045000
6	0.401138000	-0.140770000	1.841710000
8	0.323255000	-0.130956000	2.977465000
6	1.476595000	-1.682494000	-0.000334000
8	2.060764000	-2.666520000	-0.000459000
6	1.966879000	0.935707000	0.000206000
8	2.887609000	1.610238000	0.000329000
6	0.401142000	-0.140023000	-1.841793000
8	0.323221000	-0.129717000	-2.977540000

1b, TE = -2003.223939

6	0.514177000	-2.389224000	-0.066992000
6	1.252598000	-0.106728000	0.121876000
7	1.553210000	-1.421609000	0.080450000
7	-0.635952000	-1.806025000	-0.122859000
25	-0.763789000	0.232569000	0.008657000
6	-0.833580000	0.035940000	1.839997000
8	-0.842243000	-0.088087000	2.972864000

6	-0.838473000	2.029790000	0.093683000
8	-0.971314000	3.169767000	0.124486000
6	-2.577417000	0.208278000	-0.179129000
8	-3.713894000	0.217150000	-0.296340000
6	-0.471247000	0.267531000	-1.809474000
8	-0.259076000	0.292087000	-2.929181000
6	-1.801580000	-2.658918000	-0.256340000
6	2.849501000	-1.994671000	0.436371000
7	2.272257000	0.774309000	0.094264000
6	3.501763000	0.568899000	-0.663333000
1	4.377299000	0.424078000	-0.022247000
1	3.400449000	-0.279791000	-1.335783000
1	3.670055000	1.460621000	-1.275551000
6	2.104424000	2.144608000	0.539232000
1	3.044609000	2.479257000	0.987470000
1	1.858370000	2.818756000	-0.289776000
1	1.332109000	2.203503000	1.300847000
1	3.382051000	-1.326834000	1.115395000
1	2.642453000	-2.938748000	0.937320000
1	3.474498000	-2.206425000	-0.435049000
1	-1.488971000	-3.705263000	-0.282503000
1	-2.485233000	-2.507101000	0.586583000
1	-2.348373000	-2.423353000	-1.176102000

1c, TE = - 1983.858696

6	-1.131675000	-2.198018000	0.000102000
6	-1.422820000	0.171621000	-0.000117000
7	-1.970357000	-1.041195000	-0.000090000
7	0.106777000	-1.829901000	0.000205000
25	0.592742000	0.167474000	-0.000010000
6	0.502194000	0.094012000	-1.841706000
8	0.429163000	0.047091000	-2.976915000
6	0.951280000	1.933769000	-0.000398000
8	1.254434000	3.040135000	-0.000670000
6	2.388940000	-0.175466000	0.000341000

8	3.514287000	-0.365401000	0.000595000
6	0.501733000	0.094843000	1.841685000
8	0.428419000	0.048466000	2.976900000
6	1.108681000	-2.879031000	0.000343000
8	-2.350410000	1.112348000	0.000043000
6	-1.988508000	2.488936000	-0.000269000
1	-1.417720000	2.737702000	0.895498000
1	-1.417725000	2.737308000	-0.896145000
1	-2.929779000	3.036938000	-0.000384000
6	-3.413696000	-1.246382000	-0.000030000
1	-3.867067000	-0.799218000	0.887489000
1	-3.867409000	-0.797150000	-0.886308000
1	-3.573407000	-2.322048000	-0.001179000
1	0.617686000	-3.854641000	0.000388000
1	1.749053000	-2.797513000	-0.884902000
1	1.748955000	-2.797374000	0.885644000

1'a, TE = -2252.445512

6	-0.637755000	-1.243676000	0.033766000
6	-1.206510000	1.077323000	0.056813000
1	-2.020807000	1.806223000	0.117085000
7	-1.620785000	-0.168661000	0.038749000
7	0.537633000	-0.695376000	0.049556000
25	0.719481000	1.373704000	0.004985000
6	0.635880000	1.232893000	-1.835846000
8	0.564055000	1.144065000	-2.967688000
6	0.527982000	3.163675000	-0.052442000
8	0.358514000	4.294662000	-0.087312000
6	2.563738000	1.467330000	-0.057974000
8	3.696662000	1.575992000	-0.108649000
6	0.706813000	1.371152000	1.851215000
8	0.678195000	1.376379000	2.989227000
6	1.647311000	-1.586700000	-0.004549000
6	2.664150000	-1.495373000	0.943214000
6	1.726268000	-2.553988000	-1.005187000

6	3.744945000	-2.366106000	0.894798000
1	2.597545000	-0.755651000	1.733938000
6	2.814219000	-3.416091000	-1.055047000
1	0.922653000	-2.621451000	-1.729576000
6	3.827511000	-3.326537000	-0.107241000
1	4.525112000	-2.293401000	1.645572000
1	2.868236000	-4.163261000	-1.840447000
1	4.676849000	-4.000248000	-0.149300000
6	-3.004889000	-0.539991000	0.044882000
6	-3.406334000	-1.656806000	0.770929000
6	-3.933023000	0.209916000	-0.670691000
6	-4.751516000	-1.998178000	0.804356000
1	-2.657028000	-2.245373000	1.285741000
6	-5.276555000	-0.140401000	-0.630005000
1	-3.607135000	1.046847000	-1.279554000
6	-5.689886000	-1.241244000	0.110754000
1	-5.066773000	-2.865016000	1.375477000
1	-5.998169000	0.441199000	-1.193743000
1	-6.738934000	-1.516171000	0.136930000

1'b, TE = -2386.231629

6	0.261240000	-1.424424000	-0.291681000
6	1.095561000	0.839902000	-0.195697000
7	1.343374000	-0.506534000	-0.245675000
7	-0.869183000	-0.795853000	-0.181734000
25	-0.874932000	1.236730000	0.179852000
6	-0.535302000	0.835442000	1.950232000
8	-0.290921000	0.595708000	3.036319000
6	-0.854900000	3.003154000	0.509234000
8	-0.931878000	4.128048000	0.726471000
6	-2.687155000	1.279971000	0.453655000
8	-3.806742000	1.367422000	0.650233000
6	-1.007850000	1.508351000	-1.637035000
8	-1.047842000	1.689865000	-2.762097000
6	-2.040597000	-1.603050000	-0.177346000
6	-3.067270000	-1.360709000	-1.087833000

6	-2.174585000	-2.644768000	0.739803000
6	-4.210578000	-2.149961000	-1.083034000
1	-2.960726000	-0.562296000	-1.815046000
6	-3.321457000	-3.428112000	0.745293000
1	-1.363225000	-2.834389000	1.433456000
6	-4.345093000	-3.184308000	-0.163856000
1	-4.998281000	-1.955856000	-1.804030000
1	-3.414500000	-4.235157000	1.465316000
1	-5.241167000	-3.796050000	-0.156568000
6	2.628518000	-1.114437000	-0.064479000
6	3.003437000	-2.192176000	-0.862239000
6	3.465417000	-0.685384000	0.962129000
6	4.226030000	-2.814227000	-0.649883000
1	2.316131000	-2.543454000	-1.622519000
6	4.689412000	-1.312311000	1.167115000
1	3.151928000	0.125952000	1.611243000
6	5.076842000	-2.374912000	0.359933000
1	4.512177000	-3.654084000	-1.274661000
1	5.333065000	-0.976701000	1.973814000
1	6.029360000	-2.867170000	0.524955000
7	2.084665000	1.668862000	-0.542070000
6	3.212763000	1.310926000	-1.398586000
1	4.138386000	1.184223000	-0.829333000
1	3.007879000	0.392186000	-1.942545000
1	3.344337000	2.121140000	-2.121138000
6	2.024820000	3.091786000	-0.250006000
1	3.047504000	3.469468000	-0.179851000
1	1.504135000	3.646300000	-1.038778000
1	1.537842000	3.269458000	0.704004000

1'c, TE = -2366.859552

6	0.420301000	-1.411901000	-0.010218000
6	1.166502000	0.863722000	-0.069596000
7	1.469146000	-0.443919000	-0.007843000
7	-0.728537000	-0.806895000	-0.041580000

25	-0.801206000	1.257869000	0.035776000
6	-0.634488000	1.082371000	1.868127000
8	-0.511106000	0.976236000	2.994207000
6	-0.784837000	3.054873000	0.144204000
8	-0.854196000	4.197071000	0.223024000
6	-2.634402000	1.315339000	0.163294000
8	-3.765058000	1.412089000	0.260708000
6	-0.821531000	1.286755000	-1.809124000
8	-0.809159000	1.313778000	-2.947860000
6	-1.880338000	-1.643292000	-0.017309000
6	-2.858317000	-1.520993000	-1.002109000
6	-2.038266000	-2.596067000	0.988029000
6	-3.978275000	-2.342444000	-0.983634000
1	-2.731685000	-0.794528000	-1.798175000
6	-3.162506000	-3.411580000	1.006097000
1	-1.262821000	-2.693210000	1.739379000
6	-4.137807000	-3.288313000	0.022677000
1	-4.727305000	-2.244159000	-1.762804000
1	-3.274938000	-4.149205000	1.794429000
1	-5.015784000	-3.925452000	0.039652000
6	2.814690000	-0.949774000	-0.030297000
6	3.173751000	-1.852682000	-1.022919000
6	3.726227000	-0.580354000	0.951483000
6	4.461234000	-2.373740000	-1.042672000
1	2.434388000	-2.153902000	-1.755740000
6	5.011688000	-1.105772000	0.926066000
1	3.428672000	0.106007000	1.736079000
6	5.383486000	-1.999484000	-0.072085000
1	4.740873000	-3.080202000	-1.817104000
1	5.721915000	-0.821582000	1.695511000
1	6.387465000	-2.410518000	-0.087385000
8	2.241667000	1.608266000	-0.193672000
6	2.150911000	3.022317000	-0.330104000
1	1.502807000	3.289515000	-1.165759000
1	1.789431000	3.475705000	0.593886000

1 3.167553000 3.357108000 -0.531134000

2a, TE = -1908.101357

6 -2.622628000 -1.105956000 -0.015458000
6 -1.618175000 1.058386000 -0.018360000
1 -1.808713000 2.140081000 -0.025029000
7 -2.716927000 0.344718000 -0.023221000
7 -1.364940000 -1.404873000 -0.004461000
6 -4.063266000 0.892883000 -0.035954000
1 -4.606432000 0.545043000 0.844913000
1 -4.017860000 1.983165000 -0.040648000
1 -4.593077000 0.536836000 -0.921658000
6 -1.035923000 -2.815088000 0.005007000
1 -0.430059000 -3.065925000 -0.873235000
1 -0.444028000 -3.057280000 0.895128000
1 -1.948864000 -3.416609000 0.000749000
6 0.058238000 0.082699000 -1.833103000
8 0.063808000 0.105801000 -2.977712000
6 0.030164000 0.099981000 1.831012000
8 0.018110000 0.133795000 2.975301000
6 1.536029000 -1.093871000 0.015694000
7 2.446137000 -1.832444000 0.025651000
6 1.085606000 1.624679000 -0.000435000
7 1.688010000 2.633360000 -0.000653000
6 2.456839000 3.812231000 -0.000461000
1 2.235883000 4.408413000 -0.889860000
1 2.232095000 4.410568000 0.886539000
1 3.523355000 3.570122000 0.002090000
6 3.502573000 -2.762937000 0.037268000
1 4.126876000 -2.634422000 -0.850582000
1 4.120983000 -2.619003000 0.926873000
1 3.106692000 -3.782124000 0.044792000
25 0.063975000 0.085153000 -0.000876000

2b, TE = -2041.880222

6	-1.253403000	-2.489508000	0.020885000
6	-1.622067000	-0.110585000	0.096179000
7	-2.130976000	-1.361380000	0.091845000
7	-0.026861000	-2.085968000	-0.025179000
6	0.204289000	0.007447000	-1.771299000
8	0.055237000	0.100998000	-2.904136000
6	0.442439000	-0.162591000	1.873772000
8	0.441194000	-0.179813000	3.019519000
6	2.240150000	-0.429291000	-0.105549000
7	3.390726000	-0.635509000	-0.204093000
6	0.798147000	1.722074000	0.091338000
7	1.143295000	2.847848000	0.108018000
6	1.575655000	4.185769000	0.127191000
1	0.720938000	4.864870000	0.204848000
1	2.235248000	4.360016000	0.982114000
1	2.123748000	4.422019000	-0.789388000
6	4.738008000	-1.025678000	-0.323028000
1	5.160785000	-0.645634000	-1.256678000
1	5.321283000	-0.631153000	0.512980000
1	4.814139000	-2.116758000	-0.320861000
25	0.407502000	-0.082779000	0.043638000
6	0.984682000	-3.119856000	-0.083608000
6	-3.510634000	-1.703829000	0.419779000
7	-2.511691000	0.909103000	-0.002083000
6	-2.153978000	2.255402000	0.388054000
1	-1.393800000	2.230881000	1.163846000
1	-1.786372000	2.845398000	-0.462227000
1	-3.044065000	2.749629000	0.791672000
6	-3.701318000	0.856752000	-0.840364000
1	-3.684338000	-0.028721000	-1.472256000
1	-4.633275000	0.872058000	-0.264167000
1	-3.692571000	1.732908000	-1.498151000
1	-3.474762000	-2.648429000	0.960410000
1	-3.950060000	-0.931414000	1.054238000

1	-4.139039000	-1.848240000	-0.463971000
1	1.662592000	-3.040767000	0.775121000
1	0.509303000	-4.104556000	-0.077412000
1	1.587974000	-3.017403000	-0.993791000

2c, TE = -2022.517880

6	1.865768000	-2.151697000	-0.000098000
6	1.777099000	0.235701000	-0.000239000
7	2.512917000	-0.875718000	-0.000396000
7	0.584530000	-1.972927000	0.000423000
6	-0.146363000	-0.058104000	1.832369000
8	-0.112279000	-0.021229000	2.976207000
6	-0.146977000	-0.058743000	-1.831630000
8	-0.113337000	-0.022393000	-2.975491000
6	-1.951411000	-0.737653000	0.000570000
7	-3.048085000	-1.150653000	0.000710000
6	-0.880013000	1.651635000	0.000169000
7	-1.396806000	2.709033000	0.000032000
6	-2.075885000	3.941548000	-0.000166000
1	-1.364007000	4.772171000	-0.007603000
1	-2.713560000	4.023006000	-0.884873000
1	-2.702458000	4.029360000	0.891826000
6	-4.312563000	-1.770563000	-0.001387000
1	-4.814834000	-1.604932000	0.955005000
1	-4.933138000	-1.359366000	-0.801467000
1	-4.201036000	-2.846809000	-0.159438000
25	-0.198791000	-0.067596000	0.000369000
6	-0.229419000	-3.169926000	0.000933000
6	3.968104000	-0.854500000	-0.000891000
8	2.565045000	1.308135000	-0.000647000
6	1.991799000	2.605061000	-0.000686000
1	1.383497000	2.759019000	-0.893704000
1	1.383957000	2.759303000	0.892591000
1	2.833940000	3.297537000	-0.001019000
1	4.291319000	-1.893325000	-0.001216000

1	4.350149000	-0.341944000	-0.887372000
1	4.350767000	-0.342348000	0.885563000
1	-0.876363000	-3.193987000	-0.884340000
1	0.413001000	-4.054600000	0.000594000
1	-0.875619000	-3.194000000	0.886647000

2'a, TE = -2291.109734

6	-0.947680000	-1.495480000	0.051411000
6	-1.386996000	0.852277000	-0.033428000
1	-2.172056000	1.613808000	-0.110401000
7	-1.873422000	-0.376348000	0.026707000
7	0.249717000	-0.994956000	0.103141000
6	0.521796000	0.928648000	-1.860139000
8	0.513694000	0.880578000	-3.002595000
6	0.518012000	1.234714000	1.796991000
8	0.501774000	1.379852000	2.932227000
6	2.418530000	0.946647000	-0.053507000
7	3.582021000	0.833344000	-0.093783000
6	0.443880000	2.903322000	-0.176533000
7	0.337828000	4.068688000	-0.267474000
6	0.272331000	5.470922000	-0.378077000
1	-0.432443000	5.755229000	-1.163715000
1	-0.060258000	5.908389000	0.566809000
1	1.256717000	5.877168000	-0.625998000
6	4.938184000	0.448754000	-0.129684000
1	5.354644000	0.643888000	-1.120649000
1	5.508611000	1.013981000	0.611021000
1	5.016816000	-0.619822000	0.089718000
25	0.526982000	1.062725000	-0.028314000
6	1.319074000	-1.926904000	0.128814000
6	2.211729000	-1.930230000	1.200713000
6	1.504722000	-2.833960000	-0.913083000
6	3.268665000	-2.831396000	1.231916000
1	2.056590000	-1.235521000	2.019596000
6	2.570487000	-3.726186000	-0.884733000

1	0.798792000	-2.831498000	-1.736122000
6	3.458185000	-3.729994000	0.185550000
1	3.939725000	-2.841214000	2.085946000
1	2.702506000	-4.427839000	-1.702687000
1	4.284140000	-4.433572000	0.209997000
6	-3.271299000	-0.670452000	0.053764000
6	-3.751819000	-1.788635000	-0.622527000
6	-4.147956000	0.150484000	0.758182000
6	-5.113422000	-2.059296000	-0.617841000
1	-3.044438000	-2.434432000	-1.127585000
6	-5.509286000	-0.127101000	0.754719000
1	-3.764814000	0.988258000	1.331243000
6	-5.997744000	-1.229324000	0.063490000
1	-5.485111000	-2.928683000	-1.150411000
1	-6.186713000	0.512532000	1.311022000
1	-7.060371000	-1.448183000	0.066898000

2'b, TE = -2424.891845

6	-0.745405000	-1.611322000	-0.199377000
6	-1.258902000	0.755588000	-0.144063000
7	-1.691321000	-0.543114000	-0.191648000
7	0.451123000	-1.135531000	-0.027579000
6	0.764395000	0.951588000	-1.782748000
8	0.748776000	1.028279000	-2.925630000
6	0.589918000	0.919081000	1.872904000
8	0.457331000	0.971693000	3.010108000
6	2.614060000	0.646285000	0.083314000
7	3.773226000	0.481209000	0.070958000
6	1.057881000	2.728764000	0.060325000
7	1.349118000	3.869093000	0.063647000
6	1.786966000	5.206394000	0.067538000
1	0.932833000	5.889770000	0.053512000
1	2.379085000	5.408757000	0.964454000
1	2.405677000	5.405333000	-0.812029000
6	5.094305000	-0.012788000	0.051819000
1	5.563091000	0.210295000	-0.909667000
1	5.681901000	0.452368000	0.846964000
1	5.075601000	-1.096224000	0.200776000
25	0.754974000	0.907445000	0.047730000
6	1.498378000	-2.090441000	-0.007176000
6	2.269913000	-2.258262000	1.143412000

6	1.781284000	-2.867623000	-1.129550000
6	3.299929000	-3.190664000	1.171726000
1	2.038579000	-1.666036000	2.022901000
6	2.818150000	-3.793609000	-1.102301000
1	1.167884000	-2.741911000	-2.015030000
6	3.584149000	-3.960160000	0.046364000
1	3.873717000	-3.328130000	2.083790000
1	3.022347000	-4.394901000	-1.983173000
1	4.386694000	-4.690514000	0.069664000
6	-3.038020000	-0.973996000	0.031325000
6	-3.584531000	-1.977850000	-0.764580000
6	-3.775300000	-0.456382000	1.093520000
6	-4.872529000	-2.432719000	-0.518184000
1	-2.976761000	-2.405559000	-1.552849000
6	-5.065391000	-0.915827000	1.334225000
1	-3.331243000	0.294588000	1.738598000
6	-5.621881000	-1.900648000	0.527057000
1	-5.290931000	-3.215257000	-1.143152000
1	-5.629806000	-0.511256000	2.168467000
1	-6.626646000	-2.262071000	0.719493000
7	-2.165869000	1.711535000	-0.410220000
6	-1.928244000	3.095104000	-0.053248000
1	-1.213603000	3.153611000	0.761536000
1	-1.557730000	3.675893000	-0.907113000
1	-2.874566000	3.534473000	0.279070000
6	-3.363119000	1.538755000	-1.223670000
1	-3.307557000	0.620795000	-1.804209000
1	-4.277569000	1.517671000	-0.622009000
1	-3.414180000	2.384467000	-1.916957000

2'c, TE = -2405.522744

6	-0.893040000	-1.580165000	0.050089000
6	-1.326480000	0.779799000	-0.010056000
7	-1.805413000	-0.479743000	0.041846000
7	0.319856000	-1.116343000	0.105357000
6	0.606817000	0.824107000	-1.836966000
8	0.569196000	0.800252000	-2.980380000
6	0.620837000	1.068515000	1.821604000
8	0.585940000	1.198811000	2.958708000
6	2.520576000	0.643296000	-0.034506000
7	3.673377000	0.452640000	-0.085102000
6	0.948210000	2.748916000	-0.123583000

7	1.227241000	3.889079000	-0.194579000
6	1.645359000	5.230956000	-0.276425000
1	0.782146000	5.902532000	-0.267003000
1	2.288769000	5.478742000	0.572227000
1	2.205268000	5.396346000	-1.200887000
6	4.988850000	-0.054745000	-0.136191000
1	5.412491000	0.107274000	-1.130090000
1	5.615507000	0.450373000	0.602444000
1	4.967613000	-1.127206000	0.076905000
25	0.657325000	0.925829000	-0.005409000
6	1.356882000	-2.083338000	0.122357000
6	2.187835000	-2.196433000	1.237189000
6	1.570726000	-2.922176000	-0.970034000
6	3.210356000	-3.137258000	1.260602000
1	2.010014000	-1.553996000	2.093534000
6	2.600481000	-3.856212000	-0.948514000
1	0.911064000	-2.837581000	-1.826649000
6	3.426252000	-3.968836000	0.164736000
1	3.831824000	-3.232032000	2.146409000
1	2.751252000	-4.506692000	-1.804726000
1	4.222523000	-4.706072000	0.184448000
6	-3.202257000	-0.804382000	0.045338000
6	-3.696897000	-1.655857000	-0.935409000
6	-4.044639000	-0.321527000	1.040799000
6	-5.040738000	-2.007727000	-0.930712000
1	-3.015547000	-2.051480000	-1.679384000
6	-5.387546000	-0.676217000	1.040319000
1	-3.646908000	0.321328000	1.817578000
6	-5.890975000	-1.516526000	0.053499000
1	-5.422177000	-2.674378000	-1.697361000
1	-6.040561000	-0.301242000	1.821871000
1	-6.939710000	-1.795227000	0.057820000
8	-2.314600000	1.655350000	-0.085600000
6	-2.038201000	3.043759000	-0.175585000
1	-1.489154000	3.386256000	0.703048000

1	-1.469018000	3.264863000	-1.079859000
1	-3.012710000	3.530040000	-0.220878000

3a, TE = -1946.751934

6	-2.607549000	0.035421000	-1.055262000
6	-1.563743000	0.014121000	1.091815000
1	-1.749503000	0.012351000	2.176467000
7	-2.681432000	0.030896000	0.392632000
7	-1.351001000	0.020880000	-1.368177000
6	-4.016377000	0.045528000	0.963591000
1	-4.575881000	-0.828362000	0.621434000
1	-3.950677000	0.039805000	2.053423000
1	-4.553180000	0.936562000	0.629349000
6	-1.039677000	0.021539000	-2.779857000
1	-0.429284000	0.897754000	-3.031027000
1	-0.450012000	-0.867132000	-3.036432000
1	-1.957622000	0.034222000	-3.376206000
25	0.097531000	-0.002369000	0.113634000
6	1.560929000	-0.013449000	-1.058108000
7	2.476873000	-0.019789000	-1.799080000
6	1.109607000	-0.021272000	1.634218000
7	1.692582000	-0.032576000	2.663537000
6	0.029464000	-1.872770000	0.061260000
7	-0.031539000	-3.045654000	0.017447000
6	0.074100000	1.869375000	0.077709000
7	0.041056000	3.043735000	0.043812000
6	-0.135582000	4.436098000	-0.036350000
1	-0.297044000	4.858110000	0.959897000
1	0.747623000	4.909655000	-0.474488000
1	-1.003404000	4.671087000	-0.659538000
6	3.511203000	-0.016603000	-2.749571000
1	4.248519000	0.755964000	-2.511238000
1	4.019512000	-0.985316000	-2.764968000
1	3.112583000	0.181201000	-3.749737000
6	2.601336000	-0.050786000	3.735422000

1	2.484966000	0.844227000	4.354569000
1	2.432017000	-0.926787000	4.369342000
1	3.633326000	-0.084727000	3.369532000
6	-0.237689000	-4.433179000	-0.074659000
1	0.638013000	-4.922406000	-0.510669000
1	-0.414886000	-4.859163000	0.917212000
1	-1.106178000	-4.644605000	-0.705295000

3b, TE = -2080.528876

6	-1.366645000	0.928894000	-2.195686000
6	-1.638472000	0.215733000	0.091567000
7	-2.196783000	0.663870000	-1.058873000
7	-0.134763000	0.667269000	-1.900424000
25	0.371011000	0.020460000	-0.010141000
6	2.158302000	-0.126054000	-0.487141000
7	3.296607000	-0.228488000	-0.778273000
6	0.829343000	-0.567601000	1.641972000
7	1.182908000	-0.962211000	2.713585000
6	0.019478000	-1.723314000	-0.587527000
7	-0.218139000	-2.814067000	-0.956972000
6	0.571307000	1.816771000	0.483134000
7	0.674061000	2.949961000	0.778188000
6	0.697796000	4.335400000	1.016200000
1	0.099100000	4.582017000	1.897927000
1	1.722727000	4.677016000	1.186787000
1	0.288944000	4.872479000	0.155351000
6	4.592550000	-0.259420000	-1.321754000
1	5.251739000	0.427116000	-0.781962000
1	5.014548000	-1.266573000	-1.252576000
1	4.571770000	0.036372000	-2.375772000
6	2.209453000	-1.461578000	3.554959000
1	1.780998000	-1.917379000	4.451358000
1	2.809804000	-2.217645000	3.036690000
1	2.874601000	-0.651433000	3.873096000
6	-0.546637000	-4.056079000	-1.528010000

1	0.357752000	-4.579471000	-1.851711000
1	-1.068579000	-4.685343000	-0.801247000
1	-1.195990000	-3.912501000	-2.396674000
6	0.831939000	0.902246000	-2.949217000
6	-3.553470000	1.181823000	-1.182453000
7	-2.506579000	-0.150368000	1.072980000
6	-2.064746000	-0.272482000	2.445267000
1	-2.891166000	0.013564000	3.106147000
1	-1.760579000	-1.298178000	2.691287000
1	-1.224656000	0.391433000	2.626021000
6	-3.758250000	-0.845407000	0.817560000
1	-4.643376000	-0.251863000	1.076683000
1	-3.824677000	-1.143656000	-0.227143000
1	-3.773640000	-1.757450000	1.425817000
1	0.330780000	1.279667000	-3.846325000
1	1.583362000	1.631545000	-2.619889000
1	1.364629000	-0.024889000	-3.197553000
1	-3.902925000	1.558537000	-0.218115000
1	-3.510223000	1.996668000	-1.904143000
1	-4.269282000	0.443540000	-1.558353000

3c, TE = -2061.169314

6	-1.954169000	-0.018462000	-2.009254000
6	-1.753622000	0.001489000	0.374355000
7	-2.544103000	-0.009009000	-0.705194000
7	-0.665107000	-0.015461000	-1.881369000
25	0.199765000	0.000407000	-0.000401000
6	1.912112000	-0.005902000	-0.731549000
7	2.998569000	-0.010802000	-1.186858000
6	0.946391000	0.014651000	1.654827000
7	1.478365000	0.023507000	2.723011000
6	0.130058000	-1.872046000	-0.027177000
7	0.065686000	-3.044643000	-0.058404000
6	0.126785000	1.872112000	-0.057821000
7	0.060354000	3.043927000	-0.108034000
6	-0.139358000	4.426830000	-0.269138000

1	-0.600639000	4.852313000	0.626652000
1	0.814479000	4.932886000	-0.442391000
1	-0.796097000	4.614470000	-1.123407000
6	4.202652000	-0.021223000	-1.912616000
1	4.783233000	0.882313000	-1.704580000
1	4.807514000	-0.890681000	-1.638921000
1	3.998576000	-0.063722000	-2.987256000
6	2.636639000	0.041246000	3.538744000
1	3.345619000	0.802047000	3.194203000
1	2.371333000	0.262999000	4.575614000
1	3.137395000	-0.932617000	3.517446000
6	-0.132777000	-4.430170000	-0.197067000
1	0.820934000	-4.937512000	-0.367216000
1	-0.588981000	-4.842347000	0.707506000
1	-0.793466000	-4.631936000	-1.045046000
6	0.095218000	-0.023669000	-3.110552000
6	-3.994827000	-0.010556000	-0.618258000
8	-2.502423000	0.010089000	1.479943000
6	-1.860791000	0.022590000	2.744746000
1	-1.239164000	0.912196000	2.855942000
1	-2.664803000	0.029787000	3.482313000
1	-1.238945000	-0.864456000	2.873622000
1	-4.365554000	-0.020035000	-1.641602000
1	-4.356299000	-0.891744000	-0.080678000
1	-4.359193000	0.878661000	-0.096068000
1	0.744722000	-0.907434000	-3.154352000
1	-0.580595000	-0.030665000	-3.971613000
1	0.742984000	0.860609000	-3.167190000

3'a, TE = -2329.763863

6	-1.007156000	-1.516564000	-0.175090000
6	-1.389534000	0.828449000	0.084724000
1	-2.166897000	1.589907000	0.228472000
7	-1.907782000	-0.393332000	-0.065387000
7	0.204657000	-1.036435000	-0.181759000
25	0.502400000	1.017194000	0.100700000
6	2.384988000	0.924680000	0.159965000

7	3.556398000	0.844941000	0.229926000
6	0.410829000	2.824330000	0.369269000
7	0.280003000	3.985204000	0.538286000
6	0.493258000	0.690552000	1.951024000
7	0.483596000	0.474711000	3.103995000
6	0.535103000	1.254640000	-1.761231000
7	0.543811000	1.389516000	-2.927788000
6	0.454865000	1.440043000	-4.331086000
1	-0.430434000	2.005549000	-4.635359000
1	1.340081000	1.924226000	-4.752305000
1	0.379846000	0.428146000	-4.739216000
6	4.894252000	0.404572000	0.282511000
1	5.500655000	0.944267000	-0.449836000
1	5.312206000	0.584552000	1.276690000
1	4.939301000	-0.667266000	0.065088000
6	0.306412000	5.375380000	0.743551000
1	-0.214765000	5.893523000	-0.067135000
1	-0.184920000	5.633772000	1.686472000
1	1.338098000	5.740169000	0.779854000
6	0.430318000	0.131678000	4.466984000
1	1.014239000	0.840347000	5.060652000
1	-0.604115000	0.146225000	4.821238000
1	0.838130000	-0.871598000	4.618353000
6	1.243654000	-1.990994000	-0.269817000
6	2.245531000	-1.847337000	-1.232374000
6	1.302011000	-3.082605000	0.599341000
6	3.274505000	-2.775982000	-1.327930000
1	2.196166000	-1.005646000	-1.914580000
6	2.339156000	-4.003307000	0.509774000
1	0.511001000	-3.198069000	1.331866000
6	3.332663000	-3.857061000	-0.452596000
1	4.031127000	-2.661097000	-2.099320000
1	2.367384000	-4.846141000	1.194298000
1	4.138405000	-4.580652000	-0.525284000
6	-3.307663000	-0.655808000	-0.102249000
6	-3.804227000	-1.844619000	0.431053000
6	-4.187360000	0.262278000	-0.674188000
6	-5.170214000	-2.091346000	0.416918000
1	-3.098530000	-2.562105000	0.830697000
6	-5.553609000	0.009139000	-0.679538000
1	-3.802196000	1.164701000	-1.136681000
6	-6.053046000	-1.166004000	-0.130982000
1	-5.547626000	-3.017912000	0.838166000
1	-6.228144000	0.729614000	-1.131438000
1	-7.119698000	-1.364745000	-0.141309000

3'b, TE = -2463.542716

6	0.852991000	-1.611992000	-0.266533000
6	1.258104000	0.778996000	-0.248797000
7	1.754304000	-0.508128000	-0.277831000
7	-0.359550000	-1.181748000	-0.065182000
25	-0.724739000	0.865169000	0.091405000
6	-2.559552000	0.577627000	0.232357000
7	-3.726897000	0.427362000	0.276501000
6	-1.080895000	2.638832000	0.212874000
7	-1.377339000	3.791040000	0.303507000
6	-0.886096000	0.911791000	-1.774238000
7	-0.973424000	0.940391000	-2.945567000
6	-0.438653000	0.742663000	1.943202000
7	-0.234723000	0.654799000	3.096979000
6	0.093500000	0.430864000	4.446619000
1	0.803971000	1.185321000	4.796408000
1	-0.802831000	0.482278000	5.070989000
1	0.546664000	-0.557697000	4.563256000
6	-5.025720000	-0.120078000	0.300479000
1	-5.567994000	0.224555000	1.185443000
1	-5.584394000	0.188285000	-0.587759000
1	-4.963787000	-1.212680000	0.321871000
6	-2.341747000	4.821525000	0.433601000
1	-1.865744000	5.802504000	0.359430000
1	-3.099484000	4.746246000	-0.353763000
1	-2.845010000	4.758466000	1.404292000
6	-1.104809000	0.848315000	-4.342881000
1	-1.905218000	0.149599000	-4.602775000
1	-1.342942000	1.826932000	-4.768984000
1	-0.172438000	0.491214000	-4.789410000
6	-1.359591000	-2.178977000	-0.043485000
6	-2.177864000	-2.333274000	1.078329000
6	-1.555554000	-3.028458000	-1.134143000
6	-3.160886000	-3.314772000	1.109584000
1	-2.018649000	-1.682657000	1.931683000
6	-2.546592000	-4.002958000	-1.105572000
1	-0.904666000	-2.916633000	-1.994344000
6	-3.357289000	-4.152598000	0.014489000
1	-3.769788000	-3.435928000	2.001461000
1	-2.680843000	-4.656029000	-1.963132000
1	-4.125499000	-4.919011000	0.039290000
6	3.116346000	-0.865343000	-0.052010000
6	3.682374000	-1.936106000	-0.743889000
6	3.869422000	-0.208190000	0.921186000
6	4.990960000	-2.319476000	-0.484229000
1	3.067700000	-2.470677000	-1.457632000

6	5.180427000	-0.595469000	1.173706000
1	3.420492000	0.602069000	1.486223000
6	5.750827000	-1.649708000	0.470610000
1	5.419176000	-3.154430000	-1.030231000
1	5.752807000	-0.076533000	1.936632000
1	6.772565000	-1.954436000	0.672028000
7	2.113259000	1.744877000	-0.633902000
6	1.825027000	3.142779000	-0.384979000
1	2.771868000	3.668601000	-0.222708000
1	1.307664000	3.607665000	-1.233273000
1	1.206769000	3.247486000	0.500429000
6	3.256516000	1.555855000	-1.515919000
1	4.211639000	1.629664000	-0.984460000
1	3.210361000	0.586913000	-2.008508000
1	3.219221000	2.338458000	-2.281283000

3'c, TE = -2444.176168

6	-1.004847000	-1.559319000	-0.149810000
6	-1.320604000	0.815737000	0.040784000
7	-1.864171000	-0.421974000	-0.077855000
7	0.231860000	-1.148362000	-0.180476000
25	0.652865000	0.882255000	0.059708000
6	2.492391000	0.551384000	0.124490000
7	3.647904000	0.348999000	0.212166000
6	1.015610000	2.650325000	0.282574000
7	1.312597000	3.794559000	0.421590000
6	0.563037000	0.612945000	1.915961000
7	0.493872000	0.438697000	3.074335000
6	0.654663000	1.082844000	-1.805909000
7	0.638511000	1.202031000	-2.974370000
6	0.548955000	1.227235000	-4.378500000
1	-0.166610000	1.988867000	-4.700763000
1	1.523363000	1.456794000	-4.818400000
1	0.215693000	0.254316000	-4.750547000
6	4.918807000	-0.256230000	0.297307000
1	5.608272000	0.204850000	-0.414988000
1	5.328582000	-0.135142000	1.303828000
1	4.830729000	-1.323657000	0.072290000
6	2.222764000	4.872036000	0.538351000
1	3.098457000	4.714193000	-0.100182000
1	1.744836000	5.810545000	0.245427000
1	2.562756000	4.974197000	1.573931000
6	0.361659000	0.140170000	4.442767000
1	0.984951000	0.811031000	5.040185000
1	-0.679290000	0.256415000	4.756931000
1	0.672329000	-0.890558000	4.634854000

6	1.207975000	-2.167245000	-0.261859000
6	2.159415000	-2.145054000	-1.284472000
6	1.250329000	-3.209083000	0.666961000
6	3.125080000	-3.139753000	-1.377449000
1	2.118483000	-1.345344000	-2.016239000
6	2.223476000	-4.197728000	0.578590000
1	0.495392000	-3.233791000	1.444927000
6	3.168685000	-4.169873000	-0.441603000
1	3.841018000	-3.118096000	-2.194576000
1	2.238154000	-5.001257000	1.309300000
1	3.923120000	-4.946900000	-0.513569000
6	-3.270640000	-0.685490000	-0.092404000
6	-3.789073000	-1.619945000	0.798550000
6	-4.113089000	-0.067374000	-1.011861000
6	-5.145405000	-1.919277000	0.782529000
1	-3.110555000	-2.122171000	1.477754000
6	-5.469002000	-0.369138000	-1.023647000
1	-3.704005000	0.643866000	-1.719489000
6	-5.991917000	-1.292518000	-0.125011000
1	-5.540603000	-2.651735000	1.479364000
1	-6.118550000	0.114820000	-1.746346000
1	-7.051050000	-1.528805000	-0.138898000
8	-2.278028000	1.725407000	0.166388000
6	-1.933881000	3.092831000	0.321867000
1	-1.353837000	3.446562000	-0.531471000
1	-2.883812000	3.625638000	0.381705000
1	-1.357962000	3.245159000	1.235434000

4a, TE = -2060.057548

6	2.333228000	0.011469000	-1.107448000
6	1.463791000	0.008150000	1.193277000
1	1.554877000	0.887548000	1.852077000
7	1.046345000	0.005965000	-1.397603000
1	1.562664000	-0.868237000	1.854944000
6	-1.185388000	-0.006489000	1.705198000
6	-0.012957000	-1.823156000	0.039456000
6	-0.033762000	1.823339000	0.039615000
7	-1.721439000	-0.009224000	2.748255000
7	0.228414000	2.960340000	-0.051642000
7	0.262313000	-2.957019000	-0.052037000
6	0.885136000	-4.195807000	-0.309348000
1	1.784951000	-4.032939000	-0.909006000
1	1.165134000	-4.678376000	0.630153000
1	0.205404000	-4.856049000	-0.853379000
6	-2.310650000	-0.012558000	4.025872000
1	-1.820815000	-0.751207000	4.666050000

1	-2.211706000	0.972359000	4.490150000
1	-3.373110000	-0.260469000	3.953934000
6	0.836290000	4.206709000	-0.308013000
1	1.117137000	4.688539000	0.631624000
1	1.734017000	4.055928000	-0.913923000
1	0.146114000	4.861782000	-0.845095000
6	0.650567000	0.005234000	-2.781417000
26	-0.277754000	-0.001305000	0.128413000
6	-1.776478000	-0.009745000	-0.949718000
7	-2.727519000	-0.015083000	-1.634753000
6	-3.797741000	-0.020379000	-2.548624000
1	-4.427663000	0.860311000	-2.398761000
1	-3.415648000	-0.009675000	-3.573235000
1	-4.408949000	-0.916031000	-2.410390000
7	2.557734000	0.011388000	0.222890000
6	3.896672000	0.018289000	0.745335000
1	4.598602000	0.019839000	-0.089237000
1	4.079661000	0.906449000	1.369861000
1	4.087294000	-0.865905000	1.373132000
1	0.039512000	0.887025000	-3.030042000
1	1.542106000	0.010562000	-3.416579000
1	0.048826000	-0.882425000	-3.031911000

4b, TE = -5207.549348

6	-2.503324000	0.002844000	-1.087499000
6	-1.595868000	0.005561000	1.216244000
1	-1.696416000	-0.870035000	1.877872000
7	-1.226551000	-0.000050000	-1.426693000
1	-1.693414000	0.884460000	1.873976000
6	1.290117000	0.000979000	1.726567000
6	0.005328000	1.950019000	0.056255000
6	-0.003175000	-1.949631000	0.063954000
7	1.891293000	0.001835000	2.735589000
7	-0.251018000	-3.090560000	0.017869000
7	-0.237425000	3.091853000	0.005843000
6	-0.734067000	4.401187000	-0.148648000
1	-1.695309000	4.368143000	-0.668047000
1	-0.873234000	4.867714000	0.829545000
1	-0.033128000	5.004309000	-0.730735000
6	2.552871000	0.005116000	3.976487000
1	2.155922000	0.798735000	4.615792000
1	2.412216000	-0.953543000	4.483698000
1	3.624613000	0.172070000	3.836751000
6	-0.754129000	-4.397998000	-0.131753000
1	-0.896409000	-4.859873000	0.848200000
1	-1.714800000	-4.362181000	-0.652023000

1	-0.055793000	-5.006982000	-0.710855000
6	-0.892569000	-0.002932000	-2.828385000
6	1.780973000	-0.006378000	-1.118470000
7	2.677677000	-0.010294000	-1.874615000
6	3.673267000	-0.015798000	-2.869185000
1	4.306533000	-0.900856000	-2.765634000
1	3.212979000	-0.026184000	-3.861216000
1	4.300505000	0.875243000	-2.781485000
7	-2.697456000	0.005357000	0.246972000
6	-4.029461000	0.009173000	0.789361000
44	0.235795000	-0.000234000	0.109683000
1	-4.743983000	0.008376000	-0.034039000
1	-4.207471000	-0.875118000	1.420678000
1	-4.204294000	0.897323000	1.416164000
1	-0.299788000	-0.889316000	-3.102412000
1	-1.812847000	-0.002049000	-3.421427000
1	-0.296280000	0.880215000	-3.105199000

4'a, TE = -2443.081484

6	-0.935948000	-1.371932000	0.141017000
6	-1.386252000	1.051325000	0.144064000
1	-1.739392000	1.529142000	1.069154000
7	0.314801000	-0.939115000	0.154243000
1	-1.869307000	1.591327000	-0.681132000
6	0.575499000	2.874958000	-0.189126000
6	0.284074000	0.752587000	-1.833145000
6	0.676543000	1.083693000	1.809860000
7	0.490965000	4.039868000	-0.273505000
7	0.621478000	1.039764000	2.976215000
7	-0.006975000	0.495352000	-2.933597000
6	-0.479981000	0.004758000	-4.168185000
1	-1.058743000	-0.906617000	-3.998856000
1	-1.120287000	0.749455000	-4.646232000
1	0.359578000	-0.220031000	-4.829815000
6	0.364335000	5.438687000	-0.372778000
1	-0.409303000	5.695786000	-1.100744000
1	0.087986000	5.861036000	0.596655000
1	1.310805000	5.881999000	-0.692843000
6	0.435541000	0.791383000	4.351836000
1	-0.332704000	1.457358000	4.751570000
1	0.118041000	-0.244288000	4.496388000
1	1.368024000	0.959719000	4.895558000
6	1.322393000	-1.918750000	0.165350000
6	2.448388000	-1.781941000	0.986356000
6	1.235547000	-3.064960000	-0.637427000
6	3.451367000	-2.745033000	0.997988000

1	2.516046000	-0.920499000	1.641633000
6	2.239185000	-4.023517000	-0.625236000
1	0.351162000	-3.186030000	-1.252425000
6	3.359742000	-3.871937000	0.187349000
1	4.301738000	-2.623262000	1.664090000
1	2.145062000	-4.901122000	-1.258704000
1	4.141319000	-4.624868000	0.196995000
26	0.634444000	1.061617000	-0.038670000
6	2.467337000	0.936155000	-0.301370000
7	3.612742000	0.848448000	-0.525222000
6	4.941251000	0.426623000	-0.742556000
1	5.622909000	0.974014000	-0.087254000
1	5.015356000	-0.644232000	-0.531319000
1	5.228460000	0.610069000	-1.780601000
7	-1.833752000	-0.352027000	0.121746000
6	-3.209856000	-0.633739000	0.141673000
6	-4.157656000	0.398366000	0.184785000
6	-3.680222000	-1.958473000	0.115887000
6	-5.520653000	0.114031000	0.196765000
1	-3.834245000	1.431005000	0.213471000
6	-5.038149000	-2.225517000	0.128066000
1	-2.944819000	-2.752548000	0.092900000
6	-5.977174000	-1.195097000	0.167247000
1	-6.229227000	0.936800000	0.231535000
1	-5.370535000	-3.259690000	0.108611000
1	-7.040156000	-1.412593000	0.177118000

4'b, TE = -5590.573778

6	-1.139802000	-1.416358000	0.155018000
6	-1.445462000	1.044523000	0.198013000
1	-1.766953000	1.512537000	1.138720000
7	0.145274000	-1.088662000	0.167438000
1	-1.915134000	1.623191000	-0.607451000
6	0.782818000	2.888664000	-0.193009000
6	0.260350000	0.697436000	-1.933473000
6	0.761723000	1.021062000	1.939633000
7	0.808137000	4.057427000	-0.287345000
7	0.732418000	1.000470000	3.106587000
7	-0.061140000	0.474890000	-3.031967000
6	-0.552704000	0.064166000	-4.287931000
1	-1.348412000	-0.670554000	-4.143718000
1	-0.952446000	0.922583000	-4.832272000
1	0.251180000	-0.387209000	-4.873714000
6	0.811508000	5.460138000	-0.400277000
1	0.181752000	5.772894000	-1.237440000
1	0.424897000	5.913646000	0.516269000

1	1.828229000	5.824507000	-0.570415000
6	0.602095000	0.838844000	4.500874000
1	-0.143094000	1.537042000	4.889020000
1	0.282000000	-0.182153000	4.722210000
1	1.558657000	1.029458000	4.992889000
6	1.066740000	-2.150994000	0.167011000
6	2.230990000	-2.088772000	0.941701000
6	0.854475000	-3.303024000	-0.603414000
6	3.151448000	-3.131144000	0.940386000
1	2.394358000	-1.218777000	1.568367000
6	1.776672000	-4.339776000	-0.604683000
1	-0.059021000	-3.362412000	-1.183601000
6	2.936599000	-4.264033000	0.162268000
1	4.034597000	-3.065215000	1.570788000
1	1.587804000	-5.219291000	-1.213873000
1	3.654330000	-5.078098000	0.161182000
6	2.608915000	0.680742000	-0.318574000
7	3.737496000	0.463952000	-0.544106000
6	5.008942000	-0.103317000	-0.771993000
1	5.742645000	0.329954000	-0.088001000
1	4.954886000	-1.183758000	-0.609472000
1	5.328530000	0.091499000	-1.798498000
7	-1.965178000	-0.338870000	0.148763000
6	-3.358008000	-0.537491000	0.162640000
6	-4.240814000	0.548423000	0.241547000
6	-3.909552000	-1.828824000	0.091228000
6	-5.618638000	0.348429000	0.243322000
1	-3.856370000	1.557905000	0.306460000
6	-5.281335000	-2.012222000	0.094268000
1	-3.224427000	-2.665341000	0.041490000
6	-6.155174000	-0.928033000	0.168420000
1	-6.275022000	1.211748000	0.306515000
1	-5.676251000	-3.022803000	0.039064000
1	-7.229556000	-1.079695000	0.170157000
44	0.670524000	0.976086000	-0.024797000

5a, TE = -2482.282590

6	-0.699628000	-1.182477000	0.856066000
6	-1.282531000	1.254613000	0.473642000
6	1.158352000	0.710828000	0.874668000
7	0.012238000	1.596712000	0.603470000
7	-1.602208000	-0.045527000	0.600291000
6	0.284914000	2.988868000	0.497948000
6	1.357213000	3.567466000	1.183786000
6	-0.515280000	3.817601000	-0.297853000
6	1.620209000	4.929011000	1.072306000

1	1.974665000	2.955828000	1.829720000
6	-0.245965000	5.172982000	-0.405043000
1	-1.365417000	3.368631000	-0.795867000
6	0.826948000	5.743351000	0.275776000
1	2.451695000	5.354022000	1.626497000
1	-0.882705000	5.792163000	-1.030175000
1	1.035663000	6.804518000	0.189467000
6	-2.990763000	-0.340160000	0.501964000
6	-3.545846000	-1.432197000	1.176747000
6	-3.839954000	0.456535000	-0.275850000
6	-4.902932000	-1.719315000	1.068968000
1	-2.919569000	-2.048968000	1.809840000
6	-5.190476000	0.162528000	-0.379699000
1	-3.411257000	1.322908000	-0.763314000
6	-5.736483000	-0.931091000	0.287746000
1	-5.308692000	-2.566548000	1.613715000
1	-5.825669000	0.796896000	-0.990983000
1	-6.794024000	-1.158528000	0.204405000
1	1.221914000	0.550725000	1.958329000
1	2.052925000	1.265413000	0.584656000
1	-1.237354000	-2.078001000	0.539407000
1	-0.550281000	-1.269646000	1.939269000
26	1.126926000	-1.105373000	-0.085181000
6	0.299972000	-0.291345000	-1.519274000
7	-0.235257000	0.226687000	-2.419055000
6	0.841762000	-2.767014000	-0.814152000
7	0.609569000	-3.825406000	-1.262976000
6	1.830603000	-1.804953000	1.459468000
7	2.248787000	-2.210735000	2.475216000
6	2.785848000	-0.778277000	-0.800829000
7	3.840131000	-0.514349000	-1.241665000
6	0.250874000	-5.074996000	-1.803654000
1	0.737231000	-5.223528000	-2.771573000
1	0.558096000	-5.879967000	-1.130674000
1	-0.832387000	-5.128234000	-1.942450000
6	-1.019758000	0.981455000	-3.314684000
1	-0.767909000	0.726106000	-4.346858000
1	-2.078468000	0.772388000	-3.141093000
1	-0.837151000	2.046785000	-3.153396000
6	5.077432000	-0.118333000	-1.784311000
1	5.895116000	-0.431787000	-1.129987000
1	5.222854000	-0.573351000	-2.767944000
1	5.111095000	0.969345000	-1.891386000
6	2.729436000	-2.659011000	3.720576000
1	3.800756000	-2.458663000	3.806405000
1	2.208926000	-2.142522000	4.531061000

1 2.563359000 -3.734373000 3.824789000

5b, TE = -5629.776614

6 0.163092000 -1.366436000 0.909992000
6 -1.938112000 0.000033000 0.477161000
6 0.163149000 1.366423000 0.909984000
7 -1.268982000 1.158697000 0.619145000
7 -1.269030000 -1.158658000 0.619137000
6 -2.070067000 2.330447000 0.508434000
6 -1.742573000 3.494860000 1.209992000
6 -3.207053000 2.349041000 -0.308286000
6 -2.523787000 4.639872000 1.091802000
1 -0.885996000 3.501046000 1.872943000
6 -3.979231000 3.494462000 -0.422486000
1 -3.477513000 1.431819000 -0.816087000
6 -3.644321000 4.653888000 0.272734000
1 -2.252418000 5.526145000 1.657863000
1 -4.855523000 3.481555000 -1.064285000
1 -4.250818000 5.548885000 0.180423000
6 -2.070162000 -2.330376000 0.508422000
6 -1.742730000 -3.494802000 1.209985000
6 -3.207148000 -2.348916000 -0.308300000
6 -2.523993000 -4.639779000 1.091788000
1 -0.886157000 -3.501031000 1.872941000
6 -3.979378000 -3.494301000 -0.422506000
1 -3.477570000 -1.431678000 -0.816094000
6 -3.644521000 -4.653745000 0.272711000
1 -2.252667000 -5.526065000 1.657849000
1 -4.855670000 -3.481353000 -1.064306000
1 -4.251058000 -5.548714000 0.180395000
1 0.309202000 1.312312000 1.995905000
1 0.395667000 2.389849000 0.611905000
1 0.395583000 -2.389873000 0.611927000
1 0.309131000 -1.312313000 1.995914000
6 0.279239000 0.000003000 -1.610291000
7 -0.478845000 0.000090000 -2.497270000
6 2.547245000 -1.482680000 -0.842363000
7 3.113034000 -2.414254000 -1.277037000
6 2.541053000 -0.000052000 1.586560000
7 3.098449000 -0.000048000 2.615390000
6 2.547362000 1.482513000 -0.842388000
7 3.113204000 2.414044000 -1.277086000
6 3.744296000 -3.553597000 -1.810561000
1 4.213029000 -3.313970000 -2.768925000
1 4.515257000 -3.913710000 -1.124308000
1 3.013348000 -4.351636000 -1.966058000

6	-1.565497000	0.000225000	-3.395211000
1	-1.203715000	0.000043000	-4.426048000
1	-2.177397000	-0.889463000	-3.227801000
1	-2.177024000	0.890203000	-3.227984000
6	3.744625000	3.553370000	-1.810465000
1	4.529949000	3.900760000	-1.134011000
1	4.195216000	3.319093000	-2.778796000
1	3.017700000	4.358665000	-1.946174000
6	3.743108000	-0.000047000	3.867437000
1	4.373403000	0.887343000	3.966273000
1	3.001073000	0.003197000	4.669608000
1	4.368392000	-0.890688000	3.968853000
44	1.509187000	-0.000044000	-0.076426000

6a, TE = -2630.305071

6	1.172117000	0.670668000	0.578163000
7	0.080273000	1.597928000	0.275151000
6	-1.231371000	1.318946000	0.148526000
7	-1.656270000	0.034411000	0.185715000
6	-0.895475000	-1.204226000	0.171687000
8	2.106983000	1.138120000	1.193638000
6	0.398483000	3.000846000	0.292476000
6	1.488957000	3.473750000	-0.432890000
6	1.777025000	4.832148000	-0.453492000
6	0.981322000	5.730270000	0.249874000
6	-0.105941000	5.254966000	0.974349000
6	-0.396870000	3.896560000	0.997886000
1	2.116067000	2.774543000	-0.974886000
1	2.628321000	5.190614000	-1.024198000
1	1.207559000	6.791600000	0.233029000
1	-0.734822000	5.945448000	1.527843000
1	-1.254571000	3.512842000	1.537417000
6	-3.093095000	-0.088508000	0.141559000
6	-3.796710000	0.488229000	-0.908873000
6	-5.182043000	0.397687000	-0.956638000
6	-5.873548000	-0.272355000	0.046552000
6	-5.167448000	-0.846189000	1.097946000
6	-3.781529000	-0.757633000	1.147425000
1	-3.245454000	1.035008000	-1.665838000
1	-5.722899000	0.858066000	-1.777731000
1	-6.956123000	-0.342170000	0.012221000
1	-5.698514000	-1.365654000	1.889615000
1	-3.230836000	-1.207692000	1.963940000
8	-1.537142000	-2.229773000	0.281587000
26	1.056256000	-1.160996000	-0.114077000
6	0.894173000	-2.916395000	-0.745686000

6	1.180478000	-1.683571000	1.651121000
6	2.907935000	-1.084628000	-0.326151000
6	0.696917000	-0.420464000	-1.763462000
7	4.066772000	-0.982356000	-0.419850000
7	0.734145000	-4.007794000	-1.125211000
7	1.230452000	-1.968502000	2.780861000
7	0.427536000	0.097182000	-2.774927000
6	-0.016073000	0.836431000	-3.890962000
1	-0.895805000	0.357935000	-4.327771000
1	-0.279801000	1.848960000	-3.575585000
1	0.771885000	0.888626000	-4.645843000
6	5.443697000	-0.681352000	-0.395034000
1	5.805776000	-0.493449000	-1.408433000
1	5.609307000	0.208813000	0.216585000
1	6.003351000	-1.518187000	0.029187000
6	1.237588000	-2.202061000	4.169903000
1	0.246559000	-2.525119000	4.497180000
1	1.964061000	-2.979707000	4.417073000
1	1.505880000	-1.283004000	4.696213000
6	0.276950000	-5.291565000	-1.487761000
1	0.877015000	-6.058036000	-0.992162000
1	-0.767732000	-5.399007000	-1.186106000
1	0.355793000	-5.426711000	-2.568823000

6b, TE = -5777.794210

6	0.453943000	1.277079000	0.647254000
7	-0.974384000	1.392753000	0.328710000
6	-1.886737000	0.410793000	0.191068000
7	-1.522133000	-0.894048000	0.230814000
6	-0.204981000	-1.515449000	0.217165000
8	0.927506000	2.182931000	1.299282000
6	-1.525838000	2.721604000	0.337258000
6	-0.896636000	3.736364000	-0.379472000
6	-1.444629000	5.012025000	-0.411208000
6	-2.624331000	5.287330000	0.271973000
6	-3.249728000	4.272543000	0.987649000
6	-2.703993000	2.995389000	1.022707000
1	0.027269000	3.526427000	-0.907004000
1	-0.946958000	5.795012000	-0.975268000
1	-3.051976000	6.284483000	0.246503000
1	-4.170677000	4.474418000	1.525903000
1	-3.191735000	2.187515000	1.555028000
6	-2.652239000	-1.790501000	0.185511000
6	-3.555849000	-1.698577000	-0.866411000
6	-4.659014000	-2.540905000	-0.917696000
6	-4.865777000	-3.483704000	0.083318000

6	-3.962328000	-3.571401000	1.136406000
6	-2.857668000	-2.729814000	1.189936000
1	-3.398163000	-0.936424000	-1.621502000
1	-5.362604000	-2.455686000	-1.740126000
1	-5.728301000	-4.141472000	0.046142000
1	-4.118266000	-4.298883000	1.927012000
1	-2.152430000	-2.800644000	2.008347000
8	-0.174626000	-2.722344000	0.350389000
6	2.344761000	-2.004823000	-0.837535000
6	1.988630000	-0.742810000	1.733012000
6	3.038408000	0.880644000	-0.373276000
6	0.678732000	0.113255000	-1.869199000
7	3.893748000	1.671068000	-0.458164000
7	2.749832000	-3.031375000	-1.216916000
7	2.236941000	-0.953807000	2.851787000
7	0.127837000	0.403032000	-2.855966000
6	-0.678857000	0.778526000	-3.950142000
1	-1.202131000	-0.097048000	-4.341206000
1	-1.413846000	1.518013000	-3.623268000
1	-0.061511000	1.208523000	-4.742125000
6	4.819094000	2.734270000	-0.448141000
1	4.973199000	3.106169000	-1.463731000
1	4.436502000	3.545085000	0.176469000
1	5.777189000	2.394219000	-0.048190000
6	2.446715000	-1.157070000	4.229982000
1	1.866774000	-2.018242000	4.569555000
1	3.505724000	-1.341094000	4.424804000
1	2.129661000	-0.270579000	4.784022000
6	3.017813000	-4.365656000	-1.585812000
1	3.931884000	-4.713144000	-1.099034000
1	2.181813000	-4.998790000	-1.278963000
1	3.145657000	-4.436506000	-2.668329000
44	1.479546000	-0.341911000	-0.129098000

Cartesian coordinates for the triplet state optimized geometries of **1a-6b**, along with their total energies (in hartrees) including zero point vibrational correction in gas phase.

1a, TE = -1869.391080

6	2.053051000	0.915858000	-0.000039000
6	1.178788000	-1.207588000	0.000336000
1	1.412318000	-2.270051000	0.000442000
7	2.307517000	-0.390116000	0.000232000
7	0.889878000	1.434246000	-0.000208000
6	3.668792000	-0.897929000	0.000339000
1	3.838562000	-1.508191000	0.891229000

1	3.838697000	-1.508254000	-0.890484000
1	4.367420000	-0.060871000	0.000365000
6	0.643687000	2.859925000	-0.000469000
1	0.064067000	3.140850000	-0.884994000
1	0.063714000	3.141107000	0.883740000
1	1.579825000	3.423937000	-0.000363000
25	-0.543576000	-0.127299000	-0.000005000
6	-0.363900000	-0.226310000	-1.837776000
8	-0.194057000	-0.335568000	-2.959369000
6	-1.566741000	-1.603137000	0.000254000
8	-2.190056000	-2.563592000	0.000411000
6	-1.971042000	1.004960000	-0.000396000
8	-2.874876000	1.707506000	-0.000608000
6	-0.364218000	-0.225459000	1.837846000
8	-0.194442000	-0.334205000	2.959498000

1b, TE = -2003.161346

6	-0.244170000	2.312274000	0.109847000
6	-1.229116000	0.213434000	0.190267000
7	-1.376120000	1.626915000	0.157010000
7	0.923597000	1.811141000	0.037425000
25	0.773491000	-0.300176000	-0.001195000
6	0.699552000	-0.314044000	1.846505000
8	0.578951000	-0.315225000	2.980624000
6	0.562311000	-2.082031000	-0.073778000
8	0.472250000	-3.223774000	-0.136659000
6	2.575161000	-0.489504000	-0.151108000
8	3.708608000	-0.617631000	-0.252065000
6	0.422152000	-0.147197000	-1.803256000
8	0.148585000	-0.027736000	-2.905354000
6	2.130699000	2.603096000	-0.059677000
6	-2.653193000	2.306190000	0.326420000
7	-2.450791000	-0.460991000	0.104495000
6	-2.935906000	-0.728251000	-1.242420000
1	-3.992045000	-1.014861000	-1.205193000
1	-2.843886000	0.167508000	-1.860721000
1	-2.375179000	-1.540030000	-1.734419000
6	-2.591577000	-1.608226000	0.979839000
1	-3.646314000	-1.898819000	1.024999000
1	-2.015391000	-2.482934000	0.640912000
1	-2.266618000	-1.346042000	1.988020000
1	1.904850000	3.671703000	-0.021332000
1	2.808905000	2.357847000	0.762875000
1	2.650405000	2.387986000	-0.998775000
1	-3.145805000	1.948670000	1.232204000
1	-2.464631000	3.377327000	0.404683000

1 -3.310981000 2.117050000 -0.524094000

1c, TE = -1983.789662

6 -0.913970000 -2.126804000 -0.011762000
6 -1.407142000 0.114775000 0.276675000
7 -1.863606000 -1.215608000 0.113706000
7 0.332277000 -1.888365000 -0.137724000
25 0.650681000 0.201849000 -0.025880000
6 0.079090000 0.371595000 -1.770169000
8 -0.358317000 0.486666000 -2.817620000
6 0.884125000 1.975549000 0.141314000
8 1.092567000 3.096939000 0.261857000
6 2.417023000 -0.002890000 -0.406867000
8 3.522800000 -0.120117000 -0.678122000
6 0.802743000 0.002234000 1.812932000
8 0.837438000 -0.112976000 2.945347000
6 1.344246000 -2.921190000 -0.066523000
6 -3.274381000 -1.573012000 0.069526000
8 -2.435128000 0.949171000 -0.038379000
6 -2.273040000 2.304832000 0.317948000
1 -1.936989000 2.401587000 1.355582000
1 -1.558669000 2.803156000 -0.344548000
1 -3.250850000 2.774112000 0.203833000
1 -3.750437000 -1.136387000 -0.809813000
1 -3.352607000 -2.659359000 0.030908000
1 -3.778224000 -1.200009000 0.963469000
1 0.894624000 -3.915976000 -0.117861000
1 2.046576000 -2.811280000 -0.896882000
1 1.911798000 -2.842262000 0.867350000

1'a, TE = -2252.401539

6 -0.651682000 0.940183000 0.064456000
6 -1.162991000 -1.302120000 0.087508000
1 -1.956886000 -2.027513000 0.243057000
7 -1.615974000 0.018523000 0.081648000
7 0.605887000 0.700595000 0.098125000
25 0.856537000 -1.430883000 0.000693000
6 0.771797000 -1.482705000 1.849829000
8 0.652687000 -1.519534000 2.981720000
6 0.762587000 -3.220150000 -0.076875000
8 0.660191000 -4.359107000 -0.122529000
6 2.681083000 -1.447014000 -0.113995000
8 3.818154000 -1.525558000 -0.202965000
6 0.608385000 -1.311831000 -1.832230000
8 0.390664000 -1.249760000 -2.947789000
6 1.558668000 1.736975000 0.012428000

6	2.750336000	1.640227000	0.729785000
6	1.326250000	2.864518000	-0.781052000
6	3.693660000	2.656289000	0.654931000
1	2.924049000	0.775536000	1.359479000
6	2.272234000	3.877291000	-0.846486000
1	0.405554000	2.931517000	-1.352029000
6	3.461631000	3.778702000	-0.131912000
1	4.615199000	2.569377000	1.221143000
1	2.081308000	4.745748000	-1.468756000
1	4.202398000	4.568750000	-0.190460000
6	-2.982993000	0.420873000	0.084714000
6	-3.935878000	-0.366895000	-0.553847000
6	-3.358509000	1.597714000	0.728579000
6	-5.267197000	0.028927000	-0.545008000
1	-3.631071000	-1.269670000	-1.070869000
6	-4.689590000	1.990444000	0.718013000
1	-2.609864000	2.191752000	1.242662000
6	-5.649476000	1.206901000	0.086224000
1	-6.007861000	-0.584930000	-1.046618000
1	-4.978880000	2.907342000	1.220591000
1	-6.690233000	1.512028000	0.088223000

1'b, TE = -2386.170878

6	-0.188084000	1.258186000	-0.017920000
6	-1.117157000	-0.879078000	-0.151597000
7	-1.299717000	0.540760000	-0.089838000
7	1.003306000	0.788217000	-0.015840000
25	0.869359000	-1.335924000	0.230884000
6	0.383661000	-1.078809000	2.004675000
8	0.016923000	-0.948504000	3.074777000
6	0.678078000	-3.109427000	0.419965000
8	0.607711000	-4.245280000	0.558213000
6	2.649323000	-1.529482000	0.584813000
8	3.752033000	-1.710403000	0.826550000
6	0.955067000	-1.498786000	-1.601251000
8	0.941265000	-1.602181000	-2.738167000
6	2.124423000	1.640110000	-0.093624000
6	3.255689000	1.241505000	-0.805131000
6	2.117840000	2.890470000	0.533821000
6	4.358840000	2.080842000	-0.890158000
1	3.260292000	0.281460000	-1.307754000
6	3.222500000	3.724179000	0.439619000
1	1.244326000	3.191883000	1.102944000
6	4.350348000	3.324900000	-0.270225000
1	5.229866000	1.757976000	-1.451096000
1	3.204271000	4.690220000	0.934112000

1	5.215215000	3.976058000	-0.336338000
6	-2.554223000	1.211525000	0.057163000
6	-2.755171000	2.435175000	-0.576847000
6	-3.556967000	0.654585000	0.847204000
6	-3.954847000	3.113523000	-0.401726000
1	-1.971921000	2.847446000	-1.204985000
6	-4.757160000	1.334589000	1.002680000
1	-3.386889000	-0.296001000	1.336452000
6	-4.961329000	2.563906000	0.383571000
1	-4.104559000	4.069800000	-0.891894000
1	-5.536159000	0.903161000	1.622751000
1	-5.901696000	3.089342000	0.511419000
7	-2.199578000	-1.533422000	-0.709666000
6	-2.642031000	-1.182554000	-2.052518000
1	-3.695542000	-1.452169000	-2.175028000
1	-2.547663000	-0.109105000	-2.217779000
1	-2.055557000	-1.706581000	-2.822854000
6	-2.360386000	-2.934835000	-0.406697000
1	-3.399741000	-3.226241000	-0.589688000
1	-1.716959000	-3.581066000	-1.024707000
1	-2.133270000	-3.119176000	0.643877000

1'c, TE = -2366.797362

6	0.379891000	1.191550000	-0.048628000
6	1.190017000	-0.985141000	-0.008230000
7	1.451418000	0.411168000	-0.041107000
7	-0.836650000	0.802415000	-0.141030000
25	-0.845301000	-1.333390000	0.077902000
6	-0.680974000	-1.494208000	-1.752185000
8	-0.507449000	-1.588504000	-2.874501000
6	-0.752616000	-3.109630000	0.317578000
8	-0.740524000	-4.241966000	0.494591000
6	-2.666609000	-1.457642000	0.134735000
8	-3.799289000	-1.604031000	0.173314000
6	-0.661068000	-1.067453000	1.910209000
8	-0.494315000	-0.921437000	3.025923000
6	-1.916738000	1.708125000	-0.085225000
6	-3.030997000	1.497999000	-0.897021000
6	-1.889397000	2.815710000	0.767285000
6	-4.101919000	2.380254000	-0.854178000
1	-3.044516000	0.651474000	-1.574102000
6	-2.961898000	3.695740000	0.799851000
1	-1.025890000	2.973121000	1.405720000
6	-4.074970000	3.482050000	-0.006535000
1	-4.961261000	2.206233000	-1.493471000
1	-2.929403000	4.550697000	1.467655000

1	-4.914274000	4.168245000	0.026374000
6	2.754062000	1.000846000	-0.031463000
6	3.740671000	0.488514000	0.805078000
6	3.015203000	2.100092000	-0.842135000
6	4.992229000	1.086629000	0.827579000
1	3.519623000	-0.367017000	1.432318000
6	4.267125000	2.701684000	-0.800156000
1	2.241931000	2.473071000	-1.505706000
6	5.259645000	2.195234000	0.029898000
1	5.762276000	0.688262000	1.479964000
1	4.468204000	3.561503000	-1.430445000
1	6.239629000	2.659702000	0.053817000
8	2.222023000	-1.624020000	-0.616585000
6	2.304896000	-3.019918000	-0.429965000
1	2.232037000	-3.283777000	0.630519000
1	1.520369000	-3.540638000	-0.988352000
1	3.277526000	-3.324143000	-0.817780000

2a, TE = -1908.046290

6	-2.522565000	-0.940945000	0.006475000
6	-1.593759000	1.166813000	-0.001386000
1	-1.821037000	2.232820000	-0.006955000
7	-2.742386000	0.372864000	0.001783000
7	-1.373732000	-1.490284000	0.007465000
6	-4.090403000	0.907247000	-0.001542000
1	-4.249384000	1.528360000	0.884952000
1	-4.249759000	1.517210000	-0.895705000
1	-4.808400000	0.086077000	0.003793000
6	-1.166673000	-2.916975000	0.017001000
1	-0.588278000	-3.219216000	-0.862518000
1	-0.596476000	-3.208897000	0.905461000
1	-2.115723000	-3.461306000	0.015856000
25	0.102757000	0.051731000	0.000616000
6	-0.016863000	0.182642000	-1.826115000
8	-0.121669000	0.341156000	-2.956595000
6	-0.011939000	0.193481000	1.826931000
8	-0.113480000	0.358668000	2.956737000
6	1.199668000	1.526373000	-0.005142000
7	1.870595000	2.491503000	-0.008784000
6	1.518974000	-1.166067000	0.002033000
7	2.409292000	-1.933968000	0.002261000
6	2.635948000	3.671068000	-0.013280000
1	3.703615000	3.433409000	-0.020081000
1	2.406696000	4.268912000	-0.899933000
1	2.417863000	4.268426000	0.876506000
6	3.500383000	-2.821338000	0.002195000

1	3.159185000	-3.843348000	0.189905000
1	4.010490000	-2.796610000	-0.964918000
1	4.215173000	-2.544649000	0.782396000

2b, TE = -2041.816013

6	-0.801016000	-2.563021000	0.016691000
6	-1.551420000	-0.369048000	0.062872000
7	-1.852784000	-1.754907000	0.024847000
7	0.416894000	-2.189897000	0.020830000
25	0.485423000	-0.059660000	0.013669000
6	0.270523000	-0.070044000	-1.805877000
8	0.073587000	-0.054482000	-2.936265000
6	0.334042000	-0.029608000	1.841337000
8	0.169935000	0.016526000	2.975783000
6	0.442548000	1.777364000	-0.012242000
7	0.456556000	2.954336000	-0.037950000
6	2.351460000	-0.061074000	-0.019405000
7	3.526642000	-0.054886000	-0.039796000
6	0.280983000	4.349813000	-0.051909000
1	0.898448000	4.819174000	0.718972000
1	0.568699000	4.759419000	-1.024171000
1	-0.766891000	4.604164000	0.137869000
6	4.932764000	-0.027209000	-0.058699000
1	5.334584000	-1.026981000	0.128793000
1	5.293305000	0.316440000	-1.032304000
1	5.309598000	0.649592000	0.713309000
6	1.531555000	-3.104528000	0.019507000
6	-3.203560000	-2.292604000	0.031128000
7	-2.706014000	0.443459000	0.038803000
6	-2.928057000	1.125499000	-1.225428000
1	-2.905947000	0.406039000	-2.047115000
1	-3.912130000	1.607808000	-1.217209000
1	-2.165021000	1.896206000	-1.430201000
6	-2.815796000	1.347187000	1.168880000
1	-3.797265000	1.834322000	1.154347000
1	-2.723332000	0.788549000	2.102503000
1	-2.040274000	2.132483000	1.164939000
1	-3.139761000	-3.381464000	0.046150000
1	-3.746962000	-1.942735000	0.911069000
1	-3.750543000	-1.972014000	-0.858398000
1	2.157030000	-2.939099000	0.903322000
1	1.194598000	-4.145375000	0.020031000
1	2.155684000	-2.939280000	-0.865393000

2c, TE = -2022.444931

6	-1.643357000	-2.134260000	0.088700000
6	-1.769602000	0.179727000	0.161012000
7	-2.430304000	-1.069592000	0.069437000
7	-0.368497000	-2.115566000	0.050624000
25	0.285647000	-0.086930000	0.034645000
6	-0.071717000	0.079063000	-1.754057000
8	-0.365533000	0.237975000	-2.851188000
6	0.315709000	-0.110295000	1.874496000
8	0.298835000	-0.071608000	3.019104000
6	0.832116000	1.668692000	0.103350000
7	1.245983000	2.768644000	0.166863000
6	2.054330000	-0.638416000	-0.185919000
7	3.166919000	-0.978789000	-0.349817000
6	1.611903000	4.122998000	0.262916000
1	2.009510000	4.338926000	1.258555000
1	2.379153000	4.364351000	-0.478038000
1	0.744418000	4.767125000	0.087439000
6	4.498589000	-1.382240000	-0.556721000
1	4.594454000	-2.461784000	-0.410400000
1	4.815677000	-1.138563000	-1.574534000
1	5.162765000	-0.875115000	0.148632000
6	0.440047000	-3.283606000	0.302594000
6	-3.872517000	-1.201409000	-0.059311000
8	-2.636910000	1.130686000	-0.316029000
6	-2.268848000	2.465391000	-0.078394000
1	-2.006654000	2.620551000	0.975119000
1	-1.419462000	2.758105000	-0.705465000
1	-3.133991000	3.079572000	-0.335781000
1	-4.126942000	-2.260805000	-0.018925000
1	-4.368029000	-0.673712000	0.759096000
1	-4.213652000	-0.775780000	-1.004831000
1	0.954802000	-3.196370000	1.267111000
1	-0.166974000	-4.193680000	0.313405000
1	1.204005000	-3.382752000	-0.474368000

2'a, TE = -2291.059487

6	-1.051941000	-1.118033000	0.050398000
6	-1.277317000	1.177408000	0.093400000
1	-1.990486000	1.990820000	-0.026673000
7	-1.892069000	-0.078301000	0.041636000
7	0.225419000	-1.035795000	0.112317000
25	0.735672000	1.063205000	-0.001015000
6	0.458329000	1.062957000	-1.816478000
8	0.234278000	1.120437000	-2.938104000
6	0.750976000	1.188718000	1.834691000

8	0.710809000	1.326957000	2.970658000
6	0.915001000	2.891257000	-0.074428000
7	0.990189000	4.062185000	-0.118498000
6	2.574729000	0.754273000	-0.191535000
7	3.723355000	0.573713000	-0.351286000
6	1.065148000	5.466181000	-0.169054000
1	2.108913000	5.791954000	-0.151780000
1	0.598260000	5.836870000	-1.085622000
1	0.548052000	5.903986000	0.689124000
6	5.057782000	0.172659000	-0.551477000
1	5.141142000	-0.910956000	-0.426267000
1	5.384630000	0.437130000	-1.560569000
1	5.714520000	0.665585000	0.170112000
6	1.041632000	-2.176771000	0.146787000
6	2.191591000	-2.179949000	0.940172000
6	0.730541000	-3.320133000	-0.597970000
6	3.006580000	-3.302911000	0.988338000
1	2.421022000	-1.302290000	1.532883000
6	1.550764000	-4.438083000	-0.544857000
1	-0.154361000	-3.315341000	-1.226268000
6	2.695404000	-4.437817000	0.245721000
1	3.886352000	-3.295746000	1.624941000
1	1.295025000	-5.315295000	-1.131082000
1	3.334928000	-5.313140000	0.285797000
6	-3.294861000	-0.312020000	0.036290000
6	-4.150008000	0.584183000	0.672602000
6	-3.815719000	-1.431673000	-0.610570000
6	-5.520130000	0.355644000	0.658635000
1	-3.738464000	1.440586000	1.194002000
6	-5.184816000	-1.656515000	-0.608131000
1	-3.144641000	-2.114657000	-1.120743000
6	-6.044947000	-0.762705000	0.021945000
1	-6.180396000	1.055310000	1.160789000
1	-5.582152000	-2.530038000	-1.114653000
1	-7.115540000	-0.936676000	0.014911000

2'b, TE = -2424.827370

6	-0.652052000	-1.454029000	0.028129000
6	-1.246342000	0.807479000	0.077199000
7	-1.639384000	-0.564681000	0.006639000
7	0.596918000	-1.188181000	0.136540000
25	0.817721000	0.955004000	0.065690000
6	0.562644000	0.926181000	-1.747376000
8	0.355727000	0.942429000	-2.875719000
6	0.754911000	1.061379000	1.901847000
8	0.659363000	1.180764000	3.037325000

6	0.965220000	2.787117000	0.001156000
7	1.135709000	3.949956000	-0.037953000
6	2.675119000	0.810042000	-0.090108000
7	3.836780000	0.739050000	-0.240832000
6	1.173923000	5.355497000	-0.071440000
1	1.650132000	5.743757000	0.832988000
1	1.742298000	5.699734000	-0.939703000
1	0.159309000	5.762181000	-0.134498000
6	5.199347000	0.434868000	-0.423365000
1	5.357171000	-0.639367000	-0.288529000
1	5.517769000	0.715336000	-1.430822000
1	5.810219000	0.979132000	0.301606000
6	1.574192000	-2.195644000	0.114659000
6	2.669983000	-2.114044000	0.978096000
6	1.475631000	-3.291039000	-0.750045000
6	3.641864000	-3.105689000	0.973848000
1	2.734433000	-1.278125000	1.665148000
6	2.451099000	-4.278508000	-0.748323000
1	0.629794000	-3.352558000	-1.427245000
6	3.542387000	-4.192496000	0.110038000
1	4.476326000	-3.037105000	1.665594000
1	2.358603000	-5.120688000	-1.427171000
1	4.302568000	-4.966457000	0.110657000
6	-2.973445000	-1.069322000	0.107925000
6	-3.859343000	-0.537104000	1.042829000
6	-3.374541000	-2.114418000	-0.720768000
6	-5.142205000	-1.059104000	1.140874000
1	-3.533748000	0.270883000	1.684889000
6	-4.655732000	-2.638999000	-0.604328000
1	-2.678697000	-2.508314000	-1.454393000
6	-5.546279000	-2.109459000	0.322292000
1	-5.829337000	-0.647144000	1.873079000
1	-4.959419000	-3.457864000	-1.248319000
1	-6.550046000	-2.512365000	0.407003000
7	-2.305526000	1.674533000	-0.183962000
6	-2.907717000	1.670186000	-1.508094000
1	-3.027497000	0.648363000	-1.870436000
1	-3.900838000	2.129917000	-1.462809000
1	-2.297992000	2.227678000	-2.237914000
6	-2.212890000	2.998621000	0.378755000
1	-3.219058000	3.419190000	0.492522000
1	-1.741879000	2.950644000	1.361513000
1	-1.629989000	3.688675000	-0.254078000

2'c, TE = -2405.455495

6	-0.869120000	-1.332223000	0.046936000
6	-1.263854000	0.954065000	0.190455000
7	-1.773414000	-0.356898000	0.056445000
7	0.405040000	-1.165252000	0.115785000
25	0.789799000	0.954713000	0.007878000
6	0.341725000	1.018153000	-1.770192000
8	-0.003380000	1.117069000	-2.858096000
6	0.929759000	1.030082000	1.843160000
8	0.970872000	1.140548000	2.981904000
6	1.122165000	2.764837000	-0.023465000
7	1.410295000	3.904333000	-0.035355000
6	2.596468000	0.628051000	-0.355603000
7	3.714821000	0.429649000	-0.648222000
6	1.700924000	5.280589000	-0.034684000
1	2.201264000	5.561083000	0.896177000
1	2.356631000	5.530543000	-0.873215000
1	0.780365000	5.865095000	-0.125833000
6	4.998230000	-0.050902000	-0.974513000
1	5.058137000	-1.118106000	-0.741312000
1	5.194782000	0.091231000	-2.040269000
1	5.760428000	0.484074000	-0.402326000
6	1.281095000	-2.255182000	0.194779000
6	2.441120000	-2.168234000	0.971138000
6	1.017654000	-3.450707000	-0.487070000
6	3.312983000	-3.245600000	1.056508000
1	2.633791000	-1.258453000	1.527118000
6	1.893099000	-4.522738000	-0.394548000
1	0.122693000	-3.521269000	-1.096896000
6	3.050008000	-4.428959000	0.372954000
1	4.198260000	-3.164632000	1.680472000
1	1.670628000	-5.439359000	-0.932264000
1	3.732530000	-5.269116000	0.443789000
6	-3.159135000	-0.709725000	0.016511000
6	-4.041835000	-0.182170000	0.954305000
6	-3.609956000	-1.602954000	-0.949160000
6	-5.377174000	-0.556991000	0.921602000
1	-3.674471000	0.510660000	1.701557000
6	-4.946654000	-1.983049000	-0.965918000
1	-2.912513000	-1.987914000	-1.685494000
6	-5.834720000	-1.458911000	-0.034707000
1	-6.064603000	-0.147334000	1.654625000
1	-5.294665000	-2.682662000	-1.718806000
1	-6.879834000	-1.749511000	-0.053908000
8	-2.251916000	1.829666000	-0.147617000
6	-2.030059000	3.179585000	0.180754000

1	-1.682677000	3.283763000	1.214944000
1	-1.295311000	3.632897000	-0.492195000
1	-2.988544000	3.687990000	0.061333000

3a, TE = -1946.692359

6	-2.431975000	0.195423000	-1.088298000
6	-1.583128000	0.118049000	1.061640000
1	-1.875291000	0.119465000	2.114590000
7	-2.697592000	0.203899000	0.220124000
7	-1.268904000	0.112878000	-1.597074000
6	-4.062686000	0.290958000	0.694292000
1	-4.312130000	-0.591178000	1.293688000
1	-4.190530000	1.182848000	1.316933000
1	-4.744418000	0.348857000	-0.156100000
6	-0.999159000	0.123477000	-3.009992000
1	-0.353210000	0.971511000	-3.264179000
1	-0.466229000	-0.789355000	-3.298405000
1	-1.919546000	0.194040000	-3.599341000
25	0.155552000	-0.011087000	0.011519000
6	0.197041000	1.861457000	0.078544000
7	0.199186000	3.037349000	0.147762000
6	1.165818000	-0.097937000	1.515200000
7	1.820662000	-0.154679000	2.501345000
6	1.616160000	-0.125115000	-1.118807000
7	2.548750000	-0.199153000	-1.841414000
6	-0.104039000	-1.866590000	0.061595000
7	-0.293431000	-3.027810000	0.119003000
6	2.263929000	-0.192905000	3.835348000
1	1.959933000	-1.127866000	4.318457000
1	3.355182000	-0.125751000	3.881637000
1	1.845444000	0.641497000	4.408898000
6	0.020445000	4.408896000	0.398964000
1	-0.725742000	4.560839000	1.185497000
1	0.962119000	4.864985000	0.718442000
1	-0.318871000	4.921161000	-0.506086000
6	3.759170000	-0.294330000	-2.546502000
1	4.481923000	0.439488000	-2.174314000
1	4.193974000	-1.293209000	-2.435252000
1	3.600160000	-0.107602000	-3.613215000
6	-0.696126000	-4.353868000	0.354701000
1	0.153449000	-4.958241000	0.686078000
1	-1.471290000	-4.387998000	1.127032000
1	-1.097123000	-4.798803000	-0.560660000

3b, TE = -2080.461749

6	0.975906000	0.781642000	-2.341795000
6	1.529472000	0.430364000	-0.100528000
7	1.932614000	0.807092000	-1.420785000
7	-0.224926000	0.412945000	-2.143070000
25	-0.497245000	-0.005175000	-0.053296000
6	0.001482000	-1.767080000	-0.411273000
7	0.317805000	-2.880406000	-0.645383000
6	-0.685866000	-0.391842000	1.707044000
7	-0.927114000	-0.655380000	2.841952000
6	-2.300795000	-0.327916000	-0.303899000
7	-3.452247000	-0.543538000	-0.449576000
6	-0.745294000	1.828260000	0.289456000
7	-0.865078000	2.976951000	0.513796000
6	-0.662427000	-0.932735000	4.198643000
1	0.416217000	-0.932746000	4.398433000
1	-1.132454000	-0.183088000	4.842992000
1	-1.064470000	-1.912263000	4.475794000
6	1.035356000	-4.075994000	-0.835988000
1	2.066546000	-3.965315000	-0.481356000
1	0.563943000	-4.896737000	-0.287960000
1	1.057946000	-4.341521000	-1.896950000
6	-4.824812000	-0.824623000	-0.537426000
1	-5.038314000	-1.827445000	-0.153629000
1	-5.404995000	-0.101719000	0.045172000
1	-5.161594000	-0.776333000	-1.577859000
6	-0.821762000	4.353094000	0.796481000
1	-1.414553000	4.578264000	1.687830000
1	0.209505000	4.675244000	0.971948000
1	-1.227920000	4.926878000	-0.041503000
6	3.194125000	1.470400000	-1.709485000
6	-1.164040000	0.153124000	-3.203428000
7	2.665255000	0.192150000	0.704321000
6	2.469185000	0.408589000	2.116543000
1	1.936015000	1.347643000	2.272975000
1	1.886145000	-0.400555000	2.590952000
1	3.441575000	0.464916000	2.620041000
6	3.369183000	-1.055219000	0.452649000
1	3.491660000	-1.205632000	-0.622542000
1	4.363552000	-1.030693000	0.914987000
1	2.822574000	-1.927069000	0.857668000
1	3.191193000	1.779565000	-2.755940000
1	3.314819000	2.347624000	-1.066664000
1	4.042796000	0.805260000	-1.534920000
1	-2.087018000	0.717449000	-3.035231000
1	-0.755013000	0.429277000	-4.180842000

1 -1.429465000 -0.910722000 -3.221750000

3c, TE = -2061.092781

6	1.311593000	1.631589000	-1.662560000
6	1.606709000	0.531727000	0.366545000
7	2.153294000	1.306630000	-0.689155000
7	0.118590000	1.202638000	-1.785445000
25	-0.336926000	-0.040302000	-0.088628000
6	0.503852000	-1.498700000	-0.899208000
7	1.082969000	-2.400034000	-1.387479000
6	-0.725829000	-1.008626000	1.388988000
7	-1.088111000	-1.649140000	2.325467000
6	-2.002482000	-0.447993000	-0.785886000
7	-3.059604000	-0.732084000	-1.226835000
6	-0.917401000	1.515780000	0.796184000
7	-1.247290000	2.487897000	1.370645000
6	-0.974397000	-2.237429000	3.603268000
1	0.076356000	-2.400634000	3.871590000
1	-1.427854000	-1.594435000	4.364978000
1	-1.489295000	-3.202190000	3.628581000
6	1.989878000	-3.356732000	-1.878030000
1	2.997473000	-3.154461000	-1.501926000
1	1.692487000	-4.361052000	-1.562890000
1	2.013152000	-3.332389000	-2.971360000
6	-4.324465000	-1.134266000	-1.684597000
1	-4.327889000	-2.203660000	-1.918820000
1	-5.087576000	-0.945266000	-0.922784000
1	-4.598822000	-0.583297000	-2.589681000
6	-1.441976000	3.647963000	2.141190000
1	-2.260213000	3.500709000	2.851998000
1	-0.532479000	3.891729000	2.698798000
1	-1.693586000	4.495197000	1.496889000
6	3.543902000	1.721192000	-0.738610000
6	-0.832881000	1.764906000	-2.708321000
8	2.670891000	-0.135960000	0.949900000
6	2.372811000	-0.778477000	2.158610000
1	1.700762000	-1.630508000	1.999716000
1	3.319798000	-1.134682000	2.571512000
1	1.900173000	-0.086705000	2.868548000
1	4.204609000	0.857201000	-0.839045000
1	3.677564000	2.386126000	-1.592872000
1	3.807871000	2.249755000	0.181801000
1	-0.347456000	2.422432000	-3.437076000
1	-1.347496000	0.963212000	-3.246870000
1	-1.596349000	2.341198000	-2.170422000

3'a, TE = -2329.709702

6	1.103897000	1.154243000	0.049719000
6	1.238961000	-1.149098000	0.201932000
1	1.936360000	-1.985194000	0.142582000
7	1.901371000	0.078266000	0.122227000
7	-0.179438000	1.127359000	0.067452000
25	-0.753298000	-0.983914000	-0.022648000
6	-0.378855000	-0.986172000	-1.863073000
7	-0.110523000	-0.996425000	-3.007516000
6	-0.952565000	-2.792918000	-0.028867000
7	-1.038370000	-3.970055000	-0.026265000
6	-2.554444000	-0.696750000	-0.364936000
7	-3.699503000	-0.564596000	-0.623911000
6	-0.947492000	-0.952847000	1.849353000
7	-1.039328000	-0.939349000	3.021327000
6	-1.164960000	-5.367419000	0.007798000
1	-0.704036000	-5.775017000	0.913349000
1	-2.219925000	-5.660320000	-0.002736000
1	-0.674449000	-5.820502000	-0.859624000
6	0.334959000	-1.029759000	-4.340401000
1	1.399527000	-1.279209000	-4.380727000
1	-0.222116000	-1.779813000	-4.909134000
1	0.186108000	-0.055460000	-4.814483000
6	-4.978913000	-0.100580000	-0.979901000
1	-5.228663000	-0.408965000	-1.999787000
1	-5.737350000	-0.507401000	-0.304415000
1	-5.013625000	0.992942000	-0.928843000
6	-0.989381000	-0.899402000	4.425831000
1	-1.703122000	-1.609347000	4.853261000
1	0.013945000	-1.155736000	4.779128000
1	-1.239990000	0.102888000	4.784883000
6	3.308249000	0.269430000	0.149359000
6	4.129246000	-0.670643000	0.770211000
6	3.879165000	1.392434000	-0.451250000
6	5.505897000	-0.482572000	0.788178000
1	3.684909000	-1.531920000	1.254800000
6	5.253774000	1.575489000	-0.419207000
1	3.237519000	2.113870000	-0.946166000
6	6.077358000	0.637653000	0.197068000
1	6.135167000	-1.218427000	1.278871000
1	5.685024000	2.453405000	-0.889646000
1	7.152682000	0.779333000	0.214353000
6	-0.938374000	2.299074000	0.090670000
6	-2.208421000	2.290629000	0.678568000
6	-0.463344000	3.502254000	-0.453678000
6	-2.974893000	3.447189000	0.718662000

1	-2.568701000	1.368921000	1.118211000
6	-1.236533000	4.652774000	-0.409223000
1	0.517187000	3.516414000	-0.918914000
6	-2.499923000	4.637069000	0.174638000
1	-3.952261000	3.420835000	1.192081000
1	-0.848752000	5.571332000	-0.839736000
1	-3.102876000	5.538364000	0.206997000

3'b, TE = -2463.476683

6	-0.715294000	-1.484957000	0.025242000
6	-1.245090000	0.796093000	0.097742000
7	-1.677432000	-0.561473000	0.037195000
7	0.545128000	-1.263955000	0.103392000
25	0.818189000	0.900685000	0.044660000
6	0.581368000	0.848660000	-1.812625000
7	0.428514000	0.812130000	-2.979161000
6	1.002229000	2.707946000	0.017807000
7	1.234658000	3.870022000	0.003677000
6	2.652859000	0.761457000	-0.163271000
7	3.817723000	0.732938000	-0.349464000
6	0.859275000	0.900766000	1.928937000
7	0.858039000	0.898798000	3.104504000
6	1.107260000	5.270691000	0.028616000
1	0.053394000	5.567469000	-0.034678000
1	1.525682000	5.678797000	0.954062000
1	1.643308000	5.720953000	-0.812355000
6	0.038593000	0.793591000	-4.329620000
1	-1.020119000	1.058455000	-4.424833000
1	0.630942000	1.508298000	-4.907859000
1	0.189436000	-0.202914000	-4.754325000
6	5.159935000	0.403646000	-0.610927000
1	5.451034000	0.744707000	-1.609092000
1	5.821397000	0.878299000	0.119931000
1	5.297832000	-0.681494000	-0.558698000
6	0.738157000	0.841697000	4.504315000
1	1.290936000	1.663582000	4.967978000
1	-0.312545000	0.915108000	4.800472000
1	1.140500000	-0.103257000	4.880513000
6	-3.017023000	-1.038414000	0.166505000
6	-3.896616000	-0.444030000	1.071678000
6	-3.440684000	-2.120008000	-0.604376000
6	-5.187840000	-0.939768000	1.197773000
1	-3.558067000	0.394729000	1.665115000
6	-4.729537000	-2.617322000	-0.459824000
1	-2.751218000	-2.565921000	-1.313981000
6	-5.611754000	-2.025327000	0.437470000

1	-5.867653000	-0.476780000	1.906347000
1	-5.046299000	-3.465441000	-1.058456000
1	-6.622168000	-2.406208000	0.543524000
6	1.477703000	-2.304600000	0.075231000
6	2.663443000	-2.193816000	0.809972000
6	1.256028000	-3.475547000	-0.663389000
6	3.598424000	-3.219746000	0.798488000
1	2.823378000	-1.300662000	1.401801000
6	2.195302000	-4.496569000	-0.668758000
1	0.339001000	-3.567588000	-1.236743000
6	3.376379000	-4.377466000	0.057669000
1	4.505519000	-3.119884000	1.387912000
1	2.003932000	-5.393538000	-1.250399000
1	4.109455000	-5.177212000	0.051483000
7	-2.297763000	1.680217000	-0.179934000
6	-2.132818000	3.027234000	0.303998000
1	-1.654818000	3.007093000	1.284357000
1	-1.514387000	3.646399000	-0.368264000
1	-3.114525000	3.507557000	0.396318000
6	-2.895729000	1.645343000	-1.503139000
1	-3.082968000	0.615820000	-1.812676000
1	-3.856929000	2.171311000	-1.490374000
1	-2.248253000	2.127138000	-2.258130000

3'c, TE = -2444.107526

6	0.989416000	1.322384000	-0.155272000
6	1.214072000	-0.913843000	0.427237000
7	1.814303000	0.292525000	0.166042000
7	-0.312058000	1.228907000	-0.053144000
25	-0.771250000	-0.886160000	-0.033007000
6	-0.168954000	-1.046720000	-1.810451000
7	0.226928000	-1.163170000	-2.909320000
6	-1.182671000	-2.658432000	0.030071000
7	-1.501150000	-3.798898000	0.060697000
6	-2.486651000	-0.565591000	-0.662284000
7	-3.558672000	-0.399408000	-1.125999000
6	-1.213528000	-0.693295000	1.788412000
7	-1.462178000	-0.569687000	2.929639000
6	-2.218266000	-5.008515000	-0.013502000
1	-1.641922000	-5.826600000	0.428425000
1	-3.168650000	-4.927932000	0.524574000
1	-2.432725000	-5.265924000	-1.055910000
6	0.769687000	-1.262711000	-4.202806000
1	1.828461000	-1.532177000	-4.150473000
1	0.241501000	-2.027668000	-4.778650000
1	0.676335000	-0.306653000	-4.725526000

6	-4.741677000	0.201122000	-1.602857000
1	-4.810057000	0.098545000	-2.689635000
1	-5.619264000	-0.274883000	-1.156424000
1	-4.744216000	1.266277000	-1.348879000
6	-1.690732000	-0.279354000	4.287132000
1	-2.500652000	-0.900856000	4.678539000
1	-0.788190000	-0.470723000	4.874664000
1	-1.967579000	0.772323000	4.403631000
6	3.222206000	0.553596000	0.143858000
6	4.013249000	0.290761000	1.257648000
6	3.785519000	1.108465000	-1.001196000
6	5.369821000	0.583614000	1.218670000
1	3.561918000	-0.140015000	2.142429000
6	5.141954000	1.409959000	-1.027630000
1	3.150145000	1.305492000	-1.857939000
6	5.938811000	1.145198000	0.079735000
1	5.985462000	0.378932000	2.088712000
1	5.576728000	1.848770000	-1.920006000
1	6.998765000	1.376315000	0.057152000
6	-1.103544000	2.357954000	0.005945000
6	-2.416120000	2.296284000	0.509292000
6	-0.625900000	3.618737000	-0.414483000
6	-3.208321000	3.432628000	0.575380000
1	-2.788022000	1.348600000	0.877909000
6	-1.429110000	4.745385000	-0.344241000
1	0.383609000	3.686079000	-0.807953000
6	-2.730802000	4.670221000	0.145957000
1	-4.211743000	3.354047000	0.985953000
1	-1.032063000	5.699007000	-0.681188000
1	-3.355636000	5.555288000	0.199088000
8	2.148338000	-1.825476000	0.783895000
6	1.693255000	-3.134850000	1.041252000
1	1.339291000	-3.616116000	0.125251000
1	2.551796000	-3.681199000	1.436230000
1	0.880769000	-3.130971000	1.773443000

4a, TE = -2060.017139

6	3.178133000	-1.125279000	-0.428813000
6	0.957194000	-0.980861000	0.634374000
1	1.537105000	-0.357574000	1.317056000
7	3.829320000	-0.208737000	0.143283000
1	0.618360000	-1.860531000	1.199973000
6	-1.136566000	0.692703000	1.617589000
6	-1.627983000	-1.492974000	-0.054580000
6	0.588745000	1.362582000	-0.486950000
7	-1.328453000	1.030618000	2.728353000

7	1.447679000	2.127057000	-0.714747000
7	-2.197338000	-2.520911000	-0.004173000
6	-2.894657000	-3.738473000	0.081093000
1	-2.206435000	-4.555583000	0.314430000
1	-3.654864000	-3.688632000	0.866544000
1	-3.389867000	-3.960763000	-0.868532000
6	-1.515249000	1.447570000	4.058230000
1	-1.867414000	0.614467000	4.673265000
1	-0.573964000	1.814659000	4.477216000
1	-2.255031000	2.252071000	4.105841000
6	2.700557000	2.758336000	-0.863464000
1	2.732389000	3.676539000	-0.270934000
1	3.472166000	2.060835000	-0.520817000
1	2.870894000	3.012586000	-1.912849000
6	5.265053000	-0.262156000	0.278824000
26	-0.695146000	0.091264000	-0.088828000
6	-2.002235000	0.950787000	-1.037309000
7	-2.833187000	1.508382000	-1.657796000
6	-3.791773000	2.198257000	-2.418555000
1	-3.711261000	3.275797000	-2.247255000
1	-3.646430000	2.005196000	-3.486049000
1	-4.800837000	1.878173000	-2.142812000
7	1.896790000	-1.456747000	-0.387265000
6	1.373794000	-2.361220000	-1.383049000
1	2.180550000	-2.676307000	-2.046083000
1	0.937767000	-3.247828000	-0.904081000
1	0.584375000	-1.871030000	-1.965559000
1	5.544981000	-0.526273000	1.306506000
1	5.725728000	-0.993929000	-0.396861000
1	5.701816000	0.721998000	0.072587000

4b, TE = -5207.489050

6	-2.005533000	1.511782000	-1.226483000
6	-1.294436000	1.264270000	1.038096000
1	-1.916928000	0.803785000	1.817492000
7	-1.178472000	0.668237000	-1.692791000
1	-0.739125000	2.092556000	1.495845000
6	0.962031000	-0.461584000	1.571330000
6	1.281630000	1.421427000	-0.275065000
6	-1.378756000	-1.534852000	0.369704000
7	1.602829000	-0.596396000	2.547675000
7	-2.148809000	-2.357056000	0.702119000
7	2.233456000	1.963113000	0.295546000
6	2.935286000	3.133784000	-0.203440000
1	2.529451000	3.486524000	-1.161845000
1	2.866531000	3.942423000	0.531698000

1	3.997140000	2.897710000	-0.330269000
6	2.563522000	-0.353363000	3.553310000
1	3.165186000	0.517823000	3.280665000
1	2.069787000	-0.163421000	4.510080000
1	3.218280000	-1.221146000	3.669651000
6	-3.051686000	-3.352844000	1.115954000
1	-2.919298000	-3.567623000	2.180287000
1	-4.080935000	-3.022442000	0.951294000
1	-2.885641000	-4.273496000	0.549765000
6	-0.726188000	0.698725000	-3.064160000
6	1.120074000	-1.298247000	-1.083638000
7	1.832776000	-1.955618000	-1.743748000
6	2.742298000	-2.680252000	-2.535701000
1	2.617803000	-3.753989000	-2.371373000
1	2.573799000	-2.466171000	-3.594647000
1	3.768443000	-2.401457000	-2.281559000
7	-2.219012000	1.823716000	0.032565000
6	-3.323979000	2.659765000	0.435168000
44	-0.032807000	-0.147430000	0.004971000
1	-3.884069000	2.986472000	-0.443146000
1	-3.996639000	2.110605000	1.104789000
1	-2.954294000	3.541684000	0.970111000
1	-0.697911000	-0.318736000	-3.465210000
1	-1.381679000	1.309642000	-3.692365000
1	0.288676000	1.112543000	-3.099988000

4'a, TE = -2443.003083

6	0.631062000	-1.458814000	-0.060873000
6	1.091851000	0.525927000	-1.257702000
1	0.784782000	0.380093000	-2.299543000
7	-0.602607000	-0.989090000	0.113053000
1	1.898551000	1.261088000	-1.239096000
6	-0.167909000	2.823198000	-0.429266000
6	0.834211000	1.063212000	1.295946000
6	-1.612181000	0.844217000	-1.483467000
7	0.057818000	3.934856000	-0.717564000
7	-2.275505000	0.595117000	-2.409724000
7	1.713421000	0.999586000	2.056580000
6	2.866450000	0.713726000	2.822565000
1	3.428868000	-0.084111000	2.329321000
1	3.490086000	1.606761000	2.900065000
1	2.574927000	0.391397000	3.824257000
6	0.363937000	5.259602000	-1.085677000
1	1.436533000	5.359855000	-1.269937000
1	-0.176253000	5.529891000	-1.996328000
1	0.076712000	5.949154000	-0.287879000

6	-3.120758000	0.026060000	-3.386974000
1	-2.529575000	-0.301792000	-4.244674000
1	-3.632705000	-0.836090000	-2.951076000
1	-3.857836000	0.759571000	-3.720750000
6	-1.678864000	-1.837084000	0.138588000
6	-3.010231000	-1.372931000	0.245860000
6	-1.501367000	-3.244594000	0.054560000
6	-4.082707000	-2.250571000	0.244350000
1	-3.198149000	-0.309129000	0.310947000
6	-2.584294000	-4.106065000	0.052369000
1	-0.489734000	-3.633714000	-0.003334000
6	-3.891862000	-3.630632000	0.147607000
1	-5.090490000	-1.848851000	0.318703000
1	-2.403114000	-5.175564000	-0.016557000
1	-4.734833000	-4.312895000	0.156786000
26	-0.484274000	1.075727000	-0.028341000
6	-1.813421000	1.415794000	1.229327000
7	-2.600204000	1.641592000	2.064745000
6	-3.583347000	1.699780000	3.073747000
1	-4.294780000	2.501114000	2.861083000
1	-4.117634000	0.747102000	3.118664000
1	-3.114763000	1.890789000	4.041977000
7	1.594252000	-0.732332000	-0.702115000
6	2.933956000	-1.014479000	-0.536105000
6	3.943780000	-0.280186000	-1.187435000
6	3.328474000	-2.083272000	0.301750000
6	5.280879000	-0.577862000	-0.974421000
1	3.678831000	0.513064000	-1.876131000
6	4.671544000	-2.364452000	0.499678000
1	2.559894000	-2.679369000	0.783119000
6	5.666727000	-1.615822000	-0.124729000
1	6.036422000	0.006593000	-1.491829000
1	4.944555000	-3.191659000	1.149414000
1	6.715015000	-1.848805000	0.026634000

4'b, TE = -5590.497210

6	0.797619000	-1.537389000	-0.055080000
6	1.143756000	0.457143000	-1.305442000
1	0.852855000	0.259718000	-2.343434000
7	-0.469228000	-1.153422000	0.128648000
1	1.913824000	1.229932000	-1.310551000
6	-0.321113000	2.866386000	-0.428728000
6	0.890972000	1.069132000	1.355588000
6	-1.717483000	0.694661000	-1.565338000
7	-0.180943000	4.000951000	-0.688159000
7	-2.370700000	0.411272000	-2.488561000

7	1.792867000	1.032281000	2.090248000
6	2.974721000	0.781913000	2.824106000
1	3.544269000	-0.002018000	2.316375000
1	3.574484000	1.692573000	2.880669000
1	2.719832000	0.455393000	3.834328000
6	0.014045000	5.356258000	-1.014476000
1	1.076223000	5.608023000	-0.956707000
1	-0.337909000	5.553390000	-2.030447000
1	-0.537468000	5.996883000	-0.321020000
6	-3.195162000	-0.171309000	-3.474694000
1	-2.604950000	-0.401830000	-4.364068000
1	-3.624205000	-1.094752000	-3.076795000
1	-3.998126000	0.517034000	-3.747127000
6	-1.482311000	-2.077996000	0.153345000
6	-2.840500000	-1.703449000	0.254870000
6	-1.205219000	-3.468525000	0.085552000
6	-3.850233000	-2.652780000	0.261416000
1	-3.095391000	-0.652704000	0.314345000
6	-2.226385000	-4.402734000	0.092400000
1	-0.168957000	-3.787107000	0.033143000
6	-3.563311000	-4.016933000	0.179903000
1	-4.883512000	-2.321495000	0.331500000
1	-1.972312000	-5.457965000	0.036059000
1	-4.357171000	-4.755668000	0.195121000
6	-1.968275000	1.290148000	1.294109000
7	-2.781941000	1.447871000	2.120054000
6	-3.768699000	1.440488000	3.126946000
1	-4.562843000	2.149331000	2.881069000
1	-4.196691000	0.438336000	3.214037000
1	-3.327065000	1.723221000	4.085446000
7	1.712402000	-0.759506000	-0.708714000
6	3.065584000	-0.968817000	-0.551630000
6	4.032697000	-0.193373000	-1.221141000
6	3.521960000	-2.003316000	0.299232000
6	5.384534000	-0.418845000	-1.013651000
1	3.724349000	0.575156000	-1.919586000
6	4.879004000	-2.211306000	0.491446000
1	2.789252000	-2.632749000	0.793842000
6	5.830146000	-1.422094000	-0.151288000
1	6.105000000	0.195749000	-1.545937000
1	5.198443000	-3.013931000	1.150805000
1	6.890077000	-1.598248000	-0.004660000
44	-0.523120000	1.005092000	-0.032857000

5a, TE = -2482.221088

6	-0.675173000	-0.178030000	1.286531000
6	0.000318000	-2.077725000	-0.000959000
6	0.676248000	-0.176851000	-1.286664000
7	1.036630000	-1.402641000	-0.568350000
7	-1.035869000	-1.403272000	0.567450000
6	2.342433000	-1.828663000	-0.387826000
6	2.617532000	-2.864379000	0.532517000
6	3.430136000	-1.289953000	-1.104169000
6	3.911801000	-3.305627000	0.743372000
1	1.784286000	-3.310485000	1.065161000
6	4.720642000	-1.752941000	-0.887618000
1	3.274396000	-0.510222000	-1.838102000
6	4.985222000	-2.757919000	0.039893000
1	4.085052000	-4.100453000	1.463341000
1	5.534308000	-1.318575000	-1.461723000
1	5.996078000	-3.118086000	0.196830000
6	-2.341660000	-1.829320000	0.387230000
6	-2.616769000	-2.865705000	-0.532373000
6	-3.429390000	-1.289961000	1.103058000
6	-3.911054000	-3.307033000	-0.742968000
1	-1.783524000	-3.312261000	-1.064639000
6	-4.719903000	-1.753057000	0.886785000
1	-3.273724000	-0.509481000	1.836202000
6	-4.984482000	-2.758753000	-0.039954000
1	-4.084306000	-4.102405000	-1.462333000
1	-5.533591000	-1.318140000	1.460443000
1	-5.995349000	-3.118988000	-0.196668000
1	-0.112530000	-0.445494000	-1.995559000
1	1.529057000	0.153802000	-1.877303000
1	0.114503000	-0.447178000	1.994228000
1	-1.527374000	0.151654000	1.878596000
26	-0.000226000	1.329828000	0.000278000
6	1.632946000	1.158728000	0.838892000
7	2.644597000	0.985631000	1.397224000
6	-1.633016000	1.157822000	-0.838884000
7	-2.644194000	0.984329000	-1.397947000
6	0.621922000	2.550683000	-1.218095000
7	1.031217000	3.294747000	-2.026933000
6	-0.623499000	2.549413000	1.219325000
7	-1.033514000	3.292575000	2.028631000
6	3.865590000	0.567620000	1.969421000
1	3.729412000	0.377407000	3.036577000
1	4.201496000	-0.349356000	1.477580000
1	4.623418000	1.344558000	1.842418000
6	1.522556000	4.180731000	-3.004508000

1	1.150130000	3.897137000	-3.992320000
1	1.199139000	5.202312000	-2.787372000
1	2.615246000	4.155118000	-3.021792000
6	-1.525696000	4.177439000	3.006795000
1	-1.204035000	5.199609000	2.789821000
1	-2.618333000	4.150078000	3.024712000
1	-1.152240000	3.894104000	3.994293000
6	-3.864547000	0.565758000	-1.971098000
1	-3.727129000	0.374325000	-3.037876000
1	-4.201065000	-0.350651000	-1.478620000
1	-4.622474000	1.342888000	-1.845864000

5b, TE = - 5629.716668

6	-0.655139000	-0.360017000	1.332180000
6	0.000056000	-2.242037000	-0.000141000
6	0.655283000	-0.359875000	-1.332247000
7	1.030546000	-1.565319000	-0.580688000
7	-1.030418000	-1.565410000	0.580549000
6	2.340737000	-1.972605000	-0.399200000
6	2.628576000	-3.017229000	0.507270000
6	3.423798000	-1.401315000	-1.097507000
6	3.928404000	-3.442178000	0.716020000
1	1.800042000	-3.485045000	1.028360000
6	4.720397000	-1.848936000	-0.883513000
1	3.260740000	-0.605433000	-1.811999000
6	4.996313000	-2.867182000	0.025761000
1	4.110743000	-4.246507000	1.423047000
1	5.530004000	-1.389951000	-1.444113000
1	6.011726000	-3.215505000	0.180033000
6	-2.340604000	-1.972731000	0.399134000
6	-2.628459000	-3.017391000	-0.507292000
6	-3.423649000	-1.401439000	1.097466000
6	-3.928289000	-3.442364000	-0.715982000
1	-1.799938000	-3.485209000	-1.028401000
6	-4.720248000	-1.849091000	0.883536000
1	-3.260580000	-0.605524000	1.811919000
6	-4.996182000	-2.867367000	-0.025700000
1	-4.110640000	-4.246721000	-1.422975000
1	-5.529841000	-1.390100000	1.444150000
1	-6.011595000	-3.215713000	-0.179923000
1	-0.163523000	-0.651941000	-1.996190000
1	1.483240000	-0.064001000	-1.974792000
1	0.163742000	-0.652110000	1.996020000
1	-1.483048000	-0.064250000	1.974836000
6	1.747413000	1.077014000	0.883699000
7	2.757753000	0.884191000	1.435529000

6	-1.747438000	1.076884000	-0.883697000
7	-2.757765000	0.884056000	-1.435548000
6	0.660576000	2.557822000	-1.303583000
7	1.075202000	3.299732000	-2.112333000
6	-0.660767000	2.557688000	1.303661000
7	-1.075491000	3.299505000	2.112445000
6	3.978396000	0.442148000	1.990228000
1	3.852410000	0.253351000	3.058730000
1	4.287568000	-0.480003000	1.490552000
1	4.748254000	1.205138000	1.852824000
6	1.569847000	4.192718000	-3.081494000
1	1.197680000	3.918656000	-4.072145000
1	1.248908000	5.213322000	-2.855756000
1	2.662539000	4.164120000	-3.098040000
6	-1.570245000	4.192399000	3.081635000
1	-1.249150000	5.213003000	2.856116000
1	-2.662944000	4.163915000	3.097945000
1	-1.198317000	3.918150000	4.072324000
6	-3.978390000	0.442018000	-1.990288000
1	-3.852380000	0.253254000	-3.058794000
1	-4.287556000	-0.480159000	-1.490655000
1	-4.748261000	1.204992000	-1.852875000
44	-0.000021000	1.255713000	0.000010000

6a, TE = -2630.247721

6	0.467927000	1.478148000	0.205024000
7	-0.895883000	1.293325000	-0.204535000
6	-1.200561000	0.063319000	-0.731073000
7	-1.057457000	-1.146887000	-0.082377000
6	0.283778000	-1.470036000	0.317309000
8	0.768821000	2.536785000	0.724709000
6	-1.933484000	2.238045000	0.013829000
6	-1.717068000	3.609693000	-0.142118000
6	-2.765248000	4.500324000	0.050127000
6	-4.036227000	4.047472000	0.387923000
6	-4.251892000	2.681778000	0.535598000
6	-3.210036000	1.782402000	0.354686000
1	-0.729908000	3.967779000	-0.397898000
1	-2.583773000	5.563936000	-0.071470000
1	-4.849685000	4.750863000	0.532805000
1	-5.236619000	2.309127000	0.800076000
1	-3.382642000	0.717658000	0.476353000
6	-2.174694000	-2.015117000	0.000036000
6	-3.215142000	-1.857203000	-0.923850000
6	-4.347087000	-2.657564000	-0.860894000
6	-4.459938000	-3.640435000	0.115280000

6	-3.425452000	-3.802046000	1.029911000
6	-2.290469000	-3.001758000	0.985246000
1	-3.125033000	-1.098216000	-1.694398000
1	-5.141520000	-2.513443000	-1.586716000
1	-5.341798000	-4.270706000	0.163275000
1	-3.500648000	-4.560789000	1.803061000
1	-1.492392000	-3.136519000	1.699693000
8	0.474345000	-2.535299000	0.876208000
26	1.696687000	-0.088956000	-0.072987000
6	2.836158000	-1.548295000	-0.249957000
6	3.012645000	1.191767000	-0.358716000
6	1.224142000	-0.127674000	-1.854946000
7	3.806651000	2.032081000	-0.519741000
7	3.510364000	-2.496497000	-0.342225000
7	1.008018000	-0.156160000	-3.007372000
6	0.309430000	-0.157368000	-4.233912000
1	0.474679000	-1.100650000	-4.759665000
1	-0.760801000	-0.034611000	-4.041846000
1	0.657756000	0.662196000	-4.866674000
6	4.607779000	3.186967000	-0.621564000
1	4.821070000	3.404972000	-1.670639000
1	4.079947000	4.035395000	-0.179295000
1	5.552756000	3.037283000	-0.094094000
6	4.118177000	-3.768280000	-0.347545000
1	5.046603000	-3.744095000	0.227751000
1	3.436149000	-4.495994000	0.098867000
1	4.346671000	-4.071293000	-1.371942000
6	1.887378000	-0.017222000	1.762770000
7	1.960074000	0.043043000	2.924738000
6	1.897887000	0.166170000	4.326192000
1	1.326318000	-0.664982000	4.745914000
1	2.904453000	0.155463000	4.750817000
1	1.408844000	1.106739000	4.590811000

6b, TE = -5777.740800

6	0.296174000	1.536577000	0.219806000
7	-1.063257000	1.297520000	-0.180301000
6	-1.327576000	0.059580000	-0.715893000
7	-1.198373000	-1.156806000	-0.072096000
6	0.139392000	-1.517642000	0.312713000
8	0.562627000	2.604827000	0.738526000
6	-2.130285000	2.209797000	0.033731000
6	-1.957880000	3.586695000	-0.131568000
6	-3.032806000	4.445298000	0.058515000
6	-4.288033000	3.955109000	0.402753000
6	-4.460261000	2.584282000	0.558941000

6	-3.391159000	1.716825000	0.381029000
1	-0.983420000	3.974383000	-0.392662000
1	-2.884977000	5.513296000	-0.070043000
1	-5.122665000	4.633576000	0.546037000
1	-5.432100000	2.182401000	0.828216000
1	-3.530679000	0.648286000	0.509995000
6	-2.327425000	-2.010549000	0.008915000
6	-3.352232000	-1.863262000	-0.933139000
6	-4.492803000	-2.651376000	-0.868442000
6	-4.628703000	-3.611096000	0.127599000
6	-3.609282000	-3.762084000	1.060871000
6	-2.466577000	-2.973151000	1.014266000
1	-3.243619000	-1.121369000	-1.717660000
1	-5.275885000	-2.516073000	-1.608138000
1	-5.517215000	-4.231872000	0.176852000
1	-3.703036000	-4.502564000	1.849507000
1	-1.680091000	-3.099251000	1.743230000
8	0.313044000	-2.596300000	0.850179000
6	2.847999000	-1.641128000	-0.261349000
6	3.005533000	1.342915000	-0.362335000
6	1.153768000	-0.108702000	-1.984077000
7	3.748683000	2.232990000	-0.501907000
7	3.488443000	-2.614307000	-0.339690000
7	0.894983000	-0.129945000	-3.125242000
6	0.222064000	-0.133464000	-4.364785000
1	0.402710000	-1.076051000	-4.886558000
1	-0.852062000	-0.016021000	-4.194752000
1	0.579577000	0.688769000	-4.988767000
6	4.482206000	3.432902000	-0.591466000
1	4.698846000	3.662580000	-1.637397000
1	3.898579000	4.249185000	-0.158798000
1	5.425852000	3.338730000	-0.048941000
6	4.065052000	-3.900364000	-0.348812000
1	4.990088000	-3.902077000	0.232491000
1	3.363300000	-4.615141000	0.087892000
1	4.292727000	-4.201609000	-1.373962000
6	1.857617000	-0.003894000	1.879850000
7	1.930418000	0.053238000	3.041394000
6	1.897119000	0.163778000	4.445088000
1	1.359354000	-0.686834000	4.870077000
1	2.913694000	0.178802000	4.844783000
1	1.387500000	1.087743000	4.728102000
44	1.642965000	-0.072232000	-0.078580000

Cartesian coordinates for the optimized structure of GaCl₃ adducts of **1a-6b**, along with their total energies (in hartrees) including zero point vibrational correction.

1a-GaCl₃, TE = -5174.419187

6	-0.492551000	0.313884000	-0.081212000
6	1.378018000	1.715330000	-0.053211000
1	1.732939000	2.749431000	-0.061393000
7	0.070228000	1.633472000	-0.086502000
7	0.432751000	-0.576405000	-0.055984000
6	-0.803754000	2.806518000	-0.134761000
1	-1.453996000	2.826599000	0.739330000
1	-0.177400000	3.697464000	-0.156686000
1	-1.431106000	2.769336000	-1.025107000
6	0.113967000	-1.994170000	-0.052950000
1	0.642602000	-2.472452000	-0.881530000
1	0.469354000	-2.434616000	0.882742000
1	-0.950678000	-2.195978000	-0.155669000
25	2.379011000	0.054185000	0.000560000
6	2.403112000	0.044893000	-1.854475000
8	2.417201000	0.056549000	-2.989245000
6	3.976006000	0.911076000	0.040928000
8	4.954087000	1.497476000	0.063892000
6	3.149696000	-1.631742000	0.053300000
8	3.646936000	-2.654040000	0.087575000
6	2.280858000	0.098754000	1.853073000
8	2.221802000	0.144570000	2.985392000
31	-2.528387000	-0.124616000	-0.074362000
17	-2.799533000	-1.276698000	1.766799000
17	-2.840990000	-1.267781000	-1.914128000
17	-3.850475000	1.614889000	-0.052570000

1b-GaCl₃, TE = -5308.210679

6	0.675345000	-0.127745000	0.248841000
6	-1.256721000	1.231562000	0.146490000
7	0.087104000	1.143241000	0.361242000
7	-0.170850000	-1.090249000	0.161429000
25	-2.147583000	-0.593330000	0.028326000
6	-2.263201000	-0.582763000	1.874545000
8	-2.328949000	-0.541284000	3.008668000
6	-3.889008000	-0.135194000	-0.133959000
8	-5.007873000	0.075198000	-0.250573000
6	-2.665055000	-2.349529000	-0.097829000
8	-3.019600000	-3.429020000	-0.179454000
6	-1.917096000	-0.429853000	-1.803745000

8	-1.784683000	-0.297326000	-2.924163000
6	0.281841000	-2.468436000	0.095952000
6	0.849193000	2.187072000	1.065823000
7	-1.739954000	2.458873000	-0.045609000
6	-0.961059000	3.547210000	-0.640568000
1	-0.684847000	4.311012000	0.091262000
1	-0.065243000	3.155160000	-1.119211000
1	-1.583853000	4.012328000	-1.409096000
6	-3.160033000	2.752875000	0.052393000
1	-3.272047000	3.793941000	0.363625000
1	-3.666136000	2.622583000	-0.910294000
1	-3.629940000	2.128120000	0.806294000
1	0.152436000	2.778327000	1.661050000
1	1.548098000	1.696446000	1.744241000
1	1.417877000	2.826808000	0.392894000
1	1.356960000	-2.556328000	0.247805000
1	-0.236049000	-3.045628000	0.866533000
1	0.035903000	-2.901194000	-0.878137000
31	2.729936000	-0.157464000	-0.020718000
17	3.479089000	-1.931343000	-1.048288000
17	3.649263000	0.064838000	1.957276000
17	3.072702000	1.578168000	-1.341093000

1c-GaCl₃, TE = -5288.837493

6	-0.648593000	0.193823000	0.203892000
6	1.329973000	1.443515000	0.020890000
7	-0.005152000	1.448328000	0.155360000
7	0.177781000	-0.789888000	0.248265000
25	2.163066000	-0.375968000	0.007144000
6	1.891768000	-0.414925000	-1.831272000
8	1.736017000	-0.418911000	-2.954880000
6	3.909015000	0.040467000	-0.232920000
8	5.026539000	0.231090000	-0.382320000
6	2.641274000	-2.155095000	0.029952000
8	2.970364000	-3.243953000	0.037017000
6	2.334378000	-0.235389000	1.845915000
8	2.438659000	-0.131183000	2.972065000
6	-0.301692000	-2.157118000	0.373944000
8	1.792783000	2.667707000	-0.045563000
6	3.189643000	2.929709000	-0.167347000
1	3.732188000	2.521808000	0.685986000
1	3.574121000	2.522366000	-1.102901000
1	3.277211000	4.014654000	-0.175577000
6	-0.762272000	2.692468000	0.316261000
1	-0.169765000	3.394263000	0.899867000
1	-0.998986000	3.131957000	-0.653857000

1	-1.691364000	2.474746000	0.834637000
1	-1.349649000	-2.203912000	0.669658000
1	-0.179410000	-2.687937000	-0.574077000
1	0.289235000	-2.663798000	1.140785000
31	-2.703595000	-0.071633000	-0.004237000
17	-3.808688000	1.736172000	-0.544746000
17	-2.877113000	-1.487647000	-1.669455000
17	-3.383202000	-0.857709000	1.922226000

1'a-GaCl₃, TE = -5557.420885

6	0.318892000	-0.008877000	-0.028262000
6	-0.436485000	-2.228726000	0.007528000
1	-0.129118000	-3.276667000	0.054278000
7	0.599572000	-1.414519000	0.006935000
7	-0.953574000	0.197808000	-0.014713000
25	-2.201742000	-1.438956000	-0.004559000
6	-2.186443000	-1.464757000	-1.858103000
8	-2.168518000	-1.503586000	-2.992901000
6	-3.017177000	-3.054955000	0.025552000
8	-3.480561000	-4.097313000	0.046234000
6	-3.810322000	-0.499381000	0.012421000
8	-4.816454000	0.027023000	0.031269000
6	-2.152459000	-1.403974000	1.850401000
8	-2.113178000	-1.395755000	2.984662000
6	-1.463150000	1.527144000	0.091251000
6	-1.219785000	2.261483000	1.247109000
6	-2.239707000	2.057737000	-0.934700000
6	-1.747757000	3.541272000	1.366938000
1	-0.606599000	1.841227000	2.036997000
6	-2.752633000	3.339286000	-0.809320000
1	-2.405996000	1.486110000	-1.841599000
6	-2.512485000	4.082034000	0.342653000
1	-1.546248000	4.117809000	2.263186000
1	-3.334930000	3.763905000	-1.619946000
1	-2.915946000	5.084487000	0.435790000
6	1.945326000	-1.927303000	0.112403000
6	2.697049000	-1.635547000	1.240860000
6	2.434006000	-2.744919000	-0.897320000
6	3.974332000	-2.170068000	1.349689000
1	2.304480000	-0.982267000	2.012017000
6	3.708188000	-3.279868000	-0.772318000
1	1.837647000	-2.929686000	-1.784652000
6	4.477913000	-2.992064000	0.349270000
1	4.575911000	-1.936165000	2.220916000
1	4.105876000	-3.907881000	-1.561887000
1	5.478389000	-3.401568000	0.437794000

31	1.825392000	1.426622000	-0.201049000
17	2.399087000	1.861485000	1.879678000
17	3.459859000	0.590707000	-1.386380000
17	1.087924000	3.181470000	-1.256967000

1'b-GaCl₃, TE = -5691.209135

6	0.363513000	0.179400000	-0.021581000
6	-0.679864000	-1.961383000	0.037749000
7	0.479715000	-1.222519000	0.078230000
7	-0.859345000	0.582663000	-0.085681000
25	-2.350261000	-0.800565000	-0.047931000
6	-2.310979000	-0.895211000	-1.894870000
8	-2.270693000	-0.990910000	-3.027701000
6	-3.665885000	-2.036854000	0.042376000
8	-4.553543000	-2.755631000	0.119596000
6	-3.674016000	0.486232000	-0.025296000
8	-4.533124000	1.230369000	0.002129000
6	-2.231306000	-0.799060000	1.800442000
8	-2.153257000	-0.830533000	2.933771000
6	-1.183902000	1.973575000	-0.066247000
6	-1.087740000	2.680996000	1.127075000
6	-1.664732000	2.590945000	-1.216776000
6	-1.465747000	4.017644000	1.162582000
1	-0.695155000	2.193101000	2.013253000
6	-2.035172000	3.926470000	-1.172403000
1	-1.718104000	2.034708000	-2.146903000
6	-1.941582000	4.641375000	0.017131000
1	-1.374061000	4.573125000	2.089717000
1	-2.388374000	4.414301000	-2.074664000
1	-2.229957000	5.686602000	0.046558000
6	1.792697000	-1.813096000	-0.051357000
6	2.696953000	-1.751415000	1.000006000
6	2.125511000	-2.440712000	-1.245328000
6	3.946437000	-2.339691000	0.855687000
1	2.433019000	-1.229525000	1.913492000
6	3.372780000	-3.035915000	-1.377061000
1	1.418846000	-2.447114000	-2.068769000
6	4.281810000	-2.989515000	-0.325789000
1	4.662146000	-2.277255000	1.667999000
1	3.642164000	-3.517452000	-2.310927000
1	5.261133000	-3.442821000	-0.436293000
7	-0.605254000	-3.278886000	0.222462000
6	0.411021000	-4.004103000	0.989823000
1	1.180500000	-4.443838000	0.350416000
1	0.881580000	-3.354232000	1.721078000
1	-0.110421000	-4.802618000	1.524079000

6	-1.664500000	-4.161349000	-0.243321000
1	-1.195999000	-5.063488000	-0.646332000
1	-2.335201000	-4.454444000	0.570710000
1	-2.230487000	-3.693295000	-1.042907000
31	2.035412000	1.441969000	-0.007627000
17	2.472037000	1.548648000	2.157937000
17	3.694395000	0.655405000	-1.200704000
17	1.664418000	3.427252000	-0.829015000

1'*c*-GaCl₃, TE = -5671.838024

6	-0.376096000	0.122574000	-0.130594000
6	0.598327000	-2.023877000	-0.006005000
7	-0.528583000	-1.278249000	-0.081469000
7	0.863355000	0.478179000	-0.127820000
25	2.295334000	-0.979333000	-0.010857000
6	2.166418000	-0.895390000	1.838882000
8	2.084959000	-0.867499000	2.970771000
6	3.524999000	-2.301683000	0.106006000
8	4.354436000	-3.086029000	0.177309000
6	3.685881000	0.246889000	-0.010552000
8	4.576340000	0.951206000	0.004608000
6	2.302987000	-1.102055000	-1.858326000
8	2.299322000	-1.200754000	-2.990379000
6	1.236728000	1.857173000	-0.082047000
6	1.768269000	2.464557000	-1.215292000
6	1.127318000	2.559779000	1.112606000
6	2.176206000	3.788594000	-1.153506000
1	1.830227000	1.911277000	-2.146762000
6	1.542997000	3.884820000	1.165057000
1	0.690152000	2.082196000	1.983115000
6	2.068882000	4.499999000	0.036904000
1	2.568782000	4.270082000	-2.042779000
1	1.440309000	4.438630000	2.092021000
1	2.385518000	5.536527000	0.080258000
6	-1.833311000	-1.902499000	-0.054760000
6	-2.332548000	-2.476824000	-1.215179000
6	-2.543261000	-1.939219000	1.135445000
6	-3.572922000	-3.095490000	-1.182214000
1	-1.764542000	-2.418365000	-2.137434000
6	-3.789711000	-2.553337000	1.155790000
1	-2.143074000	-1.464611000	2.024302000
6	-4.301244000	-3.133217000	0.002294000
1	-3.979827000	-3.532932000	-2.087365000
1	-4.363240000	-2.566698000	2.076020000
1	-5.277783000	-3.605379000	0.021477000
8	0.305402000	-3.292233000	0.067385000

6	1.317037000	-4.292180000	0.166295000
1	1.960974000	-4.273483000	-0.713356000
1	1.899857000	-4.157725000	1.077998000
1	0.777800000	-5.236622000	0.209526000
31	-2.023379000	1.405998000	-0.046420000
17	-2.298217000	1.527458000	2.142097000
17	-1.603754000	3.342696000	-0.952147000
17	-3.779942000	0.613715000	-1.070183000

2a-GaCl₃, TE = -5213.092635

6	-0.892256000	-0.379771000	-0.076381000
6	0.970492000	-1.781959000	-0.055159000
1	1.308734000	-2.823622000	-0.065147000
7	-0.346809000	-1.697213000	-0.083138000
7	0.041386000	0.503927000	-0.050907000
6	-1.225216000	-2.863989000	-0.126560000
1	-1.855306000	-2.833117000	-1.015609000
1	-0.601507000	-3.757218000	-0.147514000
1	-1.874386000	-2.885911000	0.748710000
6	-0.275726000	1.918933000	-0.048740000
1	0.092873000	2.361833000	0.880727000
1	0.245534000	2.393296000	-0.884341000
1	-1.341047000	2.127068000	-0.138804000
6	1.978669000	-0.193039000	1.838292000
8	2.016979000	-0.239342000	2.977665000
6	2.086476000	-0.126760000	-1.841216000
8	2.190618000	-0.131417000	-2.977494000
6	2.752371000	1.589270000	0.055750000
7	3.222993000	2.657639000	0.095282000
6	3.609670000	-1.049035000	0.027478000
7	4.605709000	-1.664251000	0.043243000
6	5.822425000	-2.377044000	0.061249000
1	5.854932000	-3.039538000	0.929353000
1	5.917382000	-2.977470000	-0.846525000
1	6.663672000	-1.681734000	0.115127000
6	3.748190000	3.966230000	0.145045000
1	4.319995000	4.102087000	1.065611000
1	4.403914000	4.136362000	-0.711648000
1	2.933981000	4.694316000	0.120769000
25	1.979829000	-0.152655000	-0.002915000
31	-2.909454000	0.071677000	-0.076709000
17	-3.253449000	1.225395000	-1.913889000
17	-3.232338000	1.243905000	1.752711000
17	-4.273491000	-1.644908000	-0.056771000

2b-GaCl₃, TE = -5346.878061

6	1.023102000	0.029373000	0.246032000
6	-0.800289000	-1.472833000	0.161504000
7	0.547109000	-1.291250000	0.309901000
7	0.096276000	0.917409000	0.225883000
6	-1.695576000	0.141508000	-1.726494000
8	-1.655346000	0.030560000	-2.862834000
6	-2.010311000	0.217202000	1.931906000
8	-2.150679000	0.154247000	3.064740000
6	-2.484454000	2.024519000	-0.006140000
7	-2.902084000	3.114167000	-0.084379000
6	-3.590272000	-0.327443000	-0.061324000
7	-4.725126000	-0.602327000	-0.181747000
6	-6.088310000	-0.926198000	-0.329544000
1	-6.242045000	-1.999282000	-0.185675000
1	-6.686010000	-0.385013000	0.408320000
1	-6.432816000	-0.653806000	-1.330347000
6	-3.322576000	4.456826000	-0.181438000
1	-3.851208000	4.616033000	-1.124079000
1	-3.990972000	4.700425000	0.647543000
1	-2.455463000	5.120987000	-0.144964000
25	-1.834364000	0.256646000	0.103107000
6	0.441654000	2.324920000	0.235017000
6	1.418827000	-2.291902000	0.942645000
7	-1.183520000	-2.744270000	-0.023674000
6	-2.559010000	-3.159717000	0.165793000
1	-3.048024000	-2.515192000	0.889962000
1	-3.118621000	-3.146424000	-0.777387000
1	-2.559898000	-4.182042000	0.554898000
6	-0.365445000	-3.747087000	-0.702565000
1	0.464381000	-3.271771000	-1.223049000
1	0.020622000	-4.509506000	-0.019251000
1	-0.996461000	-4.240033000	-1.447969000
1	2.110060000	-1.773120000	1.608117000
1	0.799092000	-2.954529000	1.548214000
1	2.002836000	-2.866100000	0.224740000
1	-0.120645000	2.814881000	1.034396000
1	1.506579000	2.492210000	0.395420000
1	0.159874000	2.789990000	-0.714444000
31	3.049640000	0.264517000	-0.044595000
17	3.617622000	-1.388559000	-1.396698000
17	4.030558000	0.113017000	1.918158000
17	3.620911000	2.128281000	-1.046705000

2c-GaCl₃, TE = -5327.508677

6	-1.023601000	-0.278479000	0.205651000
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6	0.868300000	-1.658582000	0.079388000
7	-0.473336000	-1.573890000	0.175833000
7	-0.127972000	0.641777000	0.262237000
6	2.039222000	-0.041632000	1.886194000
8	2.206985000	-0.134605000	3.012183000
6	1.677217000	0.106500000	-1.773434000
8	1.630059000	0.102973000	-2.913216000
6	2.413023000	1.874912000	0.061539000
7	2.783990000	2.982431000	0.045455000
6	3.602484000	-0.451341000	-0.141347000
7	4.743649000	-0.690882000	-0.269148000
6	6.119616000	-0.955295000	-0.424815000
1	6.291757000	-2.031007000	-0.517294000
1	6.496833000	-0.461117000	-1.323519000
1	6.672981000	-0.584264000	0.441390000
6	3.141599000	4.347187000	0.021159000
1	3.799150000	4.575406000	0.862811000
1	3.660264000	4.579539000	-0.911523000
1	2.243635000	4.965685000	0.092203000
25	1.827843000	0.073148000	0.063670000
6	-0.519296000	2.034026000	0.379530000
6	-1.317816000	-2.758658000	0.327098000
8	1.227182000	-2.927501000	0.036019000
6	2.598699000	-3.288402000	-0.047283000
1	3.035731000	-2.913961000	-0.973962000
1	3.150152000	-2.906372000	0.812825000
1	2.610483000	-4.377778000	-0.044018000
1	-2.256606000	-2.468217000	0.789530000
1	-1.533849000	-3.212921000	-0.641505000
1	-0.806370000	-3.482062000	0.959728000
1	-0.338784000	2.556502000	-0.564081000
1	-1.568607000	2.155209000	0.650497000
1	0.089405000	2.497514000	1.159749000
31	-3.037989000	0.125813000	-0.036840000
17	-3.739130000	0.930142000	1.882983000
17	-4.274425000	-1.584344000	-0.636903000
17	-3.142880000	1.592705000	-1.673440000

2'a-GaCl₃, TE = -5596.096064

6	0.629009000	0.007036000	-0.065844000
6	-0.543281000	2.033075000	-0.033706000
1	-0.427573000	3.121019000	0.003529000
7	0.641804000	1.429867000	-0.036898000
7	-0.584102000	-0.432898000	-0.061092000
6	-2.123252000	0.970754000	1.818641000
8	-2.161866000	1.019277000	2.957709000

6	-2.232987000	0.995547000	-1.859847000
8	-2.337439000	1.066592000	-2.994329000
6	-3.485049000	-0.381460000	0.036195000
7	-4.290406000	-1.222774000	0.092437000
6	-3.251530000	2.418093000	0.016722000
7	-3.921232000	3.377542000	0.041388000
6	-4.755868000	4.513979000	0.070683000
1	-4.524660000	5.124481000	0.946621000
1	-4.602192000	5.113249000	-0.829708000
1	-5.803718000	4.207841000	0.118396000
6	-5.101545000	-2.376457000	0.152161000
1	-5.561917000	-2.453871000	1.139286000
1	-5.886165000	-2.319679000	-0.605159000
1	-4.480964000	-3.258007000	-0.028532000
25	-2.112289000	0.948851000	-0.023313000
6	-0.841304000	-1.832586000	-0.000189000
6	-1.388100000	-2.483874000	-1.102916000
6	-0.605215000	-2.528820000	1.180274000
6	-1.674515000	-3.838967000	-1.027737000
1	-1.551187000	-1.934313000	-2.023825000
6	-0.905039000	-3.884632000	1.250161000
1	-0.167198000	-2.015214000	2.029395000
6	-1.438966000	-4.543062000	0.150391000
1	-2.062971000	-4.352875000	-1.901400000
1	-0.699527000	-4.428201000	2.166253000
1	-1.653276000	-5.605458000	0.202205000
6	1.861191000	2.192970000	0.046341000
6	2.639773000	2.121148000	1.192667000
6	2.204598000	3.027439000	-1.009105000
6	3.790838000	2.894691000	1.273089000
1	2.365053000	1.450398000	1.999194000
6	3.351407000	3.802683000	-0.914198000
1	1.593952000	3.042824000	-1.905753000
6	4.145181000	3.735686000	0.225608000
1	4.413206000	2.831981000	2.158958000
1	3.634785000	4.446188000	-1.740106000
1	5.048534000	4.332693000	0.292025000
31	2.369766000	-1.117382000	-0.123713000
17	2.891681000	-1.367969000	2.008642000
17	2.072425000	-3.044414000	-1.106771000
17	3.925906000	-0.069621000	-1.252323000

2'b-GaCl₃, TE = -5729.878996

6	-0.686036000	0.126060000	-0.016720000
6	0.625501000	-1.860757000	0.019496000
7	-0.624449000	-1.277326000	0.080926000

7	0.477347000	0.678202000	-0.085402000
6	2.110269000	-0.602995000	1.758928000
8	2.132090000	-0.701129000	2.897370000
6	2.175107000	-0.602833000	-1.911791000
8	2.226921000	-0.703459000	-3.049826000
6	3.279146000	0.977521000	-0.015436000
7	3.989913000	1.901564000	0.047876000
6	3.646727000	-1.600132000	-0.022829000
7	4.658294000	-2.192463000	0.030203000
6	5.891215000	-2.871414000	0.094445000
1	5.747617000	-3.939074000	-0.092887000
1	6.579178000	-2.473329000	-0.655737000
1	6.337644000	-2.745525000	1.084037000
6	4.636898000	3.154522000	0.113550000
1	5.091847000	3.286517000	1.097673000
1	5.415533000	3.213454000	-0.650063000
1	3.900305000	3.944467000	-0.053731000
25	2.130800000	-0.525887000	-0.075969000
6	0.610983000	2.095207000	-0.071389000
6	0.998233000	2.771568000	-1.225524000
6	0.430301000	2.791949000	1.119098000
6	1.176913000	4.146884000	-1.190496000
1	1.127135000	2.220413000	-2.150984000
6	0.617320000	4.169141000	1.148097000
1	0.119154000	2.257039000	2.010383000
6	0.990049000	4.850472000	-0.003414000
1	1.441671000	4.675368000	-2.100993000
1	0.448751000	4.710614000	2.073120000
1	1.114800000	5.928286000	0.016617000
6	-1.850639000	-2.027823000	-0.044545000
6	-2.756122000	-2.078385000	1.006614000
6	-2.105791000	-2.697643000	-1.235442000
6	-3.922714000	-2.818917000	0.866869000
1	-2.558195000	-1.525149000	1.918402000
6	-3.267911000	-3.446031000	-1.363160000
1	-1.403908000	-2.618468000	-2.059073000
6	-4.175270000	-3.510789000	-0.311119000
1	-4.639784000	-2.843171000	1.680162000
1	-3.475447000	-3.961149000	-2.295157000
1	-5.089730000	-4.084584000	-0.418709000
7	0.694744000	-3.185047000	0.206336000
6	1.826466000	-3.943664000	-0.292563000
1	2.343152000	-3.385156000	-1.066590000
1	2.527030000	-4.200067000	0.510524000
1	1.446327000	-4.872896000	-0.729035000
6	-0.203408000	-4.006532000	1.017912000

1	-0.707186000	-3.403643000	1.768062000
1	-0.951570000	-4.532343000	0.418792000
1	0.419583000	-4.742010000	1.534912000
31	-2.497983000	1.154898000	0.000259000
17	-4.068031000	0.180499000	-1.183506000
17	-2.407609000	3.179618000	-0.824055000
17	-2.970999000	1.234322000	2.164505000

2'^c-GaCl₃, TE = -5710.511336

6	-0.700510000	0.068159000	-0.131069000
6	0.590124000	-1.905873000	-0.053832000
7	-0.645076000	-1.336255000	-0.100946000
7	0.473969000	0.602048000	-0.128844000
6	2.056008000	-0.659634000	1.798379000
8	2.061093000	-0.706146000	2.938839000
6	2.210598000	-0.743954000	-1.875182000
8	2.305364000	-0.844428000	-3.009192000
6	3.290145000	0.838471000	0.001200000
7	4.010513000	1.753997000	0.051259000
6	3.578231000	-1.781392000	0.043180000
7	4.561503000	-2.418180000	0.095331000
6	5.761801000	-3.155232000	0.155469000
1	5.550622000	-4.227534000	0.128234000
1	6.400206000	-2.900999000	-0.694168000
1	6.296094000	-2.925470000	1.080535000
6	4.685613000	2.993123000	0.102773000
1	5.140861000	3.126053000	1.086404000
1	5.466126000	3.024173000	-0.660298000
1	3.965905000	3.795970000	-0.075786000
25	2.105303000	-0.648004000	-0.042054000
6	0.627293000	2.017390000	-0.081603000
6	1.038781000	2.706933000	-1.219253000
6	0.435328000	2.695633000	1.117236000
6	1.232642000	4.079559000	-1.159759000
1	1.172898000	2.168699000	-2.151684000
6	0.637091000	4.070197000	1.170326000
1	0.099532000	2.151644000	1.993586000
6	1.035377000	4.765567000	0.035765000
1	1.516192000	4.619626000	-2.057690000
1	0.459774000	4.598791000	2.101088000
1	1.171761000	5.841398000	0.075416000
6	-1.842352000	-2.141498000	-0.045918000
6	-2.525173000	-2.259884000	1.155302000
6	-2.273719000	-2.803224000	-1.187488000
6	-3.671026000	-3.044664000	1.207044000
1	-2.183080000	-1.718140000	2.030044000

6	-3.411379000	-3.593141000	-1.124179000
1	-1.732726000	-2.680076000	-2.119413000
6	-4.110794000	-3.713214000	0.072315000
1	-4.224007000	-3.122111000	2.136795000
1	-3.764381000	-4.100428000	-2.015623000
1	-5.009670000	-4.319411000	0.115071000
8	0.467183000	-3.211125000	0.001559000
6	1.611871000	-4.050119000	0.066550000
1	2.237488000	-3.913616000	-0.816570000
1	2.184587000	-3.845987000	0.972182000
1	1.219184000	-5.065730000	0.094038000
31	-2.510978000	1.084683000	-0.044362000
17	-4.146118000	0.056592000	-1.071266000
17	-2.406899000	3.073528000	-0.947813000
17	-2.845265000	1.202303000	2.139880000

3a-GaCl₃, TE = -5251.757287

6	-0.949256000	0.413872000	-0.331209000
6	0.907644000	0.427219000	-1.734319000
1	1.239596000	0.587542000	-2.767635000
7	-0.413231000	0.583183000	-1.630244000
7	-0.017143000	0.244675000	0.541150000
6	-1.274723000	0.939230000	-2.752824000
1	-1.912543000	1.784613000	-2.491137000
1	-0.637863000	1.213679000	-3.593817000
1	-1.918834000	0.105663000	-3.034951000
6	-0.340017000	0.061110000	1.939824000
1	-0.150561000	-0.979184000	2.220867000
1	0.323277000	0.697359000	2.531386000
1	-1.374061000	0.311772000	2.183413000
25	1.890622000	0.001681000	-0.170797000
6	2.688472000	-0.408646000	1.501109000
7	3.182086000	-0.666922000	2.533967000
6	3.444819000	-0.237331000	-1.129236000
7	4.400118000	-0.374492000	-1.803262000
6	2.283441000	1.817984000	0.118985000
7	2.503367000	2.953492000	0.310083000
6	1.375022000	-1.815558000	-0.335157000
7	0.923514000	-2.892207000	-0.400633000
6	0.175589000	-4.089873000	-0.443436000
1	0.187635000	-4.501839000	-1.455221000
1	0.603057000	-4.824383000	0.242976000
1	-0.856979000	-3.877971000	-0.151701000
6	3.749025000	-1.003763000	3.777772000
1	4.718707000	-1.488099000	3.633987000
1	3.892171000	-0.104803000	4.382907000

1	3.090788000	-1.688460000	4.319252000
6	5.567619000	-0.596682000	-2.555715000
1	5.397461000	-1.378212000	-3.301761000
1	5.867252000	0.318197000	-3.074658000
1	6.388389000	-0.910917000	-1.904143000
6	2.698676000	4.330155000	0.533089000
1	3.471016000	4.485264000	1.290845000
1	3.010210000	4.822541000	-0.391864000
1	1.768833000	4.788812000	0.879309000
31	-2.934989000	0.141056000	0.082902000
17	-2.983859000	-1.934213000	0.873928000
17	-4.309900000	0.216851000	-1.629372000
17	-3.611965000	1.615199000	1.566689000

3b-GaCl₃, TE = -5385.539736

6	-1.064621000	-0.146683000	0.466162000
6	0.790128000	-1.558986000	0.084544000
7	-0.557330000	-1.451216000	0.337701000
7	-0.166210000	0.766857000	0.527861000
25	1.743895000	0.201274000	0.046044000
6	2.351383000	1.967700000	0.010474000
7	2.751033000	3.073004000	-0.018543000
6	3.411262000	-0.304576000	-0.545237000
7	4.496021000	-0.542837000	-0.945424000
6	1.102166000	0.364894000	-1.728884000
7	0.593786000	0.486949000	-2.776202000
6	2.217209000	0.039177000	1.854623000
7	2.491765000	-0.060086000	2.992433000
6	2.745947000	-0.167226000	4.372686000
1	2.987231000	-1.200707000	4.636559000
1	3.587689000	0.470908000	4.654937000
1	1.865475000	0.142002000	4.942487000
6	3.145736000	4.423033000	-0.058024000
1	3.842845000	4.639668000	0.756137000
1	3.638407000	4.648082000	-1.008023000
1	2.274189000	5.075851000	0.045874000
6	5.779630000	-0.737436000	-1.483754000
1	5.983510000	-1.804092000	-1.622118000
1	5.867488000	-0.241588000	-2.455458000
1	6.542635000	-0.326309000	-0.815774000
6	-0.221389000	0.680503000	-3.913855000
1	0.169368000	1.500932000	-4.520532000
1	-0.242386000	-0.228515000	-4.519751000
1	-1.237320000	0.922095000	-3.588105000
6	-0.562686000	2.148514000	0.703268000
6	-1.339632000	-2.515813000	0.977608000

7	1.201211000	-2.813412000	-0.185181000
6	2.601898000	-3.171537000	-0.116274000
1	2.683784000	-4.187619000	0.284176000
1	3.074017000	-3.149697000	-1.106342000
1	3.124580000	-2.487623000	0.545874000
6	0.383875000	-3.814727000	-0.859480000
1	0.080497000	-4.633922000	-0.198790000
1	-0.503039000	-3.353618000	-1.290803000
1	0.976598000	-4.238160000	-1.676824000
1	-1.600408000	2.250231000	1.031792000
1	0.088055000	2.598789000	1.457593000
1	-0.436318000	2.700661000	-0.232428000
1	-0.655145000	-3.168143000	1.524000000
1	-2.020709000	-2.058389000	1.695978000
1	-1.937144000	-3.099929000	0.278947000
31	-3.047915000	0.209981000	0.146183000
17	-4.022851000	0.948155000	1.969445000
17	-4.086336000	-1.576369000	-0.624941000
17	-3.125123000	1.700685000	-1.498259000

3c-GaCl₃, TE = -5366.174146

6	1.058657000	-0.451199000	0.294284000
6	-0.817582000	-1.576857000	-0.543820000
7	0.515942000	-1.602898000	-0.296947000
7	0.161162000	0.382819000	0.684329000
25	-1.754467000	0.057685000	0.007408000
6	-2.367917000	1.699155000	0.681877000
7	-2.766400000	2.722559000	1.097355000
6	-3.423420000	-0.191175000	-0.732440000
7	-4.509984000	-0.271273000	-1.184866000
6	-2.243665000	-0.794793000	1.605689000
7	-2.525975000	-1.327638000	2.612734000
6	-1.111387000	0.918571000	-1.558303000
7	-0.601343000	1.437382000	-2.473479000
6	0.213010000	2.028614000	-3.465431000
1	0.209461000	1.412235000	-4.367429000
1	-0.161643000	3.024286000	-3.713654000
1	1.234663000	2.108607000	-3.083216000
6	-3.148755000	3.982120000	1.596742000
1	-3.590149000	4.587237000	0.800344000
1	-3.884546000	3.865847000	2.396849000
1	-2.277812000	4.509955000	1.995351000
6	-5.811637000	-0.245321000	-1.716976000
1	-5.930667000	0.605562000	-2.394493000
1	-6.018872000	-1.162706000	-2.276477000
1	-6.551150000	-0.156491000	-0.915530000

6	-2.778064000	-1.954502000	3.848332000
1	-3.700424000	-1.567087000	4.288951000
1	-2.881112000	-3.034404000	3.712302000
1	-1.952071000	-1.766706000	4.539460000
6	0.548334000	1.603044000	1.360138000
6	1.322445000	-2.803652000	-0.499305000
8	-1.168145000	-2.741243000	-1.074915000
6	-2.525815000	-2.971457000	-1.417033000
1	-2.840361000	-2.289815000	-2.208384000
1	-2.566323000	-4.001810000	-1.771021000
1	-3.170103000	-2.844815000	-0.545828000
1	2.263273000	-2.695181000	0.033119000
1	0.782447000	-3.668195000	-0.112345000
1	1.538436000	-2.963363000	-1.557171000
1	-0.101662000	1.733173000	2.229598000
1	1.585318000	1.588186000	1.703285000
1	0.410052000	2.460797000	0.695973000
31	3.045719000	0.035892000	0.171510000
17	3.056804000	1.998682000	-0.873874000
17	4.258089000	-1.304069000	-1.080938000
17	3.920033000	0.175264000	2.181354000

3'a-GaCl₃, TE = -5634.760432

6	-0.723102000	-0.002188000	-0.010126000
6	0.541041000	1.967133000	-0.010866000
1	0.460452000	3.059131000	0.033849000
7	-0.682821000	1.410106000	0.008222000
7	0.472935000	-0.496259000	0.002860000
25	2.050214000	0.842601000	-0.024761000
6	3.411450000	-0.489010000	0.027637000
7	4.231492000	-1.323864000	0.083090000
6	3.201377000	2.278654000	-0.050912000
7	3.878319000	3.240507000	-0.066444000
6	2.072699000	0.826272000	1.862154000
7	2.066752000	0.800591000	3.032267000
6	2.063195000	0.769415000	-1.912306000
7	2.037897000	0.716433000	-3.081751000
6	1.893801000	0.640690000	-4.482077000
1	1.733955000	1.638697000	-4.897812000
1	2.792338000	0.210843000	-4.931331000
1	1.035431000	0.012377000	-4.732997000
6	5.012400000	-2.495310000	0.156446000
1	5.743067000	-2.512807000	-0.655897000
1	5.546764000	-2.531013000	1.108910000
1	4.362078000	-3.371365000	0.076938000
6	4.736419000	4.355363000	-0.086886000

1	4.520474000	4.986176000	-0.953676000
1	4.604289000	4.953737000	0.818826000
1	5.780073000	4.032414000	-0.142199000
6	1.995494000	0.734621000	4.437777000
1	2.956599000	1.013229000	4.877014000
1	1.226004000	1.416928000	4.807461000
1	1.744675000	-0.282013000	4.750686000
6	0.662273000	-1.898354000	0.109825000
6	1.311151000	-2.595465000	-0.908427000
6	0.254665000	-2.572451000	1.257631000
6	1.524146000	-3.959956000	-0.786561000
1	1.615775000	-2.062962000	-1.802254000
6	0.480697000	-3.939118000	1.377633000
1	-0.259041000	-2.027869000	2.042385000
6	1.114567000	-4.637772000	0.359419000
1	1.994513000	-4.503761000	-1.600340000
1	0.140042000	-4.458976000	2.267090000
1	1.274195000	-5.707424000	0.447537000
6	-1.863766000	2.215203000	0.140839000
6	-2.683576000	2.068739000	1.252030000
6	-2.141767000	3.173536000	-0.826697000
6	-3.802295000	2.882077000	1.383307000
1	-2.465663000	1.307557000	1.993006000
6	-3.253109000	3.990840000	-0.680563000
1	-1.504338000	3.253037000	-1.700947000
6	-4.086436000	3.845016000	0.423371000
1	-4.454800000	2.754822000	2.240354000
1	-3.480662000	4.729683000	-1.441778000
1	-4.963986000	4.474283000	0.528107000
31	-2.486423000	-1.050027000	-0.205036000
17	-3.932078000	0.106900000	-1.387531000
17	-3.226368000	-1.431083000	1.848055000
17	-2.190873000	-2.927530000	-1.295898000

3'b-GaCl₃, TE = -5768.538928

6	-0.762451000	0.143317000	0.142936000
6	0.526562000	-1.853487000	0.005352000
7	-0.727721000	-1.256958000	-0.001522000
7	0.409312000	0.672269000	0.235853000
25	2.037869000	-0.547339000	-0.016312000
6	3.212461000	0.908244000	-0.143524000
7	3.950665000	1.816754000	-0.229182000
6	3.468184000	-1.645428000	-0.385894000
7	4.427088000	-2.278782000	-0.654566000
6	1.633620000	-0.407412000	-1.856967000
7	1.284293000	-0.286234000	-2.968571000

6	2.322018000	-0.660548000	1.837794000
7	2.491207000	-0.733699000	2.997959000
6	2.665452000	-0.768842000	4.394544000
1	2.939074000	-1.776682000	4.718663000
1	3.457534000	-0.077864000	4.695753000
1	1.738602000	-0.480022000	4.897674000
6	4.586730000	3.073667000	-0.293656000
1	5.350291000	3.151029000	0.484813000
1	5.067141000	3.204127000	-1.266925000
1	3.846597000	3.865759000	-0.150059000
6	5.643047000	-2.878747000	-1.027788000
1	5.598760000	-3.962840000	-0.885078000
1	5.860642000	-2.678739000	-2.081404000
1	6.466158000	-2.485198000	-0.423532000
6	0.665805000	-0.039665000	-4.213914000
1	1.224636000	0.718343000	-4.768334000
1	0.634589000	-0.956736000	-4.807370000
1	-0.355360000	0.315724000	-4.046097000
6	0.585981000	2.078605000	0.310204000
6	0.945693000	2.665616000	1.521035000
6	0.492632000	2.861329000	-0.837299000
6	1.181401000	4.031466000	1.586471000
1	1.019454000	2.045107000	2.407464000
6	0.736448000	4.227317000	-0.766905000
1	0.200283000	2.398735000	-1.773541000
6	1.080426000	4.818422000	0.442730000
1	1.430994000	4.487467000	2.539538000
1	0.632404000	4.834947000	-1.660160000
1	1.250275000	5.888785000	0.499505000
6	-1.952041000	-1.987326000	0.213261000
6	-2.898937000	-2.106522000	-0.795980000
6	-2.165252000	-2.580820000	1.452435000
6	-4.054471000	-2.842335000	-0.569370000
1	-2.736876000	-1.607720000	-1.745601000
6	-3.319396000	-3.320862000	1.671552000
1	-1.427475000	-2.454668000	2.237981000
6	-4.262333000	-3.458128000	0.658491000
1	-4.800819000	-2.920009000	-1.352596000
1	-3.490129000	-3.778225000	2.640652000
1	-5.168863000	-4.027712000	0.834601000
7	0.560929000	-3.189281000	-0.141869000
6	1.711896000	-3.939421000	0.321722000
1	1.351950000	-4.819481000	0.866878000
1	2.335653000	-4.280237000	-0.512673000
1	2.307769000	-3.326546000	0.990967000
6	-0.385910000	-4.027961000	-0.871245000

1	-1.115843000	-4.516576000	-0.218827000
1	-0.916303000	-3.449941000	-1.623169000
1	0.197047000	-4.798203000	-1.385440000
31	-2.531242000	1.196723000	-0.021405000
17	-2.499268000	3.266026000	0.690497000
17	-4.272007000	0.337062000	1.003482000
17	-2.763563000	1.168741000	-2.251919000

3'^c-GaCl₃, TE = -5749.175088

6	0.770931000	0.086806000	-0.261842000
6	-0.515811000	-1.884446000	-0.072244000
7	0.725403000	-1.311219000	-0.186213000
7	-0.407186000	0.613671000	-0.277817000
25	-2.013712000	-0.647283000	0.056806000
6	-3.208414000	0.809535000	0.165333000
7	-3.940448000	1.721470000	0.238327000
6	-3.415432000	-1.771964000	0.458560000
7	-4.360980000	-2.423916000	0.726965000
6	-1.573172000	-0.445117000	1.888233000
7	-1.198402000	-0.293260000	2.986018000
6	-2.352127000	-0.813059000	-1.784480000
7	-2.553904000	-0.917363000	-2.935705000
6	-2.759512000	-1.010661000	-4.325787000
1	-3.024576000	-2.034730000	-4.601961000
1	-3.568606000	-0.343508000	-4.634627000
1	-1.848476000	-0.728811000	-4.860304000
6	-4.586474000	2.973897000	0.298294000
1	-5.391252000	3.018780000	-0.439727000
1	-5.013460000	3.129144000	1.292281000
1	-3.862056000	3.766181000	0.090794000
6	-5.569201000	-3.048081000	1.088590000
1	-6.325864000	-2.892935000	0.313788000
1	-5.423791000	-4.124689000	1.217973000
1	-5.945677000	-2.634816000	2.029137000
6	-0.556441000	-0.041375000	4.218661000
1	-1.124303000	0.693077000	4.794696000
1	-0.482510000	-0.964678000	4.798238000
1	0.448594000	0.345886000	4.026925000
6	-0.585714000	2.021743000	-0.312708000
6	-1.006670000	2.628001000	-1.494436000
6	-0.426059000	2.787225000	0.838709000
6	-1.236011000	3.996074000	-1.529109000
1	-1.130718000	2.020546000	-2.384479000
6	-0.663438000	4.155975000	0.799230000
1	-0.083841000	2.311583000	1.750619000
6	-1.067368000	4.766347000	-0.381782000

1	-1.532512000	4.466753000	-2.461393000
1	-0.507163000	4.750134000	1.693871000
1	-1.231630000	5.838562000	-0.414760000
6	1.921994000	-2.113192000	-0.214555000
6	2.622904000	-2.337059000	0.961573000
6	2.340160000	-2.678875000	-1.411536000
6	3.764411000	-3.128432000	0.934544000
1	2.293344000	-1.866189000	1.880954000
6	3.477163000	-3.473340000	-1.431063000
1	1.782501000	-2.481237000	-2.320697000
6	4.189530000	-3.699130000	-0.258180000
1	4.328728000	-3.286834000	1.847292000
1	3.816663000	-3.905331000	-2.366591000
1	5.085865000	-4.310370000	-0.277981000
8	-0.366939000	-3.195602000	-0.055447000
6	-1.505606000	-4.036202000	0.042869000
1	-2.227641000	-3.801131000	-0.740038000
1	-1.126353000	-5.050512000	-0.081656000
1	-1.975414000	-3.928800000	1.021529000
31	2.550750000	1.105279000	-0.057335000
17	4.331774000	0.140398000	-0.885609000
17	2.532901000	3.118172000	-0.913355000
17	2.668617000	1.171046000	2.179238000

4'a-GaCl₃, TE = -5748.079515

6	0.638627000	0.062453000	0.097641000
6	-0.559655000	2.108903000	-0.416151000
1	-0.487898000	2.444293000	-1.457866000
7	-0.564210000	-0.464371000	0.180939000
1	-0.628658000	3.011023000	0.201905000
6	-3.247351000	2.169641000	-0.560205000
6	-1.961181000	1.278857000	1.640210000
6	-1.797818000	0.308037000	-1.934423000
7	-3.941528000	3.067292000	-0.839277000
7	-1.407801000	-0.052757000	-2.970357000
7	-1.771101000	1.563949000	2.753956000
6	-1.414469000	1.885108000	4.081259000
1	-0.411713000	2.318200000	4.096763000
1	-2.123627000	2.605546000	4.494266000
1	-1.423877000	0.981736000	4.694870000
6	-4.759113000	4.159396000	-1.194589000
1	-4.291803000	5.094907000	-0.878286000
1	-4.899836000	4.182908000	-2.277743000
1	-5.735412000	4.069555000	-0.712475000
6	-0.702778000	-0.589435000	-4.076032000
1	-0.237923000	0.220019000	-4.641895000

1	0.073781000	-1.262641000	-3.700273000
1	-1.388589000	-1.137057000	-4.725146000
6	-0.718316000	-1.829770000	0.508018000
6	-1.500393000	-2.680628000	-0.278350000
6	-0.121368000	-2.342679000	1.660603000
6	-1.668087000	-4.010485000	0.075986000
1	-1.940713000	-2.301591000	-1.193033000
6	-0.283869000	-3.679155000	2.007526000
1	0.488171000	-1.690532000	2.276066000
6	-1.061558000	-4.518765000	1.222333000
1	-2.249212000	-4.665930000	-0.566298000
1	0.210361000	-4.061825000	2.894578000
1	-1.181569000	-5.563747000	1.488643000
26	-2.093811000	0.812082000	-0.150973000
6	-3.449001000	-0.427113000	0.190429000
7	-4.295900000	-1.185727000	0.454344000
6	-5.128486000	-2.273663000	0.792299000
1	-5.872317000	-2.434385000	0.008881000
1	-4.512979000	-3.171105000	0.900164000
1	-5.642697000	-2.072544000	1.734588000
7	0.678707000	1.405717000	-0.058888000
6	1.830947000	2.162623000	0.246876000
6	2.112699000	3.333806000	-0.459007000
6	2.666721000	1.784279000	1.299500000
6	3.229024000	4.090615000	-0.134601000
1	1.471111000	3.635642000	-1.278623000
6	3.793497000	2.535832000	1.602894000
1	2.443924000	0.891522000	1.873911000
6	4.079991000	3.694249000	0.891887000
1	3.445018000	4.990517000	-0.701971000
1	4.446267000	2.210775000	2.406419000
1	4.958699000	4.282986000	1.133006000
31	2.314775000	-1.053678000	-0.346626000
17	3.671705000	0.127730000	-1.611662000
17	1.633014000	-2.692803000	-1.676517000
17	3.366868000	-1.829028000	1.427627000

4'b-GaCl₃, TE = -8895.571549

6	-0.796338000	-0.081245000	0.145251000
6	0.516529000	-2.078869000	-0.360031000
1	0.442053000	-2.439763000	-1.392382000
7	0.362198000	0.540240000	0.242718000
1	0.629407000	-2.962886000	0.276370000
6	3.416701000	-1.953813000	-0.614010000
6	2.081421000	-1.156681000	1.749438000
6	1.647048000	-0.145137000	-2.026113000

7	4.194650000	-2.775701000	-0.912464000
7	1.172013000	0.187352000	-3.034420000
7	1.983444000	-1.457184000	2.871117000
6	1.771307000	-1.797204000	4.223880000
1	0.795312000	-2.275125000	4.333556000
1	2.548430000	-2.486571000	4.560791000
1	1.799847000	-0.895966000	4.840118000
6	5.110760000	-3.774615000	-1.296825000
1	4.927248000	-4.690506000	-0.729677000
1	5.001806000	-3.992262000	-2.362170000
1	6.133830000	-3.440248000	-1.107536000
6	0.387719000	0.666672000	-4.112595000
1	-0.021505000	-0.177748000	-4.670066000
1	-0.431444000	1.266818000	-3.704439000
1	1.003285000	1.276612000	-4.776279000
6	0.400101000	1.915486000	0.569386000
6	1.133970000	2.820997000	-0.201138000
6	-0.265882000	2.382454000	1.703036000
6	1.187595000	4.160972000	0.149805000
1	1.625339000	2.472628000	-1.101871000
6	-0.217586000	3.728874000	2.045931000
1	-0.836061000	1.686574000	2.308048000
6	0.512658000	4.624033000	1.276816000
1	1.732111000	4.857924000	-0.480746000
1	-0.762650000	4.074726000	2.918167000
1	0.543786000	5.675979000	1.540848000
6	3.414175000	0.793112000	0.153223000
7	4.174670000	1.649834000	0.382136000
6	4.894850000	2.824391000	0.685913000
1	5.553264000	3.085778000	-0.145529000
1	4.189102000	3.641120000	0.860927000
1	5.499660000	2.671502000	1.582458000
7	-0.753311000	-1.423962000	-0.004510000
6	-1.869350000	-2.237429000	0.298899000
6	-2.091153000	-3.423476000	-0.403077000
6	-2.727008000	-1.894683000	1.345524000
6	-3.171736000	-4.230945000	-0.080298000
1	-1.432540000	-3.698238000	-1.218396000
6	-3.819036000	-2.696697000	1.646333000
1	-2.548379000	-0.991199000	1.917940000
6	-4.046372000	-3.870449000	0.939515000
1	-3.341532000	-5.142736000	-0.644290000
1	-4.490317000	-2.399306000	2.445232000
1	-4.897323000	-4.499273000	1.178954000
44	2.082020000	-0.650723000	-0.147165000
31	-2.530028000	0.909281000	-0.345410000

17	-3.751625000	-0.367413000	-1.649658000
17	-1.939777000	2.584684000	-1.670019000
17	-3.696754000	1.625537000	1.373072000

5a-GaCl₃, TE = - 5787.273151

6	1.319622000	1.291931000	-0.972713000
6	-0.765603000	-0.000448000	-0.476887000
6	1.319646000	-1.293031000	-0.972192000
7	-0.105393000	-1.155697000	-0.614229000
7	-0.105396000	1.154774000	-0.614628000
6	-0.743867000	-2.402404000	-0.317676000
6	-0.793608000	-3.392641000	-1.297714000
6	-1.238024000	-2.660202000	0.953887000
6	-1.358955000	-4.623110000	-1.007732000
1	-0.413081000	-3.178352000	-2.290353000
6	-1.817085000	-3.893188000	1.236165000
1	-1.196085000	-1.888737000	1.712030000
6	-1.875850000	-4.877102000	0.260507000
1	-1.417470000	-5.382327000	-1.780917000
1	-2.226550000	-4.076509000	2.224043000
1	-2.331656000	-5.836929000	0.480185000
6	-0.743787000	2.401613000	-0.318454000
6	-0.793366000	3.391614000	-1.298743000
6	-1.237920000	2.659833000	0.953034000
6	-1.358498000	4.622258000	-1.009100000
1	-0.412843000	3.177032000	-2.291318000
6	-1.816738000	3.893011000	1.234991000
1	-1.196097000	1.888569000	1.711387000
6	-1.875333000	4.876682000	0.259077000
1	-1.416865000	5.381287000	-1.782480000
1	-2.226172000	4.076665000	2.222820000
1	-2.330945000	5.836657000	0.478505000
1	1.402000000	-1.155459000	-2.055349000
1	1.566443000	-2.334037000	-0.763319000
1	1.566544000	2.333015000	-0.764394000
1	1.401617000	1.154047000	-2.055881000
26	2.599087000	-0.000343000	-0.037032000
6	1.543628000	-0.000387000	1.490281000
7	0.911942000	-0.000201000	2.471250000
6	3.572775000	1.404696000	0.646407000
7	4.149626000	2.336159000	1.060959000
6	3.576960000	0.000231000	-1.595420000
7	4.158408000	0.001093000	-2.610325000
6	3.573673000	-1.404918000	0.646170000
7	4.151459000	-2.335954000	1.060354000
6	4.783846000	3.490337000	1.562221000

1	5.385003000	3.240266000	2.440088000
1	5.437318000	3.921028000	0.799600000
1	4.036041000	4.235213000	1.845820000
6	0.099949000	0.000192000	3.627544000
1	0.309604000	-0.888860000	4.226986000
1	0.308476000	0.890462000	4.225573000
1	-0.955624000	-0.000669000	3.338069000
6	4.788071000	-3.488517000	1.562290000
1	5.444608000	-3.916668000	0.800879000
1	5.386452000	-3.237153000	2.441682000
1	4.041924000	-4.235871000	1.843735000
6	4.842826000	0.000848000	-3.842655000
1	4.953033000	-1.022001000	-4.210738000
1	4.285110000	0.582902000	-4.580055000
1	5.835055000	0.442044000	-3.721168000
31	-2.835822000	-0.000381000	-0.260229000
17	-3.288592000	0.000121000	1.930461000
17	-3.796801000	1.723935000	-1.215407000
17	-3.797119000	-1.724913000	-1.214651000

5b-GaCl₃, TE = -8934.767330

6	-1.129940000	1.325845000	1.019317000
6	0.939372000	-0.000011000	0.497492000
6	-1.129964000	-1.325902000	1.019239000
7	0.288983000	-1.160878000	0.641217000
7	0.288990000	1.160856000	0.641245000
6	0.937095000	-2.401592000	0.334852000
6	1.017455000	-3.388287000	1.316206000
6	1.406917000	-2.657176000	-0.946011000
6	1.588577000	-4.613765000	1.017415000
1	0.655702000	-3.175330000	2.316094000
6	1.992529000	-3.885087000	-1.237159000
1	1.340658000	-1.888072000	-1.704776000
6	2.081281000	-4.865831000	-0.260773000
1	1.670847000	-5.370262000	1.791048000
1	2.383247000	-4.066927000	-2.232837000
1	2.541850000	-5.821651000	-0.487747000
6	0.937073000	2.401575000	0.334844000
6	1.017453000	3.388282000	1.316183000
6	1.406838000	2.657157000	-0.946042000
6	1.588545000	4.613767000	1.017358000
1	0.655748000	3.175330000	2.316089000
6	1.992419000	3.885074000	-1.237226000
1	1.340530000	1.888057000	-1.704805000
6	2.081196000	4.865829000	-0.260850000
1	1.670832000	5.370270000	1.790983000

1	2.383086000	4.066916000	-2.232923000
1	2.541742000	5.821652000	-0.487853000
1	-1.203027000	-1.177087000	2.101600000
1	-1.357874000	-2.373370000	0.825812000
1	-1.357857000	2.373331000	0.825996000
1	-1.202981000	1.176929000	2.101666000
6	-1.381238000	-0.000066000	-1.588656000
7	-0.731684000	-0.000199000	-2.556925000
6	-3.561447000	1.492392000	-0.697942000
7	-4.135499000	2.427281000	-1.109830000
6	-3.531602000	-0.000062000	1.705339000
7	-4.100548000	-0.000155000	2.726648000
6	-3.561659000	-1.492165000	-0.698045000
7	-4.135929000	-2.426888000	-1.110008000
6	-4.779951000	3.573882000	-1.614579000
1	-5.401769000	3.310710000	-2.474184000
1	-5.414880000	4.017417000	-0.843642000
1	-4.038370000	4.313412000	-1.927158000
6	0.099993000	-0.000425000	-3.699130000
1	-0.100180000	0.889056000	-4.300988000
1	1.149823000	0.000171000	-3.389300000
1	-0.099389000	-0.890722000	-4.300046000
6	-4.780680000	-3.573283000	-1.614840000
1	-5.415679000	-4.016744000	-0.843918000
1	-5.402468000	-3.309883000	-2.474397000
1	-4.039290000	-4.312964000	-1.927517000
6	-4.785217000	-0.000276000	3.958723000
1	-5.416453000	-0.888735000	4.036382000
1	-4.068564000	-0.002136000	4.783246000
1	-5.413753000	0.889948000	4.038055000
44	-2.507877000	0.000013000	0.035117000
31	3.001995000	0.000006000	0.258221000
17	3.436338000	0.000032000	-1.933269000
17	3.984517000	1.715571000	1.196523000
17	3.984602000	-1.715572000	1.196416000

6a-GaCl₃, TE = -5935.294079

6	-1.343456000	1.330888000	-0.710792000
7	0.140817000	1.168069000	-0.553702000
6	0.775533000	-0.000038000	-0.376963000
7	0.140882000	-1.168230000	-0.553493000
6	-1.343371000	-1.331177000	-0.710401000
8	-1.672774000	2.327366000	-1.301938000
6	0.919502000	2.356580000	-0.754143000
6	0.661353000	3.494320000	0.005235000
6	1.402488000	4.642927000	-0.208012000

6	2.406290000	4.662202000	-1.173909000
6	2.654616000	3.529642000	-1.934219000
6	1.898148000	2.378789000	-1.737911000
1	-0.103624000	3.464919000	0.772085000
1	1.211089000	5.524979000	0.394105000
1	2.994791000	5.560685000	-1.327855000
1	3.436442000	3.532251000	-2.685843000
1	2.076260000	1.497494000	-2.343281000
6	0.919687000	-2.356656000	-0.753975000
6	0.661740000	-3.494431000	0.005418000
6	1.403036000	-4.642928000	-0.207863000
6	2.406800000	-4.662060000	-1.173803000
6	2.654922000	-3.529469000	-1.934132000
6	1.898291000	-2.378729000	-1.737792000
1	-0.103199000	-3.465147000	0.772307000
1	1.211793000	-5.525006000	0.394265000
1	2.995427000	-5.560457000	-1.327770000
1	3.436716000	-3.531963000	-2.685791000
1	2.076244000	-1.497411000	-2.343177000
8	-1.672702000	-2.327853000	-1.301212000
26	-2.497636000	-0.000048000	0.119219000
6	-3.538108000	-1.401527000	0.794797000
6	-3.438435000	-0.000351000	-1.481255000
6	-3.538254000	1.401560000	0.794297000
6	-1.435971000	0.000291000	1.660987000
7	-4.144142000	2.323477000	1.170922000
7	-4.143910000	-2.323367000	1.171747000
7	-3.984390000	-0.000568000	-2.507955000
7	-0.767690000	0.000542000	2.612671000
6	0.131143000	0.000757000	3.707456000
1	0.773668000	-0.879870000	3.643612000
1	0.767075000	0.886465000	3.648749000
1	-0.431560000	-0.004029000	4.643184000
6	-4.808516000	3.511887000	1.539634000
1	-4.478643000	3.830366000	2.530868000
1	-4.578918000	4.297729000	0.816554000
1	-5.887864000	3.346240000	1.560757000
6	-4.524590000	-0.000887000	-3.810322000
1	-4.188402000	-0.891782000	-4.345122000
1	-5.615602000	-0.000422000	-3.763468000
1	-4.187680000	0.889295000	-4.345853000
6	-4.808250000	-3.511688000	1.540805000
1	-5.887300000	-3.344777000	1.566650000
1	-4.582530000	-4.296392000	0.815272000
1	-4.474729000	-3.832524000	2.530057000
31	2.682435000	0.000099000	0.477115000

17	2.815636000	1.723062000	1.853233000
17	4.327804000	0.000212000	-0.966536000
17	2.815904000	-1.723123000	1.852978000

6b-GaCl₃, TE = - 9082.783511

6	-1.169678000	-1.384206000	0.746976000
7	0.311332000	-1.175580000	0.581096000
6	0.930582000	0.000129000	0.388368000
7	0.311928000	1.176300000	0.580515000
6	-1.169020000	1.385509000	0.746211000
8	-1.467399000	-2.388499000	1.340457000
6	1.117956000	-2.345256000	0.788053000
6	0.882838000	-3.497674000	0.043156000
6	1.647925000	-4.627671000	0.269873000
6	2.652826000	-4.614468000	1.234754000
6	2.879060000	-3.467598000	1.980052000
6	2.098944000	-2.335153000	1.769752000
1	0.116519000	-3.494324000	-0.722598000
1	1.473995000	-5.520847000	-0.320967000
1	3.259634000	-5.498805000	1.399221000
1	3.661871000	-3.444500000	2.730246000
1	2.259202000	-1.442964000	2.363995000
6	1.119359000	2.345323000	0.787719000
6	0.884119000	3.498568000	0.044152000
6	1.650756000	4.627602000	0.270489000
6	2.657384000	4.612582000	1.233517000
6	2.883698000	3.464890000	1.977549000
6	2.101995000	2.333460000	1.767791000
1	0.116696000	3.496591000	-0.720509000
1	1.476736000	5.521415000	-0.319363000
1	3.265444000	5.496132000	1.397571000
1	3.667802000	3.440376000	2.726350000
1	2.262420000	1.440659000	2.361099000
8	-1.466432000	2.390157000	1.339268000
6	-3.550374000	1.501509000	-0.814608000
6	-3.384972000	0.001206000	1.612571000
6	-3.551482000	-1.499403000	-0.814354000
6	-1.307642000	-0.000534000	-1.759877000
7	-4.146757000	-2.436743000	-1.170542000
7	-4.144689000	2.439573000	-1.170503000
7	-3.898149000	0.001373000	2.656231000
7	-0.626565000	-0.001879000	-2.701703000
6	0.275733000	-0.002262000	-3.793277000
1	0.969772000	0.833681000	-3.681848000
1	0.855878000	-0.926704000	-3.776813000
1	-0.282239000	0.083544000	-4.727889000

6	-4.799382000	-3.632919000	-1.534664000
1	-4.552787000	-3.891203000	-2.566803000
1	-4.474697000	-4.441556000	-0.876019000
1	-5.881157000	-3.510264000	-1.447272000
6	-4.418787000	0.001439000	3.966589000
1	-4.074255000	0.891972000	4.496553000
1	-5.510333000	0.001477000	3.934823000
1	-4.074316000	-0.889089000	4.496600000
6	-4.795712000	3.636869000	-1.533823000
1	-5.877676000	3.515439000	-1.447065000
1	-4.470350000	4.444479000	-0.874253000
1	-4.548309000	3.895844000	-2.565595000
44	-2.426482000	0.000700000	-0.112736000
31	2.805895000	-0.001510000	-0.516536000
17	4.505267000	-0.007530000	0.853795000
17	2.891733000	-1.714979000	-1.902948000
17	2.905753000	1.720652000	-1.892713000

Cartesian coordinates for the optimized geometries of protonated complex **1a-6b**, along with their total energies (in hartrees) including zero point vibrational correction in gas phase.

[1a-H]⁺, TE = -1869.856379

6	-2.133774000	0.901086000	-0.000211000
6	-1.166596000	-1.171495000	0.000351000
1	-1.339120000	-2.250916000	0.000575000
7	-2.298009000	-0.485620000	0.000166000
7	-0.939171000	1.335599000	-0.000379000
6	-3.653687000	-1.047209000	0.000248000
1	-4.190972000	-0.723262000	-0.892873000
1	-3.578608000	-2.132956000	0.000777000
1	-4.191204000	-0.722420000	0.892921000
6	-0.702484000	2.769454000	-0.000747000
1	-0.116983000	3.035052000	0.882634000
1	-0.117107000	3.034617000	-0.884342000
1	-1.634983000	3.339490000	-0.000820000
25	0.481176000	-0.145533000	0.000040000
6	0.503328000	-0.161670000	1.865793000
8	0.516033000	-0.188109000	2.997464000
6	1.513810000	-1.655768000	0.000588000
8	2.114416000	-2.618366000	0.000958000
6	1.951386000	1.012073000	-0.000441000
8	2.845442000	1.707531000	-0.000752000
6	0.503253000	-0.163086000	-1.865692000
8	0.515945000	-0.190420000	-2.997343000
1	-3.026267000	1.523459000	-0.000335000

[1b-H]⁺, TE = -2003.658090

6	-0.576209000	2.254972000	-0.101899000
6	-1.270429000	0.042590000	0.098112000
7	-1.626384000	1.377573000	0.032369000
7	0.617556000	1.819610000	-0.150723000
25	0.769240000	-0.208421000	0.012823000
6	0.860245000	-0.059476000	1.866165000
8	0.885461000	0.022443000	2.996899000
6	0.906914000	-2.020511000	0.135385000
8	1.073273000	-3.145947000	0.191035000
6	2.604311000	-0.141403000	-0.164279000
8	3.733870000	-0.107065000	-0.273110000
6	0.528202000	-0.372934000	-1.823024000
8	0.353064000	-0.490727000	-2.937591000
6	1.708395000	2.768329000	-0.297035000
6	-2.911284000	1.957709000	0.455700000
7	-2.254893000	-0.841213000	0.057405000
6	-3.555856000	-0.636649000	-0.589280000
1	-4.367250000	-0.531265000	0.134884000
1	-3.527910000	0.222791000	-1.253857000
1	-3.754771000	-1.521616000	-1.198171000
6	-2.049615000	-2.227600000	0.465347000
1	-2.985013000	-2.594273000	0.893144000
1	-1.787579000	-2.859003000	-0.388793000
1	-1.284100000	-2.288200000	1.232529000
1	-3.398577000	1.282309000	1.156500000
1	-2.710820000	2.890822000	0.982776000
1	-3.577122000	2.163579000	-0.383237000
1	1.345259000	3.799372000	-0.329607000
1	2.399861000	2.662754000	0.542348000
1	2.258368000	2.558732000	-1.217551000
1	-0.828699000	3.312929000	-0.153907000

[1c-H]⁺, TE = -1984.284153

6	1.181236000	-2.049837000	-0.000091000
6	1.408839000	0.247470000	0.000090000
7	2.026134000	-0.963587000	0.000071000
7	-0.074917000	-1.847498000	-0.000180000
25	-0.596018000	0.135239000	-0.000002000
6	-0.563444000	0.148936000	1.863529000
8	-0.533300000	0.170199000	2.995762000
6	-1.009742000	1.912191000	0.000218000
8	-1.329957000	3.003910000	0.000360000
6	-2.408134000	-0.261479000	-0.000172000
8	-3.517498000	-0.494743000	-0.000282000
6	-0.563231000	0.149416000	-1.863523000
8	-0.532960000	0.170980000	-2.995747000
6	-0.976366000	-2.987639000	-0.000318000
8	2.302834000	1.186927000	0.000095000
6	1.943303000	2.578543000	0.000173000
1	1.378652000	2.817802000	-0.900462000
1	1.378670000	2.817708000	0.900844000
1	2.889377000	3.114773000	0.000190000
6	3.482574000	-1.130367000	0.000053000
1	3.911622000	-0.667795000	-0.888953000
1	3.911716000	-0.666736000	0.888451000
1	3.712110000	-2.194869000	0.000690000
1	-0.430405000	-3.934834000	-0.000363000
1	-1.616576000	-2.947334000	0.884137000
1	-1.616480000	-2.947194000	-0.884837000
1	1.640072000	-3.036480000	-0.000129000

[1'a-H]⁺, TE = -2252.868116

6	0.635507000	1.083356000	0.050584000
6	1.173904000	-1.146952000	0.024030000
1	1.990883000	-1.872355000	0.046490000
7	1.626455000	0.101565000	0.043065000
7	-0.575056000	0.677529000	0.071872000

25	-0.749171000	-1.383104000	0.002079000
6	-0.754249000	-1.293064000	-1.861115000
8	-0.741415000	-1.246981000	-2.992560000
6	-0.587626000	-3.197213000	-0.099766000
8	-0.436768000	-4.320892000	-0.163651000
6	-2.622881000	-1.435938000	-0.013562000
8	-3.752945000	-1.504708000	-0.032709000
6	-0.752464000	-1.505625000	1.861925000
8	-0.743097000	-1.593338000	2.991278000
6	-1.613121000	1.652785000	0.001865000
6	-2.635627000	1.628451000	0.947551000
6	-1.602106000	2.614334000	-1.007559000
6	-3.634674000	2.589653000	0.894755000
1	-2.632480000	0.883694000	1.736078000
6	-2.615597000	3.563000000	-1.058644000
1	-0.826135000	2.598868000	-1.766734000
6	-3.628579000	3.554968000	-0.107613000
1	-4.422102000	2.583732000	1.640223000
1	-2.615679000	4.303930000	-1.850412000
1	-4.419162000	4.295733000	-0.150906000
6	3.018320000	0.483035000	0.059706000
6	3.480901000	1.327573000	1.061726000
6	3.863606000	-0.010649000	-0.925804000
6	4.824272000	1.680833000	1.072719000
1	2.811722000	1.686129000	1.837707000
6	5.206369000	0.343879000	-0.897242000
1	3.476362000	-0.647691000	-1.714552000
6	5.685063000	1.188869000	0.097553000
1	5.199420000	2.333275000	1.853166000
1	5.875723000	-0.032795000	-1.662464000
1	6.733082000	1.466590000	0.112552000
1	0.945535000	2.124412000	0.036815000

[1'b-H]⁺, TE = -2386.671707

6	0.274674000	-1.263642000	-0.286630000
6	1.098893000	0.919249000	-0.140528000
7	1.372864000	-0.436290000	-0.290819000
7	-0.896404000	-0.769041000	-0.177607000
25	-0.917062000	1.260060000	0.116988000
6	-0.701361000	0.978125000	1.941730000
8	-0.533378000	0.814409000	3.051907000
6	-0.950865000	3.056831000	0.381866000
8	-1.059840000	4.180232000	0.542019000
6	-2.760049000	1.283138000	0.270753000
8	-3.887732000	1.334206000	0.382377000
6	-0.976367000	1.549147000	-1.717263000
8	-0.982666000	1.745812000	-2.835108000
6	-2.003827000	-1.670852000	-0.136121000
6	-2.997716000	-1.577166000	-1.106600000
6	-2.089685000	-2.626393000	0.873502000
6	-4.071002000	-2.456600000	-1.073207000
1	-2.922161000	-0.833625000	-1.893113000
6	-3.171983000	-3.498632000	0.901453000
1	-1.325906000	-2.672219000	1.643825000
6	-4.161309000	-3.416455000	-0.070259000
1	-4.839675000	-2.391776000	-1.835434000
1	-3.242207000	-4.238800000	1.691029000
1	-5.005812000	-4.096018000	-0.043959000
6	2.650174000	-1.095125000	-0.111220000
6	3.135501000	-1.942394000	-1.100590000
6	3.335970000	-0.924632000	1.085862000
6	4.331862000	-2.617926000	-0.890340000
1	2.589835000	-2.065170000	-2.031315000
6	4.539021000	-1.593278000	1.279923000
1	2.931754000	-0.281704000	1.861229000
6	5.036937000	-2.438745000	0.294672000
1	4.714798000	-3.280956000	-1.658264000
1	5.079514000	-1.463647000	2.211172000

1	5.972012000	-2.964335000	0.453418000
7	2.101199000	1.758735000	-0.322975000
6	3.338347000	1.484108000	-1.063156000
1	4.174185000	1.277846000	-0.390575000
1	3.208131000	0.650622000	-1.747057000
1	3.564728000	2.378256000	-1.647644000
6	2.009110000	3.153417000	0.100423000
1	3.012419000	3.489935000	0.367995000
1	1.634060000	3.789050000	-0.707046000
1	1.379423000	3.247029000	0.979379000
1	0.468816000	-2.330138000	-0.373706000

[1'e-H]⁺, TE = -2367.293052

6	0.403227000	-1.272704000	-0.043064000
6	1.159534000	0.918643000	0.008649000
7	1.474729000	-0.410067000	-0.009541000
7	-0.776659000	-0.784243000	-0.065618000
25	-0.815580000	1.274985000	0.041062000
6	-0.767007000	1.147262000	1.898945000
8	-0.721248000	1.077228000	3.029111000
6	-0.796433000	3.090096000	0.171199000
8	-0.850788000	4.224192000	0.256153000
6	-2.674756000	1.326533000	0.074632000
8	-3.804883000	1.396402000	0.107598000
6	-0.791509000	1.406778000	-1.814605000
8	-0.760398000	1.501635000	-2.944121000
6	-1.880932000	-1.689891000	-0.052226000
6	-2.818894000	-1.636505000	-1.079985000
6	-2.016683000	-2.612331000	0.982599000
6	-3.885150000	-2.524624000	-1.078346000
1	-2.702564000	-0.922860000	-1.888769000
6	-3.092549000	-3.492710000	0.978229000
1	-1.299245000	-2.625005000	1.797438000
6	-4.025323000	-3.451529000	-0.050292000
1	-4.608603000	-2.493333000	-1.885563000

1	-3.202421000	-4.206825000	1.786970000
1	-4.864827000	-4.137726000	-0.049391000
6	2.821451000	-0.940474000	-0.049163000
6	3.381683000	-1.267526000	-1.276730000
6	3.509882000	-1.134465000	1.140737000
6	4.662546000	-1.805428000	-1.309470000
1	2.825475000	-1.102918000	-2.193945000
6	4.790657000	-1.670938000	1.095599000
1	3.051180000	-0.871085000	2.088124000
6	5.364377000	-2.005928000	-0.126135000
1	5.110724000	-2.067801000	-2.261297000
1	5.339071000	-1.829980000	2.017374000
1	6.363599000	-2.426397000	-0.155857000
8	2.241335000	1.626785000	-0.006401000
6	2.212249000	3.062089000	-0.005925000
1	1.664075000	3.427024000	-0.874220000
1	1.774251000	3.426808000	0.922864000
1	3.255004000	3.364245000	-0.069633000
1	0.626926000	-2.336620000	-0.061141000

[2a-H]⁺, TE = - 1908.552354

6	-2.597699000	-0.931457000	0.002254000
6	-1.569227000	1.108268000	-0.000695000
1	-1.725240000	2.191670000	-0.002040000
7	-2.731065000	0.450124000	0.000762000
7	-1.408572000	-1.388958000	0.002020000
6	-4.066618000	1.047470000	0.000525000
1	-4.617756000	0.744444000	0.893099000
1	-3.960187000	2.130814000	-0.000560000
1	-4.618220000	0.742686000	-0.891164000
6	-1.208403000	-2.824653000	0.003212000
1	-0.630814000	-3.105378000	-0.880684000
1	-0.627040000	-3.103700000	0.885089000
1	-2.153915000	-3.374909000	0.005648000
6	0.132297000	0.099991000	-1.847576000

8	0.221478000	0.156118000	-2.980691000
6	0.133809000	0.103646000	1.846758000
8	0.223659000	0.161866000	2.979733000
6	1.513737000	-1.170595000	0.000220000
7	2.418376000	-1.903594000	0.000721000
6	1.122674000	1.595273000	-0.002141000
7	1.762799000	2.569227000	-0.003119000
6	2.565777000	3.734293000	-0.003387000
1	2.369095000	4.316625000	-0.905481000
1	2.335123000	4.340551000	0.874577000
1	3.620656000	3.454130000	0.020586000
6	3.539495000	-2.767491000	-0.000077000
1	4.374717000	-2.282198000	-0.508407000
1	3.825704000	-2.996231000	1.028077000
1	3.290796000	-3.694032000	-0.520764000
25	0.032357000	0.063086000	-0.000310000
1	-3.501431000	-1.537555000	0.003549000

[2b-H]⁺, TE = - 2042.344581

6	-1.411252000	-2.286100000	-0.005474000
6	-1.635639000	0.028808000	0.067233000
7	-2.263191000	-1.208750000	0.053861000
7	-0.155072000	-2.094175000	-0.045149000
6	0.265363000	0.060036000	-1.789195000
8	0.181292000	0.230940000	-2.914296000
6	0.465557000	-0.166019000	1.883138000
8	0.502358000	-0.145032000	3.022720000
6	2.228456000	-0.588261000	-0.103560000
7	3.361332000	-0.850553000	-0.193601000
6	0.926353000	1.665923000	0.105457000
7	1.361796000	2.750539000	0.131766000
6	1.911158000	4.052503000	0.165406000
1	1.122892000	4.788235000	0.340824000
1	2.647192000	4.123086000	0.969018000
1	2.398431000	4.273623000	-0.786512000

6	4.737688000	-1.157226000	-0.302347000
1	5.116050000	-0.818817000	-1.268916000
1	5.290636000	-0.658595000	0.496113000
1	4.884423000	-2.235952000	-0.218144000
25	0.388097000	-0.129669000	0.038332000
6	0.721369000	-3.246136000	-0.114766000
6	-3.639674000	-1.484691000	0.484973000
7	-2.446064000	1.079285000	-0.049460000
6	-1.994637000	2.417527000	0.299037000
1	-1.219051000	2.364041000	1.056287000
1	-1.623353000	2.953056000	-0.581118000
1	-2.845273000	2.967964000	0.708993000
6	-3.722441000	1.085868000	-0.766765000
1	-3.817209000	0.202758000	-1.394188000
1	-4.581658000	1.163522000	-0.095042000
1	-3.724150000	1.959450000	-1.423577000
1	-3.644744000	-2.411387000	1.059832000
1	-3.976858000	-0.686103000	1.144196000
1	-4.334713000	-1.587275000	-0.349916000
1	1.407411000	-3.231664000	0.735504000
1	0.161584000	-4.186680000	-0.104805000
1	1.317303000	-3.199094000	-1.029410000
1	-1.871060000	-3.273469000	-0.009629000

[2c-H]⁺, TE = - 2022.975482

6	1.980024000	-1.918921000	0.000484000
6	1.741250000	0.376021000	0.000319000
7	2.594325000	-0.690242000	0.001014000
7	0.707907000	-1.958599000	-0.000315000
6	-0.208501000	-0.043332000	1.845416000
8	-0.240365000	0.040105000	2.981181000
6	-0.207644000	-0.043036000	-1.846194000
8	-0.238975000	0.040567000	-2.981945000
6	-1.926335000	-0.885515000	-0.000584000
7	-2.999392000	-1.338978000	-0.000207000

6	-0.982296000	1.588475000	-0.000291000
7	-1.566277000	2.599939000	-0.000082000
6	-2.294965000	3.812212000	0.000482000
1	-1.608625000	4.661778000	-0.014023000
1	-2.936292000	3.857579000	-0.882001000
1	-2.914204000	3.869960000	0.897888000
6	-4.308194000	-1.876988000	0.000975000
1	-4.767183000	-1.724493000	0.979566000
1	-4.909994000	-1.380282000	-0.762364000
1	-4.267704000	-2.946452000	-0.214562000
25	-0.178354000	-0.110838000	-0.000367000
6	0.050106000	-3.249999000	-0.001314000
6	4.051484000	-0.568059000	0.001898000
8	2.455722000	1.471288000	0.000420000
6	1.827724000	2.755165000	-0.000450000
1	1.220270000	2.874199000	-0.897569000
1	1.220359000	2.875464000	0.896559000
1	2.645218000	3.473466000	-0.000983000
1	4.486405000	-1.566801000	0.002686000
1	4.385390000	-0.030272000	-0.885964000
1	4.384192000	-0.029427000	0.889692000
1	-0.585286000	-3.333707000	-0.886307000
1	0.768862000	-4.075189000	-0.000462000
1	-0.587880000	-3.334021000	0.881732000
1	2.622422000	-2.797519000	0.000709000

[2'a-H]⁺, TE = - 2291.561750

6	-0.992580000	-1.299813000	0.096848000
6	-1.307377000	0.969380000	-0.003006000
1	-2.062565000	1.759700000	-0.049078000
7	-1.886325000	-0.241796000	0.043058000
7	0.250276000	-0.996406000	0.099220000
6	0.621722000	0.992851000	-1.873181000
8	0.638596000	1.008202000	-3.010839000
6	0.693316000	1.255900000	1.810498000

8	0.753095000	1.440050000	2.932435000
6	2.516124000	0.848988000	-0.073848000
7	3.671418000	0.724511000	-0.124302000
6	0.605550000	2.907069000	-0.154507000
7	0.568714000	4.069140000	-0.237694000
6	0.556664000	5.479854000	-0.342906000
1	-0.071817000	5.781167000	-1.183075000
1	0.160778000	5.914338000	0.576935000
1	1.572447000	5.845681000	-0.505015000
6	5.068427000	0.515401000	-0.188814000
1	5.435935000	0.801058000	-1.176069000
1	5.566295000	1.120517000	0.570969000
1	5.284871000	-0.540460000	-0.013378000
25	0.596063000	1.034239000	-0.023090000
6	1.193357000	-2.063682000	0.121332000
6	2.123967000	-2.135116000	1.155755000
6	1.189692000	-3.022447000	-0.889237000
6	3.031801000	-3.184774000	1.187310000
1	2.114585000	-1.388039000	1.941908000
6	2.112613000	-4.061698000	-0.856458000
1	0.483583000	-2.939601000	-1.709575000
6	3.031511000	-4.147415000	0.181604000
1	3.737781000	-3.256636000	2.008029000
1	2.111225000	-4.804157000	-1.647100000
1	3.746117000	-4.962633000	0.209244000
6	-3.304065000	-0.487376000	0.054099000
6	-3.862288000	-1.318450000	-0.910265000
6	-4.090399000	0.117436000	1.026935000
6	-5.232718000	-1.546129000	-0.895380000
1	-3.238694000	-1.765610000	-1.677973000
6	-5.460978000	-0.108880000	1.025050000
1	-3.632733000	0.743641000	1.785784000
6	-6.031415000	-0.940853000	0.068220000
1	-5.677109000	-2.189414000	-1.646720000
1	-6.081746000	0.357063000	1.782254000

1	-7.101008000	-1.118992000	0.074183000
1	-1.389169000	-2.309241000	0.160878000

[2'b-H]⁺, TE = - 2425.357137

6	-0.800775000	-1.417178000	-0.156980000
6	-1.207178000	0.884443000	-0.105589000
7	-1.729976000	-0.405208000	-0.221244000
7	0.435589000	-1.133059000	-0.021339000
6	0.825311000	0.975502000	-1.807968000
8	0.817550000	1.088240000	-2.943569000
6	0.767917000	0.952641000	1.872929000
8	0.719539000	1.050290000	3.009244000
6	2.691966000	0.529016000	0.023653000
7	3.834717000	0.304268000	-0.001255000
6	1.232912000	2.707661000	0.023767000
7	1.593815000	3.819675000	0.005699000
6	2.067966000	5.150847000	-0.015195000
1	1.235705000	5.848229000	0.104968000
1	2.779142000	5.303756000	0.799351000
1	2.565468000	5.351745000	-0.966363000
6	5.197844000	-0.067374000	-0.030324000
1	5.620984000	0.156890000	-1.011385000
1	5.748882000	0.484225000	0.733786000
1	5.284276000	-1.138968000	0.163422000
25	0.822734000	0.880223000	0.031039000
6	1.360762000	-2.215898000	0.003462000
6	2.131333000	-2.436614000	1.143151000
6	1.503001000	-3.041751000	-1.108491000
6	3.025610000	-3.498315000	1.171705000
1	2.013050000	-1.790035000	2.006063000
6	2.407820000	-4.097714000	-1.074583000
1	0.920299000	-2.844580000	-2.002963000
6	3.168414000	-4.329930000	0.064139000
1	3.606753000	-3.683766000	2.069101000
1	2.515699000	-4.738494000	-1.943175000

1	3.868742000	-5.157570000	0.091710000
6	-3.098294000	-0.820437000	-0.004436000
6	-3.749573000	-1.574981000	-0.973557000
6	-3.719504000	-0.523678000	1.203591000
6	-5.042719000	-2.024396000	-0.735204000
1	-3.251860000	-1.799033000	-1.912158000
6	-5.018103000	-0.965660000	1.427816000
1	-3.189280000	0.043257000	1.962007000
6	-5.680189000	-1.714536000	0.461140000
1	-5.553837000	-2.613232000	-1.489001000
1	-5.507198000	-0.735748000	2.368207000
1	-6.690860000	-2.062931000	0.643182000
7	-2.069933000	1.880857000	-0.260456000
6	-1.728928000	3.232654000	0.157961000
1	-0.964659000	3.206857000	0.927642000
1	-1.385483000	3.832816000	-0.690726000
1	-2.628314000	3.696233000	0.571537000
6	-3.351737000	1.827753000	-0.967173000
1	-3.384653000	0.986914000	-1.654241000
1	-4.197963000	1.766703000	-0.278084000
1	-3.436789000	2.748430000	-1.549307000
1	-1.185776000	-2.433585000	-0.197664000

[2'c**-H]⁺, TE = - 2405.983150**

6	-0.885261000	-1.432764000	0.033181000
6	-1.276453000	0.852849000	0.050844000
7	-1.806228000	-0.415616000	0.020665000
7	0.354400000	-1.126293000	0.076768000
6	0.657572000	0.910319000	-1.828751000
8	0.630753000	0.954309000	-2.967149000
6	0.758438000	1.067717000	1.854914000
8	0.795553000	1.213292000	2.985043000
6	2.587048000	0.612515000	-0.045588000
7	3.732802000	0.418433000	-0.103126000

6	1.008016000	2.758877000	-0.077673000
7	1.296324000	3.888846000	-0.144432000
6	1.681948000	5.246925000	-0.226772000
1	0.800691000	5.890538000	-0.180245000
1	2.346704000	5.492773000	0.603816000
1	2.203991000	5.425472000	-1.169012000
6	5.106297000	0.089755000	-0.170569000
1	5.488108000	0.308799000	-1.169393000
1	5.662444000	0.673726000	0.564994000
1	5.231819000	-0.974718000	0.039450000
25	0.697650000	0.910852000	0.017178000
6	1.302260000	-2.189327000	0.052385000
6	2.164154000	-2.365084000	1.132840000
6	1.373079000	-3.039913000	-1.047694000
6	3.080336000	-3.408350000	1.116056000
1	2.097000000	-1.700529000	1.987679000
6	2.300583000	-4.076230000	-1.060129000
1	0.716169000	-2.878678000	-1.896789000
6	3.153227000	-4.264046000	0.020190000
1	3.733031000	-3.560932000	1.969346000
1	2.353333000	-4.737229000	-1.918527000
1	3.870870000	-5.077113000	0.011934000
6	-3.217246000	-0.724195000	0.020417000
6	-3.902336000	-0.769450000	-1.186674000
6	-3.856742000	-0.989998000	1.224039000
6	-5.254586000	-1.088106000	-1.185256000
1	-3.382311000	-0.556476000	-2.114834000
6	-5.209144000	-1.309968000	1.215113000
1	-3.302825000	-0.943691000	2.156014000
6	-5.906195000	-1.358485000	0.013157000
1	-5.798364000	-1.128052000	-2.122651000
1	-5.717462000	-1.521431000	2.149388000
1	-6.961428000	-1.609035000	0.010074000
8	-2.256887000	1.710120000	0.090264000
6	-2.002268000	3.114443000	0.149765000

1	-1.382325000	3.348046000	1.015202000
1	-1.521857000	3.445939000	-0.770896000
1	-2.982129000	3.577011000	0.250443000
1	-1.269533000	-2.449983000	0.017399000

[3a-H]⁺, TE = - 1947.229537

6	2.612268000	-0.009153000	-0.975517000
6	1.596729000	-0.006245000	1.071244000
1	1.777760000	-0.007580000	2.152351000
7	2.764648000	-0.010321000	0.395733000
7	1.412001000	-0.004618000	-1.413003000
6	4.101593000	-0.015912000	0.980152000
1	4.660347000	0.872505000	0.676188000
1	4.003132000	-0.014952000	2.064593000
1	4.652576000	-0.909454000	0.677017000
6	1.190923000	-0.002998000	-2.842518000
1	0.602214000	-0.882223000	-3.116511000
1	0.608624000	0.880795000	-3.115500000
1	2.126843000	-0.006062000	-3.411407000
25	-0.000183000	0.000043000	0.061832000
6	-1.502034000	0.005293000	-1.133599000
7	-2.422120000	0.008335000	-1.855191000
6	-1.029502000	0.003914000	1.609154000
7	-1.627589000	0.006288000	2.616602000
6	-0.099985000	1.895018000	0.053016000
7	-0.178243000	3.060989000	0.058527000
6	-0.113765000	-1.894126000	0.053093000
7	-0.200671000	-3.059486000	0.058725000
6	-0.321321000	-4.465927000	0.099831000
1	0.305166000	-4.871377000	0.897399000
1	-1.360579000	-4.744655000	0.287460000
1	-0.005455000	-4.895742000	-0.853196000
6	-3.561835000	0.011318000	-2.689368000
1	-4.468330000	-0.039793000	-2.081967000
1	-3.584807000	0.925810000	-3.285971000

1	-3.534948000	-0.849494000	-3.361001000
6	-2.385721000	0.009515000	3.807158000
1	-2.159620000	-0.880588000	4.398825000
1	-2.149454000	0.895870000	4.400485000
1	-3.452983000	0.015846000	3.572906000
6	-0.288078000	4.468324000	0.099281000
1	-1.317752000	4.754497000	0.324738000
1	0.370418000	4.872172000	0.871475000
1	-0.005309000	4.893005000	-0.866359000
1	3.504920000	-0.012080000	-1.598627000

[3b-H]⁺, TE = - 2081.014766

6	-1.423374000	1.099937000	-2.026819000
6	-1.649297000	0.209476000	0.110562000
7	-2.276453000	0.762570000	-1.002987000
7	-0.177968000	0.877274000	-1.897915000
25	0.343808000	0.059942000	-0.103046000
6	2.150204000	-0.073198000	-0.619406000
7	3.277983000	-0.166371000	-0.925235000
6	0.833307000	-0.696687000	1.518116000
7	1.238321000	-1.187563000	2.506485000
6	0.043477000	-1.680715000	-0.770688000
7	-0.131429000	-2.768241000	-1.170490000
6	0.667176000	1.779711000	0.622395000
7	0.874952000	2.835422000	1.085104000
6	1.148319000	4.092783000	1.664993000
1	0.915730000	4.072109000	2.732356000
1	2.204168000	4.343337000	1.538299000
1	0.542515000	4.866120000	1.187243000
6	4.641318000	-0.286147000	-1.269070000
1	5.242655000	0.396592000	-0.664061000
1	4.984736000	-1.308587000	-1.094346000
1	4.786618000	-0.041715000	-2.324177000
6	1.763199000	-1.773873000	3.676390000
1	0.977876000	-1.898220000	4.427149000

1	2.187934000	-2.755286000	3.450100000
1	2.549374000	-1.141131000	4.096230000
6	-0.282483000	-4.087702000	-1.648282000
1	0.630869000	-4.411448000	-2.153068000
1	-0.485458000	-4.766919000	-0.816875000
1	-1.113159000	-4.139041000	-2.355982000
6	0.704441000	1.230626000	-2.987836000
6	-3.606099000	1.377990000	-1.025010000
7	-2.495963000	-0.249770000	1.043676000
6	-2.036350000	-0.506919000	2.396336000
1	-2.854257000	-0.281073000	3.086817000
1	-1.745583000	-1.555023000	2.530118000
1	-1.193367000	0.136802000	2.627569000
6	-3.807586000	-0.833417000	0.772954000
1	-4.632725000	-0.208602000	1.128815000
1	-3.929494000	-1.032558000	-0.289796000
1	-3.860969000	-1.792032000	1.297223000
1	0.167073000	1.694709000	-3.822388000
1	1.467392000	1.923899000	-2.624827000
1	1.215872000	0.335055000	-3.350030000
1	-3.884699000	1.668066000	-0.012251000
1	-3.564291000	2.284500000	-1.630586000
1	-4.376476000	0.722042000	-1.435808000
1	-1.871153000	1.555434000	-2.909847000

[3c-H]⁺, TE = - 2061.650002

6	2.019733000	-0.010708000	-1.898571000
6	1.748650000	-0.000631000	0.393696000
7	2.621810000	-0.006719000	-0.666317000
7	0.746889000	-0.008631000	-1.942837000
25	-0.148009000	0.000323000	-0.098747000
6	-1.883459000	-0.001620000	-0.862644000
7	-2.962613000	-0.003032000	-1.315812000
6	-0.941508000	0.008905000	1.581674000

7	-1.525752000	0.014088000	2.600476000
6	-0.183405000	1.894687000	-0.087816000
7	-0.214794000	3.064222000	-0.071449000
6	-0.188055000	-1.893660000	-0.071285000
7	-0.222818000	-3.062928000	-0.045419000
6	-0.279059000	-4.473079000	0.000877000
1	0.617517000	-4.869039000	0.483189000
1	-1.156917000	-4.792857000	0.566836000
1	-0.344471000	-4.877928000	-1.011507000
6	-4.273836000	-0.007040000	-1.839554000
1	-4.916787000	-0.648014000	-1.232041000
1	-4.680589000	1.006711000	-1.837647000
1	-4.267182000	-0.383700000	-2.865004000
6	-2.261415000	0.021935000	3.804247000
1	-2.854042000	-0.892249000	3.889601000
1	-1.587414000	0.083070000	4.662885000
1	-2.936408000	0.881071000	3.827804000
6	-0.264701000	4.474905000	-0.036130000
1	-1.029976000	4.803147000	0.670851000
1	0.701859000	4.876996000	0.275803000
1	-0.507722000	4.865611000	-1.026806000
6	0.096651000	-0.012786000	-3.234493000
6	4.074435000	-0.009679000	-0.531236000
8	2.473385000	0.002188000	1.495243000
6	1.831262000	0.008759000	2.766635000
1	1.215754000	-0.883477000	2.883700000
1	2.637564000	0.010890000	3.498650000
1	1.218273000	0.903748000	2.875724000
1	4.520005000	-0.012897000	-1.525831000
1	4.409068000	0.877108000	0.008741000
1	4.405165000	-0.895528000	0.012732000
1	-0.542319000	0.869611000	-3.323164000
1	0.815805000	-0.016362000	-4.060886000
1	-0.543474000	-0.895045000	-3.316667000
1	2.668623000	-0.015384000	-2.773115000

[3'a-H]⁺, TE = - 2330.238460

6	-1.070965000	-1.369232000	-0.175531000
6	-1.332366000	0.899950000	0.048688000
1	-2.082487000	1.692111000	0.143688000
7	-1.943736000	-0.309935000	-0.068671000
7	0.179908000	-1.082713000	-0.148638000
25	0.543223000	0.938705000	0.080360000
6	2.458688000	0.748650000	0.143656000
7	3.617193000	0.616399000	0.200715000
6	0.538668000	2.782111000	0.294214000
7	0.476908000	3.944357000	0.426373000
6	0.591255000	0.770981000	1.971352000
7	0.628979000	0.689887000	3.135738000
6	0.700773000	1.216973000	-1.791695000
7	0.801819000	1.413165000	-2.939243000
6	0.900468000	1.677035000	-4.323232000
1	0.058531000	2.293469000	-4.646018000
1	1.831469000	2.206922000	-4.535975000
1	0.888928000	0.739287000	-4.883080000
6	5.006520000	0.375347000	0.269715000
1	5.528422000	0.987806000	-0.468523000
1	5.377913000	0.626769000	1.265364000
1	5.206611000	-0.679908000	0.068890000
6	0.446804000	5.345898000	0.590755000
1	-0.002266000	5.817313000	-0.286480000
1	-0.143518000	5.607775000	1.471875000
1	1.461493000	5.730787000	0.717925000
6	0.678114000	0.618576000	4.545166000
1	1.234840000	1.470960000	4.940681000
1	-0.334145000	0.634212000	4.954966000
1	1.174202000	-0.303962000	4.854349000
6	1.102445000	-2.158631000	-0.231031000
6	2.079322000	-2.148978000	-1.225779000
6	1.048561000	-3.214739000	0.677504000

6	2.977497000	-3.202622000	-1.321817000
1	2.111859000	-1.323267000	-1.927441000
6	1.958853000	-4.261528000	0.581223000
1	0.307254000	-3.202700000	1.470464000
6	2.922912000	-4.260732000	-0.418717000
1	3.720756000	-3.202982000	-2.112586000
1	1.913188000	-5.078593000	1.293462000
1	3.629180000	-5.080172000	-0.495353000
6	-3.359687000	-0.523774000	-0.102550000
6	-3.938309000	-1.482364000	0.723201000
6	-4.144501000	0.239626000	-0.960372000
6	-5.313092000	-1.679936000	0.681901000
1	-3.322721000	-2.055570000	1.408993000
6	-5.519306000	0.045111000	-0.983511000
1	-3.677619000	0.968413000	-1.614495000
6	-6.105102000	-0.915955000	-0.167212000
1	-5.766571000	-2.425284000	1.326158000
1	-6.132984000	0.637890000	-1.653064000
1	-7.178204000	-1.069689000	-0.193100000
1	-1.477515000	-2.367926000	-0.309171000

[3'b-H]⁺, TE = - 2464.026126

6	0.894603000	-1.475113000	-0.155971000
6	1.230197000	0.840112000	-0.113278000
7	1.795258000	-0.440121000	-0.229929000
7	-0.348538000	-1.217081000	-0.017142000
25	-0.774231000	0.796476000	0.039891000
6	-2.625533000	0.443509000	0.007946000
7	-3.775069000	0.226490000	-0.034934000
6	-1.187593000	2.601961000	0.042587000
7	-1.550361000	3.720131000	0.033721000
6	-0.803731000	0.857267000	-1.847238000
7	-0.837355000	0.920533000	-3.016682000
6	-0.774715000	0.818953000	1.933620000
7	-0.785184000	0.859287000	3.104777000

6	-0.811364000	0.927533000	4.514261000
1	-0.131199000	1.706893000	4.866415000
1	-1.821620000	1.158737000	4.860210000
1	-0.502218000	-0.029267000	4.941658000
6	-5.129698000	-0.164480000	-0.081104000
1	-5.701450000	0.367682000	0.682667000
1	-5.553706000	0.064064000	-1.061638000
1	-5.208262000	-1.240059000	0.098076000
6	-2.047404000	5.039533000	0.027033000
1	-1.225831000	5.758039000	0.093802000
1	-2.602982000	5.229755000	-0.894888000
1	-2.716830000	5.195472000	0.876934000
6	-0.958330000	1.012212000	-4.419844000
1	-1.450285000	0.119180000	-4.812659000
1	-1.553409000	1.888683000	-4.687343000
1	0.028453000	1.102829000	-4.879879000
6	-1.242395000	-2.319283000	0.006621000
6	-2.094882000	-2.492643000	1.096341000
6	-1.281864000	-3.223184000	-1.053461000
6	-2.960260000	-3.577387000	1.130168000
1	-2.059260000	-1.781216000	1.913738000
6	-2.157137000	-4.303531000	-1.016130000
1	-0.640145000	-3.065106000	-1.914731000
6	-2.996388000	-4.485649000	0.075195000
1	-3.605939000	-3.720585000	1.990730000
1	-2.182514000	-5.002161000	-1.845833000
1	-3.675741000	-5.330537000	0.105995000
6	3.171593000	-0.807955000	-0.007115000
6	3.834185000	-1.603096000	-0.936357000
6	3.806340000	-0.421674000	1.169033000
6	5.141977000	-2.004595000	-0.691228000
1	3.330937000	-1.896433000	-1.852588000
6	5.119244000	-0.814002000	1.399897000
1	3.271650000	0.180316000	1.896175000
6	5.788739000	-1.605253000	0.472694000

1	5.657770000	-2.625246000	-1.415958000
1	5.615803000	-0.511528000	2.315709000
1	6.811107000	-1.914779000	0.659757000
7	2.087841000	1.846573000	-0.299843000
6	1.748518000	3.191911000	0.129351000
1	2.654815000	3.666346000	0.517502000
1	1.370293000	3.793696000	-0.704181000
1	1.003245000	3.152955000	0.917431000
6	3.323491000	1.806436000	-1.078928000
1	4.214544000	1.791570000	-0.444675000
1	3.341917000	0.942479000	-1.738288000
1	3.350037000	2.708319000	-1.696977000
1	1.304874000	-2.482145000	-0.188764000

[3'*c*-H]⁺, TE = - 2444.656363

6	-0.998772000	-1.461758000	-0.051457000
6	-1.281819000	0.841655000	-0.016683000
7	-1.875444000	-0.410847000	-0.010398000
7	0.253612000	-1.203268000	-0.098620000
25	0.668777000	0.825616000	0.004875000
6	2.539076000	0.494302000	0.044640000
7	3.689436000	0.292385000	0.089405000
6	1.025382000	2.640796000	0.145255000
7	1.345761000	3.766665000	0.239410000
6	0.672912000	0.726678000	1.896973000
7	0.688900000	0.680140000	3.065766000
6	0.738503000	0.991641000	-1.880640000
7	0.785367000	1.115857000	-3.043596000
6	0.834764000	1.285453000	-4.444519000
1	-0.123424000	1.661166000	-4.810903000
1	1.619411000	1.998657000	-4.706969000
1	1.048505000	0.330330000	-4.929683000
6	5.053335000	-0.066588000	0.142908000
1	5.613092000	0.470469000	-0.625950000
1	5.467558000	0.183556000	1.122047000

1	5.155413000	-1.142002000	-0.023491000
6	1.778834000	5.104793000	0.348962000
1	2.467974000	5.345530000	-0.464328000
1	0.926123000	5.787142000	0.298721000
1	2.293101000	5.257406000	1.301051000
6	0.755788000	0.631157000	4.475267000
1	1.150022000	1.573511000	4.862336000
1	-0.239553000	0.466009000	4.893700000
1	1.412433000	-0.183317000	4.789574000
6	1.150539000	-2.302706000	-0.086287000
6	2.095285000	-2.431163000	-1.103831000
6	1.101661000	-3.248182000	0.936806000
6	2.965656000	-3.512617000	-1.105538000
1	2.126119000	-1.688896000	-1.893821000
6	1.981966000	-4.324722000	0.932459000
1	0.386229000	-3.127195000	1.744357000
6	2.913941000	-4.461824000	-0.088052000
1	3.683302000	-3.621574000	-1.912443000
1	1.938141000	-5.056402000	1.732308000
1	3.597131000	-5.304129000	-0.093112000
6	-3.291335000	-0.668247000	-0.040457000
6	-4.062352000	-0.426129000	1.090194000
6	-3.864812000	-1.184112000	-1.196025000
6	-5.422558000	-0.702989000	1.059200000
1	-3.597318000	-0.025035000	1.984020000
6	-5.225737000	-1.467673000	-1.216448000
1	-3.250065000	-1.357681000	-2.073500000
6	-6.004426000	-1.225287000	-0.091455000
1	-6.029121000	-0.516697000	1.938854000
1	-5.676897000	-1.874253000	-2.115013000
1	-7.066453000	-1.444584000	-0.109827000
8	-2.244555000	1.734463000	-0.047379000
6	-1.929503000	3.122558000	-0.085797000
1	-1.287814000	3.342574000	-0.939293000
1	-2.886533000	3.631973000	-0.188130000

1	-1.438079000	3.423629000	0.839953000
1	-1.423670000	-2.463059000	-0.049934000

[4'a-H]⁺, TE = - 2443.566885

6	1.045805000	-1.178553000	-0.285545000
6	1.305992000	1.190669000	-0.197513000
1	1.538900000	1.699802000	-1.139331000
7	-0.235611000	-0.979722000	-0.197713000
1	1.805304000	1.751297000	0.599582000
6	-0.843625000	2.785911000	0.309458000
6	-0.317529000	0.730708000	1.894249000
6	-0.907399000	1.156275000	-1.775208000
7	-0.886392000	3.941714000	0.449940000
7	-0.982235000	1.270248000	-2.931097000
7	-0.036447000	0.574941000	3.012251000
6	0.314008000	0.374658000	4.367611000
1	1.395444000	0.253831000	4.454560000
1	0.000026000	1.236237000	4.959752000
1	-0.181461000	-0.520994000	4.747008000
6	-0.934321000	5.344056000	0.622139000
1	-0.497270000	5.612883000	1.585722000
1	-0.370689000	5.833837000	-0.174368000
1	-1.970691000	5.686017000	0.590848000
6	-1.050792000	1.391244000	-4.339054000
1	-0.422879000	2.221404000	-4.668070000
1	-0.697513000	0.468459000	-4.803054000
1	-2.082067000	1.576811000	-4.644793000
6	-1.087557000	-2.107585000	-0.216469000
6	-2.171863000	-2.151656000	-1.094758000
6	-0.869531000	-3.185150000	0.645713000
6	-3.008568000	-3.259590000	-1.119917000
1	-2.339048000	-1.320271000	-1.770562000
6	-1.708236000	-4.292959000	0.614357000
1	-0.048734000	-3.144197000	1.355511000
6	-2.781168000	-4.335675000	-0.267361000

1	-3.835788000	-3.290035000	-1.822149000
1	-1.524970000	-5.123239000	1.288566000
1	-3.434726000	-5.200755000	-0.291483000
26	-0.703776000	0.966049000	0.076942000
6	-2.535126000	0.655109000	0.365460000
7	-3.663934000	0.456219000	0.568421000
6	-5.016804000	0.115179000	0.793920000
1	-5.665672000	0.752589000	0.190325000
1	-5.175720000	-0.929743000	0.518298000
1	-5.261904000	0.250793000	1.848958000
7	1.898607000	-0.155950000	-0.233510000
6	3.301323000	-0.361993000	-0.244307000
6	4.138439000	0.588516000	-0.828920000
6	3.864166000	-1.495639000	0.347921000
6	5.512793000	0.389940000	-0.844606000
1	3.715305000	1.478912000	-1.277947000
6	5.238149000	-1.691440000	0.314452000
1	3.235719000	-2.216806000	0.859696000
6	6.070292000	-0.751883000	-0.282447000
1	6.151613000	1.134995000	-1.307156000
1	5.660335000	-2.577636000	0.776461000
1	7.143748000	-0.903238000	-0.298960000
1	1.454742000	-2.176093000	-0.432643000

[4'b-H]⁺, TE = -5591.060377

6	-1.257691000	1.211636000	-0.263344000
6	-1.373331000	-1.189583000	-0.210650000
1	-1.595081000	-1.689721000	-1.159334000
7	0.039616000	1.127528000	-0.186307000
1	-1.841409000	-1.784683000	0.579532000
6	1.059706000	-2.763158000	0.267631000
6	0.345444000	-0.702315000	1.993813000
6	0.929207000	-1.034240000	-1.907855000
7	1.221611000	-3.911983000	0.390115000
7	1.001207000	-1.131192000	-3.065493000

7	0.082720000	-0.601300000	3.122500000
6	-0.235793000	-0.475254000	4.494323000
1	-1.318069000	-0.400142000	4.615350000
1	0.126799000	-1.350142000	5.037194000
1	0.236586000	0.421199000	4.900378000
6	1.412136000	-5.303639000	0.542686000
1	0.562679000	-5.738416000	1.073587000
1	1.498074000	-5.775394000	-0.438314000
1	2.324981000	-5.493834000	1.111032000
6	1.080489000	-1.241520000	-4.473132000
1	0.576071000	-2.152925000	-4.799517000
1	0.597864000	-0.378536000	-4.935722000
1	2.126775000	-1.278337000	-4.782371000
6	0.789701000	2.327077000	-0.212901000
6	1.880921000	2.443813000	-1.075217000
6	0.466440000	3.398010000	0.623201000
6	2.621013000	3.617637000	-1.112189000
1	2.129514000	1.613792000	-1.727242000
6	1.209063000	4.572352000	0.579199000
1	-0.356747000	3.301824000	1.324642000
6	2.288572000	4.688151000	-0.287428000
1	3.455754000	3.703323000	-1.800716000
1	0.945973000	5.396545000	1.233999000
1	2.867667000	5.604441000	-0.319959000
6	2.645537000	-0.397073000	0.333792000
7	3.753672000	-0.089110000	0.519972000
6	5.072207000	0.369795000	0.738205000
1	5.752733000	-0.106454000	0.029719000
1	5.106467000	1.452884000	0.601160000
1	5.385959000	0.125343000	1.754900000
7	-2.033621000	0.129908000	-0.218115000
6	-3.448105000	0.251741000	-0.213686000
6	-4.232456000	-0.717525000	-0.838096000
6	-4.070091000	1.322417000	0.433326000
6	-5.616048000	-0.598005000	-0.837605000

1	-3.762912000	-1.560147000	-1.330861000
6	-5.453184000	1.440532000	0.415578000
1	-3.478312000	2.053166000	0.974581000
6	-6.233854000	0.482742000	-0.220272000
1	-6.214504000	-1.356082000	-1.331678000
1	-5.922256000	2.278639000	0.920045000
1	-7.314317000	0.572551000	-0.225018000
44	0.730015000	-0.875494000	0.057653000
1	-1.746675000	2.174331000	-0.397109000

[5a-H]⁺, TE = - 2443.566885

6	0.299659000	1.369703000	-0.873617000
6	-1.724236000	0.001072000	-0.567721000
6	0.298036000	-1.369858000	-0.874097000
7	-1.142238000	-1.180183000	-0.636758000
7	-1.140841000	1.181678000	-0.636353000
6	-1.979090000	-2.331041000	-0.485419000
6	-1.846979000	-3.397923000	-1.371390000
6	-2.911357000	-2.395801000	0.547605000
6	-2.658682000	-4.514653000	-1.229242000
1	-1.119975000	-3.343803000	-2.173574000
6	-3.727702000	-3.513404000	0.676425000
1	-2.984556000	-1.581984000	1.262225000
6	-3.603465000	-4.575618000	-0.209911000
1	-2.559330000	-5.338952000	-1.927349000
1	-4.452109000	-3.558251000	1.482668000
1	-4.236388000	-5.449809000	-0.104888000
6	-1.976315000	2.333485000	-0.484645000
6	-1.842400000	3.400815000	-1.369809000
6	-2.908975000	2.398793000	0.547997000
6	-2.652701000	4.518515000	-1.227282000
1	-1.115080000	3.346337000	-2.171679000
6	-3.723908000	3.517378000	0.677198000
1	-2.983609000	1.584599000	1.262037000
6	-3.597873000	4.580037000	-0.208351000

1	-2.551916000	5.343166000	-1.924767000
1	-4.448622000	3.562622000	1.483143000
1	-4.229692000	5.454988000	-0.103021000
1	0.449000000	-1.343938000	-1.958943000
1	0.506182000	-2.389212000	-0.545775000
1	0.509063000	2.388674000	-0.544923000
1	0.450511000	1.344151000	-1.958492000
26	1.535723000	-0.000969000	0.024603000
6	0.493015000	-0.000866000	1.553588000
7	-0.133633000	-0.000852000	2.539195000
6	2.565795000	1.374674000	0.716051000
7	3.194575000	2.265050000	1.135151000
6	2.539693000	-0.001405000	-1.537677000
7	3.146904000	-0.001956000	-2.533498000
6	2.564648000	-1.377825000	0.715353000
7	3.192988000	-2.268819000	1.133792000
6	3.960920000	3.337846000	1.642662000
1	4.423885000	3.050250000	2.589047000
1	4.744504000	3.604124000	0.930234000
1	3.320944000	4.207056000	1.808344000
6	-0.826638000	-0.000985000	3.769872000
1	-0.113339000	0.002749000	4.597037000
1	-1.457372000	0.887791000	3.844343000
1	-1.451628000	-0.893554000	3.847354000
6	3.959313000	-3.341834000	1.640882000
1	4.747030000	-3.603468000	0.931297000
1	4.416913000	-3.056873000	2.590666000
1	3.320563000	-4.213175000	1.800003000
6	3.900527000	-0.004344000	-3.729216000
1	3.806747000	-0.972458000	-4.225312000
1	3.536084000	0.776709000	-4.399421000
1	4.952748000	0.181083000	-3.504032000
1	-2.803335000	0.001685000	-0.466880000

[5b-H]⁺, TE = - 5630.257423

6	0.133377000	1.413562000	-0.923417000
6	-1.872394000	0.004183000	-0.590803000
6	0.128204000	-1.410810000	-0.929588000
7	-1.303712000	-1.184116000	-0.669625000
7	-1.299538000	1.190753000	-0.665457000
6	-2.158828000	-2.320388000	-0.499087000
6	-2.080690000	-3.381701000	-1.397614000
6	-3.053071000	-2.374346000	0.567137000
6	-2.909839000	-4.482637000	-1.234074000
1	-1.381694000	-3.335914000	-2.224878000
6	-3.887167000	-3.475987000	0.717684000
1	-3.081675000	-1.564748000	1.289655000
6	-3.817611000	-4.532664000	-0.180989000
1	-2.853294000	-5.303023000	-1.941449000
1	-4.582107000	-3.513132000	1.549807000
1	-4.464195000	-5.394636000	-0.059601000
6	-2.150942000	2.329489000	-0.492488000
6	-2.068254000	3.392982000	-1.388023000
6	-3.045959000	2.383675000	0.573066000
6	-2.893669000	4.496386000	-1.222253000
1	-1.368598000	3.347058000	-2.214716000
6	-3.876293000	3.487854000	0.725864000
1	-3.078112000	1.572239000	1.293365000
6	-3.802220000	4.546723000	-0.169863000
1	-2.833575000	5.318502000	-1.927322000
1	-4.571854000	3.525171000	1.557460000
1	-4.445902000	5.410615000	-0.046718000
1	0.266914000	-1.381033000	-2.015879000
1	0.316365000	-2.436410000	-0.610592000
1	0.324912000	2.436965000	-0.599374000
1	0.272480000	1.388822000	-2.009784000
6	0.372232000	-0.005235000	1.649260000
7	-0.249021000	-0.006757000	2.638040000

6	2.573612000	1.455311000	0.745793000
7	3.203270000	2.347732000	1.160719000
6	2.512163000	-0.001751000	-1.659444000
7	3.108636000	-0.001464000	-2.661202000
6	2.570067000	-1.467563000	0.738938000
7	3.198442000	-2.362986000	1.149299000
6	3.977339000	3.414331000	1.668539000
1	4.459299000	3.114376000	2.601650000
1	4.746466000	3.692111000	0.944745000
1	3.339643000	4.280295000	1.858675000
6	-0.923508000	-0.008861000	3.878831000
1	-0.197548000	-0.017643000	4.694887000
1	-1.544623000	0.885291000	3.967845000
1	-1.555852000	-0.895976000	3.958734000
6	3.972008000	-3.432184000	1.652401000
1	4.743020000	-3.705013000	0.928735000
1	4.451599000	-3.137574000	2.588435000
1	3.334444000	-4.299686000	1.835837000
6	3.858061000	-0.002919000	-3.859298000
1	4.125280000	-1.027028000	-4.127610000
1	3.267470000	0.435534000	-4.666066000
1	4.770294000	0.581991000	-3.725324000
44	1.465245000	-0.003073000	0.014042000
1	-2.949664000	0.005865000	-0.470969000

[6a-H]⁺, TE = - 2630.770814

6	0.290279000	1.451436000	0.265721000
7	-1.207925000	1.218783000	0.143094000
6	-1.787888000	0.033612000	0.124023000
7	-1.244882000	-1.161782000	0.232478000
6	0.249045000	-1.424218000	0.429468000
8	0.553646000	2.596830000	0.507106000
6	-2.083111000	2.361075000	0.155010000
6	-1.996769000	3.297884000	-0.868259000
6	-2.854670000	4.388144000	-0.867444000

6	-3.792576000	4.542851000	0.148825000
6	-3.866689000	3.607731000	1.172835000
6	-3.003918000	2.517118000	1.183782000
1	-1.260334000	3.173339000	-1.653904000
1	-2.792466000	5.120513000	-1.665036000
1	-4.461678000	5.396366000	0.144170000
1	-4.589042000	3.728792000	1.972683000
1	-3.037867000	1.797246000	1.995916000
6	-2.143002000	-2.282529000	0.146057000
6	-2.818745000	-2.515755000	-1.046718000
6	-3.706028000	-3.581696000	-1.137582000
6	-3.899848000	-4.417651000	-0.044948000
6	-3.208861000	-4.185032000	1.139644000
6	-2.327522000	-3.116833000	1.242485000
1	-2.646597000	-1.867274000	-1.900540000
1	-4.240295000	-3.760526000	-2.064362000
1	-4.588617000	-5.252398000	-0.116195000
1	-3.358996000	-4.837478000	1.992921000
1	-1.785034000	-2.930664000	2.160767000
8	0.470227000	-2.540011000	0.807278000
26	1.534102000	-0.027508000	-0.031607000
6	2.787372000	-1.418728000	-0.288962000
6	1.950247000	0.078762000	1.783829000
6	2.828006000	1.286961000	-0.444222000
6	0.978763000	-0.123599000	-1.801603000
7	3.608328000	2.114396000	-0.679403000
7	3.539498000	-2.291721000	-0.433594000
7	2.190765000	0.150932000	2.918418000
7	0.629830000	-0.185784000	-2.911484000
6	0.250133000	-0.280597000	-4.270255000
1	-0.014919000	-1.312730000	-4.508135000
1	-0.609151000	0.365174000	-4.461714000
1	1.080034000	0.032013000	-4.907098000
6	4.482465000	3.201098000	-0.910638000
1	4.693949000	3.284882000	-1.978095000

1	4.012018000	4.121832000	-0.560335000
1	5.418070000	3.043337000	-0.371211000
6	2.465433000	0.249598000	4.301431000
1	2.109113000	-0.647454000	4.811178000
1	3.541295000	0.348442000	4.457210000
1	1.960581000	1.125536000	4.713065000
6	4.376668000	-3.424319000	-0.555394000
1	5.295727000	-3.266459000	0.011718000
1	3.855194000	-4.300562000	-0.165578000
1	4.626511000	-3.587949000	-1.605167000
1	-2.871521000	0.046837000	0.029014000

[6b-H]⁺, TE = - 5778.262690

6	0.120155000	1.512699000	0.247121000
7	-1.370911000	1.218876000	0.134921000
6	-1.927935000	0.020657000	0.126262000
7	-1.386304000	-1.175988000	0.249050000
6	0.103679000	-1.469771000	0.457164000
8	0.340989000	2.672175000	0.460918000
6	-2.278725000	2.336793000	0.127873000
6	-2.235351000	3.245306000	-0.923011000
6	-3.122051000	4.312233000	-0.937625000
6	-4.045952000	4.471359000	0.090654000
6	-4.077558000	3.564184000	1.141608000
6	-3.185784000	2.497416000	1.167815000
1	-1.509395000	3.117471000	-1.717825000
1	-3.093418000	5.022629000	-1.756675000
1	-4.737777000	5.306396000	0.073916000
1	-4.789515000	3.688707000	1.950175000
1	-3.186790000	1.799455000	1.999480000
6	-2.295693000	-2.289125000	0.165315000
6	-2.950765000	-2.536757000	-1.035772000
6	-3.847555000	-3.594942000	-1.124577000
6	-4.071521000	-4.408610000	-0.021022000
6	-3.400965000	-4.161650000	1.172358000

6	-2.510140000	-3.101178000	1.272750000
1	-2.755170000	-1.905412000	-1.897289000
1	-4.365765000	-3.785075000	-2.058174000
1	-4.767835000	-5.237212000	-0.090459000
1	-3.574367000	-4.796896000	2.034145000
1	-1.982852000	-2.904279000	2.197728000
8	0.299964000	-2.588321000	0.839337000
6	2.812841000	-1.505326000	-0.237212000
6	1.910677000	0.132615000	1.912338000
6	2.826909000	1.417598000	-0.451179000
6	0.952044000	-0.156225000	-1.922799000
7	3.567547000	2.283999000	-0.676799000
7	3.545027000	-2.401533000	-0.341097000
7	2.148667000	0.223822000	3.045733000
7	0.638846000	-0.242832000	-3.041077000
6	0.301347000	-0.364608000	-4.408659000
1	0.038651000	-1.400487000	-4.632159000
1	-0.548499000	0.280713000	-4.639396000
1	1.152657000	-0.069023000	-5.025005000
6	4.396607000	3.405035000	-0.909132000
1	4.615123000	3.487272000	-1.975342000
1	3.883874000	4.308444000	-0.573319000
1	5.332547000	3.292409000	-0.359008000
6	2.425143000	0.343625000	4.426781000
1	2.079024000	-0.550540000	4.948391000
1	3.500362000	0.455774000	4.577734000
1	1.911539000	1.219508000	4.827409000
6	4.364640000	-3.550044000	-0.425441000
1	5.268952000	-3.402267000	0.167581000
1	3.816488000	-4.413397000	-0.043499000
1	4.643017000	-3.728465000	-1.465641000
44	1.483257000	-0.014562000	-0.022171000
1	-3.011168000	0.022901000	0.024949000

Cartesian coordinates for the singlet state optimized geometries of **1a-6b**, along with their total energies (in hartrees) including zero point in aqueous phase.

1a, TE = - 1869.452223

6	2.166336000	1.060489000	-0.000028000
6	1.218843000	-1.121825000	0.000115000
1	1.416795000	-2.197346000	0.000197000
7	2.295491000	-0.386036000	0.000081000
7	0.907752000	1.346644000	-0.000081000
6	3.653031000	-0.918738000	0.000155000
1	4.180684000	-0.563520000	0.886544000
1	3.618240000	-2.007523000	0.000177000
1	4.180763000	-0.563558000	-0.886203000
6	0.532775000	2.748444000	-0.000191000
1	-0.072386000	2.974152000	-0.883979000
1	-0.072452000	2.974271000	0.883522000
1	1.422743000	3.382565000	-0.000200000
25	-0.492898000	-0.162025000	0.000000000
6	-0.398939000	-0.146966000	-1.840775000
8	-0.321719000	-0.145161000	-2.977039000
6	-1.463044000	-1.679428000	0.000109000
8	-2.047784000	-2.664155000	0.000180000
6	-1.973659000	0.923167000	-0.000134000
8	-2.907700000	1.580997000	-0.000217000
6	-0.399028000	-0.146645000	1.840779000
8	-0.321861000	-0.144638000	2.977045000

1b, TE = - 2003.238043

6	0.548635000	-2.376203000	-0.096321000
6	1.259338000	-0.092106000	0.111686000
7	1.574591000	-1.412786000	0.070180000
7	-0.613452000	-1.812785000	-0.154332000
25	-0.767137000	0.218845000	0.013727000
6	-0.812419000	0.000490000	1.841305000
8	-0.806857000	-0.142903000	2.972432000
6	-0.877897000	2.012494000	0.134000000

8	-1.049256000	3.146554000	0.187879000
6	-2.576774000	0.179192000	-0.159600000
8	-3.716110000	0.182685000	-0.266312000
6	-0.481561000	0.301855000	-1.803492000
8	-0.278270000	0.350482000	-2.924191000
6	-1.772053000	-2.669803000	-0.314621000
6	2.875610000	-1.962693000	0.454556000
7	2.255210000	0.797669000	0.068687000
6	3.515479000	0.593159000	-0.645114000
1	4.365425000	0.475234000	0.032040000
1	3.447414000	-0.265862000	-1.307358000
1	3.687458000	1.479182000	-1.261978000
6	2.069661000	2.175997000	0.490859000
1	3.013919000	2.532343000	0.909279000
1	1.799772000	2.821972000	-0.351489000
1	1.315707000	2.236877000	1.270103000
1	3.390262000	-1.272540000	1.122797000
1	2.684240000	-2.893482000	0.985647000
1	3.515002000	-2.182676000	-0.403319000
1	-1.461576000	-3.716878000	-0.363656000
1	-2.462411000	-2.541830000	0.526599000
1	-2.315416000	-2.416986000	-1.231592000

1c, TE = - 1983.870765

6	1.151849000	-2.188188000	-0.000236000
6	1.423123000	0.179983000	0.000125000
7	1.982851000	-1.032935000	0.000056000
7	-0.092221000	-1.835695000	-0.000330000
25	-0.591794000	0.154950000	0.000004000
6	-0.500926000	0.098273000	1.841928000
8	-0.428404000	0.056788000	2.977519000
6	-0.969697000	1.919352000	0.000424000
8	-1.296582000	3.018351000	0.000704000
6	-2.385044000	-0.191452000	-0.000275000
8	-3.511484000	-0.380534000	-0.000464000

6	-0.500584000	0.099175000	-1.841923000
8	-0.427853000	0.058270000	-2.977524000
6	-1.091540000	-2.887142000	-0.000587000
8	2.336085000	1.123126000	0.000150000
6	1.970287000	2.504441000	0.000318000
1	1.402977000	2.746199000	-0.898567000
1	1.403034000	2.746004000	0.899291000
1	2.910645000	3.052114000	0.000348000
6	3.430733000	-1.212741000	0.000106000
1	3.875387000	-0.757534000	-0.887195000
1	3.875446000	-0.756322000	0.886741000
1	3.620562000	-2.283321000	0.000805000
1	-0.606743000	-3.866720000	-0.000667000
1	-1.732183000	-2.806106000	0.884040000
1	-1.731993000	-2.805858000	-0.885328000

1'a, TE = - 2252.459654

6	-0.632528000	-1.256352000	0.027156000
6	-1.216668000	1.057806000	0.030081000
1	-2.035168000	1.781565000	0.060885000
7	-1.620925000	-0.192203000	0.030088000
7	0.540238000	-0.702245000	0.049580000
25	0.708759000	1.363191000	0.012123000
6	0.654436000	1.246254000	-1.831298000
8	0.602261000	1.174322000	-2.965509000
6	0.520414000	3.153857000	-0.048771000
8	0.362522000	4.286356000	-0.087483000
6	2.550278000	1.451391000	-0.006726000
8	3.687066000	1.541102000	-0.029653000
6	0.650582000	1.381684000	1.858025000
8	0.589538000	1.403145000	2.994365000
6	1.660910000	-1.577875000	-0.008518000
6	2.610812000	-1.563300000	1.011862000
6	1.824253000	-2.445147000	-1.088171000
6	3.705058000	-2.418452000	0.958729000

1	2.483445000	-0.893944000	1.856186000
6	2.926104000	-3.292338000	-1.141536000
1	1.083717000	-2.444310000	-1.880541000
6	3.869452000	-3.283922000	-0.119101000
1	4.431461000	-2.408282000	1.764950000
1	3.046017000	-3.961236000	-1.987886000
1	4.728441000	-3.945284000	-0.162337000
6	-3.006595000	-0.562264000	0.035012000
6	-3.445323000	-1.555011000	0.905481000
6	-3.896861000	0.077086000	-0.821199000
6	-4.792309000	-1.893973000	0.928451000
1	-2.733315000	-2.047803000	1.556669000
6	-5.243338000	-0.268427000	-0.789702000
1	-3.538893000	0.824676000	-1.521437000
6	-5.693871000	-1.251845000	0.084294000
1	-5.138144000	-2.662255000	1.611815000
1	-5.937455000	0.226097000	-1.460703000
1	-6.744212000	-1.522303000	0.103480000

1'b, TE = - 2386.249913

6	0.265210000	-1.424910000	-0.313727000
6	1.101517000	0.836021000	-0.191671000
7	1.345564000	-0.517366000	-0.281454000
7	-0.868832000	-0.799251000	-0.199673000
25	-0.878590000	1.229172000	0.160813000
6	-0.551087000	0.845513000	1.935536000
8	-0.317730000	0.612587000	3.025920000
6	-0.871471000	2.998441000	0.488833000
8	-0.971702000	4.121048000	0.704763000
6	-2.686568000	1.268182000	0.402879000
8	-3.813734000	1.335802000	0.578257000
6	-0.981676000	1.516271000	-1.658416000
8	-1.010060000	1.703342000	-2.782113000
6	-2.040991000	-1.601595000	-0.176483000
6	-3.027320000	-1.434765000	-1.148953000

6	-2.226083000	-2.556828000	0.823843000
6	-4.174586000	-2.219795000	-1.127667000
1	-2.887850000	-0.695648000	-1.931416000
6	-3.377489000	-3.336709000	0.845853000
1	-1.458376000	-2.679119000	1.580419000
6	-4.356445000	-3.172820000	-0.129478000
1	-4.928452000	-2.086891000	-1.897251000
1	-3.509316000	-4.075013000	1.630779000
1	-5.254620000	-3.781320000	-0.111353000
6	2.631879000	-1.124651000	-0.086455000
6	3.074237000	-2.120942000	-0.952822000
6	3.404216000	-0.766376000	1.015027000
6	4.294130000	-2.744656000	-0.723676000
1	2.456671000	-2.401159000	-1.798317000
6	4.628046000	-1.390229000	1.235144000
1	3.047218000	-0.006448000	1.702579000
6	5.077671000	-2.379892000	0.368228000
1	4.634546000	-3.518699000	-1.403788000
1	5.224412000	-1.106194000	2.095999000
1	6.030325000	-2.868223000	0.544051000
7	2.090642000	1.669020000	-0.487715000
6	3.251334000	1.340552000	-1.315850000
1	4.151471000	1.193755000	-0.713357000
1	3.062163000	0.450259000	-1.909414000
1	3.410709000	2.182322000	-1.993384000
6	2.032044000	3.082659000	-0.140471000
1	3.055225000	3.445068000	-0.028412000
1	1.541801000	3.665466000	-0.926582000
1	1.523626000	3.222669000	0.808372000

1'c, TE = - 2366.877570

6	-0.410542000	-1.433474000	0.063435000
6	-1.179180000	0.836474000	-0.013584000
7	-1.460909000	-0.479946000	0.029305000
7	0.734715000	-0.818788000	0.081759000

25	0.789387000	1.241989000	-0.038828000
6	0.719443000	1.051771000	-1.876711000
8	0.662312000	0.934851000	-3.006941000
6	0.770056000	3.040305000	-0.176274000
8	0.847805000	4.179817000	-0.265986000
6	2.621076000	1.301120000	-0.058334000
8	3.758717000	1.378185000	-0.085351000
6	0.713055000	1.330960000	1.804475000
8	0.645277000	1.392076000	2.939075000
6	1.901554000	-1.632094000	0.074092000
6	2.777941000	-1.611453000	1.158598000
6	2.187074000	-2.445572000	-1.021993000
6	3.920252000	-2.403512000	1.149911000
1	2.556107000	-0.984168000	2.015980000
6	3.333991000	-3.232685000	-1.029437000
1	1.502847000	-2.453795000	-1.863773000
6	4.205196000	-3.214697000	0.055079000
1	4.588993000	-2.387761000	2.004621000
1	3.546066000	-3.861967000	-1.888095000
1	5.099921000	-3.828411000	0.048119000
6	-2.812888000	-0.975288000	0.054158000
6	-3.431636000	-1.215259000	1.274539000
6	-3.473060000	-1.231056000	-1.141010000
6	-4.727575000	-1.719228000	1.297181000
1	-2.897703000	-1.012032000	2.196779000
6	-4.768995000	-1.734655000	-1.112028000
1	-2.971646000	-1.040837000	-2.084034000
6	-5.397145000	-1.979103000	0.105372000
1	-5.212830000	-1.910936000	2.248421000
1	-5.286760000	-1.938956000	-2.043293000
1	-6.407625000	-2.373655000	0.125261000
8	-2.269061000	1.555991000	-0.026819000
6	-2.219717000	2.985333000	-0.068340000
1	-1.687794000	3.371225000	0.801006000
1	-1.756416000	3.319856000	-0.996344000

1 -3.258286000 3.308175000 -0.037975000

2a, TE = - 1908.119697

6 -2.620328000 -1.137566000 0.000054000
6 -1.636474000 1.026565000 0.000011000
1 -1.836815000 2.104649000 0.000004000
7 -2.734355000 0.305046000 0.000041000
7 -1.361550000 -1.434378000 0.000031000
6 -4.081164000 0.858895000 0.000065000
1 -4.621372000 0.518657000 0.885821000
1 -4.027869000 1.947626000 0.000041000
1 -4.621419000 0.518619000 -0.885648000
6 -1.008421000 -2.839147000 0.000041000
1 -0.402470000 -3.074585000 -0.881404000
1 -0.402437000 -3.074565000 0.881468000
1 -1.904938000 -3.466582000 0.000065000
6 0.048323000 0.093833000 -1.826225000
8 0.053840000 0.136555000 -2.972992000
6 0.048407000 0.093892000 1.826197000
8 0.053878000 0.136614000 2.972964000
6 1.554856000 -1.094300000 -0.000022000
7 2.481236000 -1.805896000 -0.000104000
6 1.060965000 1.635188000 -0.000060000
7 1.654145000 2.644132000 -0.000012000
6 2.389090000 3.850986000 0.000083000
1 3.023273000 3.899759000 -0.887383000
1 1.706525000 4.703195000 -0.003005000
1 3.018600000 3.902466000 0.890716000
6 3.591417000 -2.680233000 -0.000076000
1 4.199797000 -2.504995000 -0.889282000
1 4.199449000 -2.505392000 0.889445000
1 3.246965000 -3.716332000 -0.000374000
25 0.048184000 0.070045000 -0.000014000

2b, TE = - 2041.901627

6 -1.291909000 -2.481656000 0.008078000
6 -1.621721000 -0.100295000 0.082946000
7 -2.155005000 -1.353263000 0.077803000
7 -0.054560000 -2.107400000 -0.034795000
6 0.218855000 0.008327000 -1.765240000
8 0.074272000 0.120644000 -2.900021000
6 0.427795000 -0.170442000 1.865859000
8 0.407991000 -0.175099000 3.015173000
6 2.257631000 -0.471906000 -0.098585000
7 3.406204000 -0.670442000 -0.190618000
6 0.827610000 1.702227000 0.095737000

7	1.189607000	2.817252000	0.113483000
6	1.538984000	4.184882000	0.148193000
1	0.639744000	4.798761000	0.242348000
1	2.193490000	4.381472000	1.000011000
1	2.062040000	4.460512000	-0.769962000
6	4.783970000	-0.960979000	-0.305351000
1	5.197674000	-0.460028000	-1.182741000
1	5.312195000	-0.614732000	0.585118000
1	4.927584000	-2.038673000	-0.408816000
25	0.408456000	-0.113977000	0.042634000
6	0.948959000	-3.149062000	-0.094587000
6	-3.539260000	-1.662343000	0.430842000
7	-2.482925000	0.928118000	-0.026181000
6	-2.105080000	2.276978000	0.352103000
1	-1.345730000	2.253041000	1.128008000
1	-1.736688000	2.851246000	-0.506164000
1	-2.990147000	2.781881000	0.749687000
6	-3.711182000	0.890829000	-0.815459000
1	-3.732577000	0.008893000	-1.451385000
1	-4.613781000	0.920304000	-0.197748000
1	-3.713779000	1.770615000	-1.465766000
1	-3.526880000	-2.595296000	0.992498000
1	-3.950847000	-0.873266000	1.061500000
1	-4.187139000	-1.798567000	-0.439198000
1	1.631238000	-3.073158000	0.759921000
1	0.476977000	-4.136895000	-0.087642000
1	1.555958000	-3.050262000	-1.001792000

2c, TE = - 2022.538278

6	1.874362000	-2.163830000	-0.000101000
6	1.769531000	0.220579000	-0.000075000
7	2.518253000	-0.892370000	-0.000126000
7	0.590667000	-1.998416000	0.000143000
6	-0.156876000	-0.059907000	1.825949000
8	-0.125562000	-0.004583000	2.971975000
6	-0.157018000	-0.060012000	-1.825503000
8	-0.125891000	-0.004892000	-2.971541000
6	-1.972902000	-0.757795000	0.000138000
7	-3.073625000	-1.147117000	0.000162000
6	-0.877143000	1.641558000	0.000225000
7	-1.390303000	2.694178000	0.000304000
6	-1.948394000	3.991688000	0.000205000
1	-1.152614000	4.740206000	-0.009974000
1	-2.575533000	4.126902000	-0.883314000
1	-2.559365000	4.133933000	0.893889000
6	-4.390185000	-1.660606000	-0.001036000

1	-4.851024000	-1.498614000	0.975068000
1	-4.983650000	-1.155811000	-0.765499000
1	-4.368091000	-2.731376000	-0.213677000
25	-0.195134000	-0.097732000	0.000207000
6	-0.228960000	-3.191807000	0.000410000
6	3.974176000	-0.848532000	-0.000356000
8	2.550142000	1.290072000	-0.000362000
6	1.981920000	2.597246000	-0.000532000
1	1.377880000	2.751987000	-0.894897000
1	1.378390000	2.752461000	0.894091000
1	2.828701000	3.282258000	-0.000957000
1	4.326360000	-1.877839000	-0.000209000
1	4.349720000	-0.331378000	-0.886560000
1	4.349978000	-0.331032000	0.885533000
1	-0.879768000	-3.210083000	-0.880909000
1	0.399836000	-4.087530000	-0.000645000
1	-0.877983000	-3.210971000	0.882987000

2'a, TE = - 2291.620781

6	0.992633000	-1.308750000	-0.110253000
6	1.298837000	0.960725000	0.016793000
1	2.044655000	1.757817000	0.072696000
7	1.880907000	-0.246284000	-0.048787000
7	-0.251391000	-1.011302000	-0.105596000
6	-0.640563000	0.962922000	1.874487000
8	-0.664396000	0.977769000	3.014886000
6	-0.669715000	1.266858000	-1.794105000
8	-0.706695000	1.476772000	-2.915247000
6	-2.527724000	0.856984000	0.052676000
7	-3.686169000	0.763923000	0.075772000
6	-0.608666000	2.891395000	0.184531000
7	-0.565977000	4.051023000	0.282285000
6	-0.527316000	5.459618000	0.404420000
1	-0.017718000	5.732406000	1.329854000
1	0.011110000	5.885848000	-0.443460000
1	-1.544612000	5.853940000	0.422104000
6	-5.092068000	0.612603000	0.092431000
1	-5.450147000	0.654600000	1.121976000
1	-5.552564000	1.415128000	-0.485482000
1	-5.357404000	-0.351084000	-0.345864000
25	-0.604703000	1.019547000	0.031330000
6	-1.186337000	-2.082963000	-0.120402000
6	-2.169487000	-2.124884000	-1.107278000
6	-1.127896000	-3.077015000	0.855158000
6	-3.076965000	-3.175617000	-1.127296000
1	-2.208230000	-1.347923000	-1.862225000

6	-2.047385000	-4.120029000	0.832759000
1	-0.379081000	-3.019875000	1.638477000
6	-3.021020000	-4.173989000	-0.157916000
1	-3.831833000	-3.213904000	-1.905579000
1	-2.002040000	-4.888548000	1.597107000
1	-3.737927000	-4.987893000	-0.173402000
6	3.297918000	-0.481962000	-0.065094000
6	3.853749000	-1.392032000	0.827241000
6	4.089926000	0.214804000	-0.970235000
6	5.226968000	-1.605717000	0.807433000
1	3.226311000	-1.914582000	1.541474000
6	5.462932000	0.001689000	-0.972347000
1	3.634979000	0.904775000	-1.672625000
6	6.031968000	-0.908830000	-0.087700000
1	5.667338000	-2.311817000	1.502822000
1	6.086128000	0.541121000	-1.677105000
1	7.103487000	-1.076428000	-0.096677000
1	1.393514000	-2.314974000	-0.181979000

2'b, TE = - 2424.916008

6	-0.762965000	-1.627799000	-0.182435000
6	-1.244580000	0.745068000	-0.152541000
7	-1.694804000	-0.558204000	-0.206726000
7	0.446880000	-1.171767000	-0.039681000
6	0.788912000	0.921588000	-1.791785000
8	0.777569000	1.002677000	-2.936974000
6	0.597286000	0.910098000	1.850566000
8	0.454158000	0.984564000	2.988022000
6	2.647328000	0.630818000	0.096576000
7	3.808990000	0.510546000	0.120761000
6	1.075213000	2.704624000	0.031590000
7	1.370471000	3.838184000	0.020913000
6	1.651270000	5.222212000	0.009584000
1	0.719421000	5.791951000	-0.021427000
1	2.206464000	5.496922000	0.908815000
1	2.250988000	5.473506000	-0.867626000
6	5.193608000	0.235590000	0.172815000
1	5.654793000	0.465965000	-0.789395000
1	5.664495000	0.842460000	0.948423000
1	5.345644000	-0.822054000	0.400862000
25	0.771601000	0.865269000	0.032743000
6	1.483932000	-2.135836000	-0.021225000
6	2.277527000	-2.293836000	1.117168000
6	1.743079000	-2.931238000	-1.138817000
6	3.300842000	-3.233963000	1.139748000
1	2.080628000	-1.676393000	1.987655000

6	2.771990000	-3.868550000	-1.116563000
1	1.129587000	-2.803965000	-2.024704000
6	3.556311000	-4.025130000	0.021623000
1	3.900253000	-3.352049000	2.037461000
1	2.960113000	-4.478636000	-1.995005000
1	4.358752000	-4.755519000	0.038783000
6	-3.049216000	-0.964182000	0.031347000
6	-3.661754000	-1.887235000	-0.813413000
6	-3.732493000	-0.491271000	1.149228000
6	-4.954893000	-2.320560000	-0.549080000
1	-3.116272000	-2.260003000	-1.672806000
6	-5.029574000	-0.923980000	1.406594000
1	-3.247846000	0.213089000	1.817371000
6	-5.646273000	-1.838474000	0.559627000
1	-5.425488000	-3.037445000	-1.214375000
1	-5.553973000	-0.549713000	2.279932000
1	-6.656589000	-2.177313000	0.763606000
7	-2.138437000	1.707442000	-0.396785000
6	-1.886286000	3.089747000	-0.026843000
1	-1.176410000	3.136929000	0.792316000
1	-1.512676000	3.670856000	-0.876890000
1	-2.830418000	3.530434000	0.305088000
6	-3.360133000	1.559146000	-1.183314000
1	-3.322651000	0.659472000	-1.792522000
1	-4.255541000	1.533357000	-0.555495000
1	-3.423610000	2.424056000	-1.849104000

2'c, TE = - 240505.5478

6	-0.877502000	-1.619040000	0.014831000
6	-1.313217000	0.741726000	0.056770000
7	-1.785273000	-0.527865000	0.016845000
7	0.341039000	-1.162622000	0.063704000
6	0.580792000	0.858278000	-1.813068000
8	0.520191000	0.876229000	-2.957593000
6	0.672289000	1.002974000	1.840321000
8	0.665580000	1.117864000	2.981662000
6	2.548200000	0.669371000	-0.044012000
7	3.707650000	0.553161000	-0.093803000
6	0.907801000	2.736991000	-0.070196000
7	1.155588000	3.878818000	-0.130462000
6	1.392208000	5.269846000	-0.200103000
1	0.442156000	5.809187000	-0.199227000
1	1.984628000	5.588818000	0.659697000
1	1.936988000	5.508097000	-1.115752000
6	5.097378000	0.300586000	-0.129859000
1	5.476972000	0.465125000	-1.139765000

1	5.613635000	0.969551000	0.560840000
1	5.284396000	-0.735369000	0.161833000
25	0.661157000	0.886582000	0.015571000
6	1.377938000	-2.127591000	0.034538000
6	2.275098000	-2.227735000	1.099943000
6	1.530371000	-2.980141000	-1.060003000
6	3.296549000	-3.169936000	1.074847000
1	2.161354000	-1.565631000	1.952175000
6	2.557814000	-3.918560000	-1.085933000
1	0.836133000	-2.895170000	-1.889436000
6	3.445683000	-4.018864000	-0.019608000
1	3.978269000	-3.243358000	1.916746000
1	2.663653000	-4.573511000	-1.945515000
1	4.247071000	-4.750250000	-0.040237000
6	-3.188681000	-0.832438000	0.017339000
6	-3.930428000	-0.693087000	-1.150501000
6	-3.792083000	-1.291757000	1.182324000
6	-5.284193000	-1.010839000	-1.149510000
1	-3.445468000	-0.340809000	-2.054868000
6	-5.145926000	-1.611298000	1.178512000
1	-3.198506000	-1.399932000	2.083923000
6	-5.894382000	-1.470054000	0.014068000
1	-5.861788000	-0.903859000	-2.061895000
1	-5.615607000	-1.971562000	2.087990000
1	-6.950283000	-1.719900000	0.012366000
8	-2.314279000	1.595038000	0.123567000
6	-2.070525000	2.999581000	0.183815000
1	-1.454267000	3.242985000	1.049241000
1	-1.591433000	3.340985000	-0.733682000
1	-3.052895000	3.458481000	0.284124000

3a, TE = - 1946.776532

6	0.293791000	2.602789000	-1.154831000
6	0.200858000	1.621918000	1.007756000
1	0.237638000	1.844263000	2.084142000
7	0.322840000	2.723250000	0.278973000
7	0.142993000	1.347292000	-1.441342000
6	0.484775000	4.059297000	0.830838000
1	-0.333060000	4.705984000	0.503329000
1	0.487044000	4.005029000	1.920154000
1	1.425354000	4.498503000	0.489342000
6	0.086204000	0.989529000	-2.840864000
1	0.883292000	0.276280000	-3.080578000
1	-0.863879000	0.490665000	-3.065018000
1	0.188764000	1.872397000	-3.482165000
25	-0.004616000	-0.043553000	0.082060000

6	-0.194109000	-1.551041000	-1.048100000
7	-0.310876000	-2.487640000	-1.747845000
6	-0.098478000	-0.999531000	1.651420000
7	-0.149600000	-1.551366000	2.692337000
6	-1.876732000	0.164836000	0.070423000
7	-3.042793000	0.295109000	0.060503000
6	1.864244000	-0.273754000	0.033451000
7	3.028557000	-0.416302000	0.003896000
6	4.430265000	-0.584028000	-0.013436000
1	4.892231000	0.031825000	0.761632000
1	4.685658000	-1.630619000	0.167682000
1	4.830980000	-0.286867000	-0.985190000
6	-0.450619000	-3.606449000	-2.597005000
1	-0.601418000	-4.513061000	-2.005842000
1	-1.309257000	-3.470999000	-3.258847000
1	0.447419000	-3.729387000	-3.206898000
6	-0.226551000	-2.280387000	3.897816000
1	0.676909000	-2.126484000	4.493420000
1	-1.089258000	-1.954456000	4.484601000
1	-0.329818000	-3.348901000	3.690484000
6	-4.445945000	0.452125000	0.054670000
1	-4.887421000	-0.091507000	0.893086000
1	-4.706508000	1.509330000	0.143312000
1	-4.863347000	0.062603000	-0.876627000

3b, TE = - 2080.555017

6	-1.129689000	1.008177000	-2.355901000
6	-1.586563000	0.332828000	-0.090807000
7	-2.048021000	0.808013000	-1.285898000
7	0.066627000	0.675686000	-1.989372000
25	0.407578000	0.014111000	-0.072094000
6	2.223459000	-0.272969000	-0.402965000
7	3.370696000	-0.467188000	-0.579733000
6	0.667943000	-0.591790000	1.636326000
7	0.965365000	-1.013376000	2.704817000
6	-0.004320000	-1.734563000	-0.624143000
7	-0.268601000	-2.829943000	-0.956553000
6	0.729459000	1.786101000	0.474532000
7	0.920059000	2.892608000	0.820711000
6	1.123568000	4.222418000	1.248327000
1	0.336217000	4.519607000	1.945377000
1	2.090107000	4.313690000	1.749470000
1	1.107419000	4.899365000	0.390919000
6	4.738236000	-0.666364000	-0.864565000
1	5.354087000	-0.019198000	-0.235171000
1	5.017546000	-1.705851000	-0.675706000

1	4.943199000	-0.433368000	-1.912847000
6	0.897626000	-1.407794000	4.061287000
1	-0.107366000	-1.241699000	4.462962000
1	1.141930000	-2.468422000	4.162315000
1	1.610917000	-0.835533000	4.660202000
6	-0.584621000	-4.147885000	-1.351631000
1	0.303420000	-4.646614000	-1.747129000
1	-0.956443000	-4.717908000	-0.496842000
1	-1.354788000	-4.134042000	-2.126427000
6	1.118019000	0.832178000	-2.968897000
6	-3.360717000	1.416108000	-1.482308000
7	-2.536992000	0.027414000	0.825441000
6	-2.206695000	-0.096511000	2.230283000
1	-3.059506000	0.254216000	2.820529000
1	-1.999815000	-1.136930000	2.512817000
1	-1.343543000	0.520300000	2.464557000
6	-3.828834000	-0.567200000	0.500799000
1	-4.671808000	0.100243000	0.709114000
1	-3.861122000	-0.872231000	-0.543087000
1	-3.950404000	-1.466707000	1.113422000
1	0.719181000	1.221897000	-3.913021000
1	1.889712000	1.517292000	-2.597007000
1	1.612768000	-0.127368000	-3.161688000
1	-3.744994000	1.794555000	-0.533629000
1	-3.232982000	2.250608000	-2.171067000
1	-4.098324000	0.732439000	-1.913615000

3c, TE = - 2061.194755

6	1.815162000	-0.000332000	-2.215939000
6	1.767959000	-0.009569000	0.173004000
7	2.494489000	-0.008714000	-0.963357000
7	0.536104000	0.006312000	-2.007916000
25	-0.192780000	0.001219000	-0.075947000
6	-1.977609000	0.013585000	-0.658176000
7	-3.102185000	0.021491000	-0.998784000
6	-0.788437000	-0.005000000	1.666638000
7	-1.273101000	-0.008536000	2.743894000
6	-0.163747000	1.884102000	-0.067305000
7	-0.144422000	3.057713000	-0.055803000
6	-0.183140000	-1.881785000	-0.087027000
7	-0.175888000	-3.055580000	-0.088246000
6	-0.158422000	-4.467304000	-0.074936000
1	0.377248000	-4.828530000	0.806097000
1	-1.179076000	-4.855936000	-0.051349000
1	0.341525000	-4.844384000	-0.970004000
6	-4.431967000	0.031261000	-1.471908000

1	-5.019988000	-0.734603000	-0.960763000
1	-4.889953000	1.006097000	-1.288683000
1	-4.450408000	-0.169750000	-2.546069000
6	-1.632045000	-0.014506000	4.108784000
1	-2.230522000	-0.899249000	4.340698000
1	-0.738203000	-0.022582000	4.739962000
1	-2.221618000	0.873505000	4.350809000
6	-0.113796000	4.468960000	-0.026706000
1	-1.130282000	4.868006000	-0.056038000
1	0.375195000	4.815660000	0.886685000
1	0.439241000	4.849743000	-0.888342000
6	-0.316147000	0.015441000	-3.175189000
6	3.949482000	-0.015620000	-0.960338000
8	2.601830000	-0.017368000	1.215754000
6	2.077910000	-0.019299000	2.537154000
1	1.473160000	-0.910248000	2.711381000
1	2.945301000	-0.023993000	3.197437000
1	1.478935000	0.874551000	2.716282000
1	4.274650000	-0.012114000	-1.999012000
1	4.348826000	0.865149000	-0.450232000
1	4.340498000	-0.905026000	-0.458804000
1	-0.964446000	0.899796000	-3.170535000
1	0.280095000	0.015240000	-4.094832000
1	-0.974802000	-0.861286000	-3.176730000

3'a, TE = - 2329.790976

6	-1.032149000	-1.561919000	-0.222744000
6	-1.385228000	0.781933000	0.057891000
1	-2.165815000	1.545078000	0.174759000
7	-1.919645000	-0.441580000	-0.099461000
7	0.187462000	-1.099866000	-0.184095000
25	0.496361000	0.946211000	0.108103000
6	2.399639000	0.858938000	0.160100000
7	3.569550000	0.797102000	0.201174000
6	0.395883000	2.765031000	0.379466000
7	0.264522000	3.922482000	0.548551000
6	0.499763000	0.661967000	1.976751000
7	0.503878000	0.493635000	3.135921000
6	0.594048000	1.235294000	-1.756411000
7	0.655235000	1.427236000	-2.910724000
6	0.710392000	1.650047000	-4.304224000
1	-0.296122000	1.807016000	-4.698226000
1	1.316886000	2.532741000	-4.518155000
1	1.155127000	0.785849000	-4.802594000
6	4.968481000	0.606859000	0.216536000
1	5.458649000	1.376009000	-0.384172000

1	5.342467000	0.667391000	1.240757000
1	5.213034000	-0.376160000	-0.194039000
6	0.167449000	5.316296000	0.748769000
1	-0.327706000	5.787273000	-0.103936000
1	-0.411791000	5.529391000	1.650476000
1	1.163182000	5.753031000	0.860693000
6	0.499379000	0.297250000	4.534571000
1	1.070139000	1.088944000	5.024727000
1	-0.525638000	0.313346000	4.911178000
1	0.951173000	-0.666985000	4.777196000
6	1.225790000	-2.054439000	-0.272539000
6	2.178598000	-1.959467000	-1.291018000
6	1.340721000	-3.089935000	0.658975000
6	3.209797000	-2.885951000	-1.384107000
1	2.095773000	-1.153345000	-2.012151000
6	2.380386000	-4.011236000	0.569386000
1	0.607563000	-3.159857000	1.455737000
6	3.319777000	-3.916404000	-0.452410000
1	3.932687000	-2.803655000	-2.190383000
1	2.455210000	-4.807095000	1.304606000
1	4.130140000	-4.634933000	-0.521771000
6	-3.324233000	-0.675070000	-0.144961000
6	-3.875013000	-1.761848000	0.533940000
6	-4.156794000	0.184677000	-0.860611000
6	-5.247834000	-1.975690000	0.504502000
1	-3.218297000	-2.427708000	1.080701000
6	-5.530415000	-0.031373000	-0.879983000
1	-3.728107000	1.012160000	-1.416220000
6	-6.082488000	-1.111204000	-0.198584000
1	-5.667841000	-2.820625000	1.040983000
1	-6.168527000	0.641975000	-1.443217000
1	-7.153905000	-1.280728000	-0.218868000

3'b, TE = - 2463.571792

6	0.800507000	-1.693281000	-0.185291000
6	1.263054000	0.687428000	-0.136444000
7	1.725590000	-0.618683000	-0.218126000
7	-0.412103000	-1.237849000	-0.034656000
25	-0.737252000	0.814125000	0.041308000
6	-2.596172000	0.618352000	0.046972000
7	-3.769553000	0.536941000	0.026925000
6	-0.993662000	2.633095000	0.049218000
7	-1.282859000	3.778919000	0.042642000
6	-0.750601000	0.844521000	-1.841120000
7	-0.755015000	0.885545000	-3.014154000
6	-0.654378000	0.802114000	1.925039000

7	-0.596230000	0.812580000	3.097944000
6	-0.499583000	0.818158000	4.506346000
1	0.549461000	0.828267000	4.811729000
1	-0.993861000	1.703276000	4.913355000
1	-0.978251000	-0.072926000	4.919388000
6	-5.146580000	0.226562000	0.044195000
1	-5.662937000	0.836207000	0.789430000
1	-5.590922000	0.421859000	-0.934696000
1	-5.285737000	-0.829562000	0.292098000
6	-1.373018000	5.187300000	0.061120000
1	-0.376902000	5.634337000	0.136375000
1	-1.849656000	5.550202000	-0.853118000
1	-1.969226000	5.519028000	0.915133000
6	-0.763942000	0.935650000	-4.425234000
1	-1.459517000	0.193142000	-4.823158000
1	-1.075244000	1.926716000	-4.763367000
1	0.235061000	0.727691000	-4.815381000
6	-1.438314000	-2.205659000	-0.004181000
6	-2.308648000	-2.274900000	1.089022000
6	-1.623952000	-3.103718000	-1.059894000
6	-3.323498000	-3.222959000	1.130654000
1	-2.174284000	-1.575711000	1.907481000
6	-2.645654000	-4.048646000	-1.019940000
1	-0.957088000	-3.046382000	-1.913820000
6	-3.501471000	-4.115707000	0.074916000
1	-3.979541000	-3.267540000	1.995215000
1	-2.773451000	-4.734543000	-1.852499000
1	-4.298522000	-4.851696000	0.105767000
6	3.082188000	-1.016194000	0.004945000
6	3.692146000	-1.941261000	-0.841285000
6	3.782824000	-0.533981000	1.109586000
6	4.991127000	-2.367059000	-0.592654000
1	3.137658000	-2.322167000	-1.691322000
6	5.085401000	-0.958439000	1.352077000
1	3.304993000	0.173776000	1.778905000
6	5.696287000	-1.875471000	0.503161000
1	5.455960000	-3.085301000	-1.260855000
1	5.619758000	-0.575509000	2.215838000
1	6.711259000	-2.207610000	0.695118000
7	2.175520000	1.644053000	-0.379104000
6	1.952045000	3.016212000	0.033847000
1	2.902796000	3.429058000	0.386286000
1	1.595048000	3.636798000	-0.796615000
1	1.233755000	3.046880000	0.847084000
6	3.361624000	1.506694000	-1.216252000
1	4.286135000	1.484509000	-0.630211000

1	3.305815000	0.607717000	-1.825688000
1	3.394926000	2.372943000	-1.884297000

3'c, TE = - 2444.206673

6	-0.933342000	-1.675842000	-0.065647000
6	-1.327821000	0.696093000	-0.060583000
7	-1.826829000	-0.575087000	-0.047656000
7	0.291783000	-1.228070000	-0.091972000
25	0.626985000	0.827938000	0.019912000
6	2.496081000	0.618321000	0.110501000
7	3.662773000	0.514068000	0.182601000
6	0.860067000	2.651320000	0.162601000
7	1.116107000	3.797992000	0.262075000
6	0.532290000	0.704931000	1.900916000
7	0.469731000	0.639283000	3.069821000
6	0.706068000	0.965490000	-1.859061000
7	0.754133000	1.068268000	-3.026665000
6	0.801935000	1.189634000	-4.432691000
1	-0.194128000	1.407015000	-4.824999000
1	1.478153000	1.999267000	-4.716056000
1	1.160983000	0.258315000	-4.876632000
6	5.044522000	0.229442000	0.235575000
1	5.594370000	0.905444000	-0.422992000
1	5.415171000	0.353414000	1.255554000
1	5.221351000	-0.801056000	-0.084009000
6	1.255830000	5.198190000	0.366673000
1	1.886403000	5.577764000	-0.441211000
1	0.277875000	5.684497000	0.305123000
1	1.718075000	5.462828000	1.320957000
6	0.384684000	0.564480000	4.477537000
1	0.911663000	1.407804000	4.929293000
1	-0.661029000	0.590978000	4.791994000
1	0.836977000	-0.364884000	4.830782000
6	1.315632000	-2.199872000	-0.080041000
6	2.254723000	-2.242085000	-1.115490000
6	1.430529000	-3.121495000	0.964490000
6	3.271735000	-3.188880000	-1.112077000
1	2.172793000	-1.524745000	-1.925406000
6	2.454696000	-4.064519000	0.970194000
1	0.708125000	-3.084416000	1.773266000
6	3.380612000	-4.105136000	-0.067416000
1	3.983665000	-3.213508000	-1.931944000
1	2.528470000	-4.770237000	1.792529000
1	4.179201000	-4.840044000	-0.062738000
6	-3.229763000	-0.864187000	-0.074641000
6	-4.018032000	-0.623762000	1.047060000

6	-3.799309000	-1.414640000	-1.218372000
6	-5.374126000	-0.929845000	1.021246000
1	-3.564871000	-0.201320000	1.937733000
6	-5.155662000	-1.723384000	-1.240587000
1	-3.173573000	-1.602835000	-2.084289000
6	-5.946782000	-1.480214000	-0.122029000
1	-5.983766000	-0.743049000	1.899529000
1	-5.594131000	-2.154827000	-2.134768000
1	-7.004632000	-1.721417000	-0.139506000
8	-2.337823000	1.554382000	-0.142957000
6	-2.078217000	2.952349000	-0.198494000
1	-1.415784000	3.187159000	-1.032148000
1	-3.049573000	3.423852000	-0.346437000
1	-1.635791000	3.296965000	0.736823000

4'a, TE = - 2443.113820

6	1.056732000	-1.415549000	-0.194321000
6	1.380494000	1.031410000	-0.118775000
1	1.706582000	1.554665000	-1.028860000
7	-0.210889000	-1.039661000	-0.177402000
1	1.842592000	1.566226000	0.721959000
6	-0.667560000	2.756758000	0.250428000
6	-0.353693000	0.671453000	1.874947000
6	-0.721907000	1.085284000	-1.807580000
7	-0.643047000	3.917290000	0.372011000
7	-0.732055000	1.180034000	-2.969261000
7	-0.145047000	0.497005000	3.007749000
6	0.118749000	0.264399000	4.377380000
1	0.730439000	-0.632961000	4.486076000
1	0.654096000	1.116812000	4.798996000
1	-0.820261000	0.127195000	4.916284000
6	-0.616215000	5.322970000	0.520950000
1	-0.003029000	5.591369000	1.383131000
1	-0.193748000	5.781449000	-0.374986000
1	-1.629966000	5.698694000	0.671514000
6	-0.736516000	1.271853000	-4.380278000
1	-0.215669000	2.178873000	-4.691891000
1	-0.230995000	0.403550000	-4.806591000
1	-1.764502000	1.304590000	-4.745315000
6	-1.176312000	-2.062449000	-0.188760000
6	-2.273246000	-1.999254000	-1.058045000
6	-1.084849000	-3.167065000	0.670468000
6	-3.231759000	-3.005850000	-1.077833000
1	-2.359359000	-1.153585000	-1.731574000
6	-2.045292000	-4.172524000	0.650223000
1	-0.245206000	-3.220033000	1.354900000

6	-3.126940000	-4.101347000	-0.223748000
1	-4.064875000	-2.936000000	-1.771413000
1	-1.950941000	-5.015085000	1.329565000
1	-3.878139000	-4.884528000	-0.236887000
26	-0.633691000	0.932790000	0.048280000
6	-2.487011000	0.772429000	0.251872000
7	-3.641436000	0.713185000	0.410214000
6	-5.036604000	0.556738000	0.571154000
1	-5.563379000	1.337291000	0.019324000
1	-5.340204000	-0.420914000	0.190442000
1	-5.297604000	0.627358000	1.628589000
7	1.908499000	-0.346929000	-0.144103000
6	3.294662000	-0.548193000	-0.168088000
6	4.176490000	0.542308000	-0.260033000
6	3.861373000	-1.835469000	-0.087339000
6	5.555430000	0.349823000	-0.278104000
1	3.784924000	1.549365000	-0.321118000
6	5.235799000	-2.012918000	-0.107272000
1	3.193245000	-2.682618000	-0.008542000
6	6.103167000	-0.924440000	-0.204081000
1	6.204935000	1.217400000	-0.352528000
1	5.636611000	-3.020703000	-0.042164000
1	7.178277000	-1.069633000	-0.217655000

4'b, TE = - 5590.607449

6	1.282774000	1.421448000	0.180077000
6	1.427422000	-1.059741000	0.155658000
1	1.718691000	-1.572898000	1.082225000
7	-0.019185000	1.174272000	0.163128000
1	1.866159000	-1.640661000	-0.665766000
6	-0.919902000	-2.758410000	-0.215287000
6	-0.360904000	-0.660579000	-1.981637000
6	-0.798107000	-0.977013000	1.933026000
7	-1.024957000	-3.918249000	-0.316515000
7	-0.826708000	-1.056467000	3.095044000
7	-0.140317000	-0.549865000	-3.119713000
6	0.126888000	-0.408021000	-4.501057000
1	0.881344000	0.366124000	-4.650659000
1	0.496536000	-1.353212000	-4.902144000
1	-0.787735000	-0.126570000	-5.025564000
6	-1.156636000	-5.320170000	-0.436920000
1	-0.594931000	-5.671945000	-1.304461000
1	-0.769003000	-5.807174000	0.460012000
1	-2.208454000	-5.585476000	-0.561018000
6	-0.862843000	-1.140804000	4.506087000
1	-0.373871000	-2.060511000	4.831608000

1	-0.342181000	-0.284267000	4.937630000
1	-1.899051000	-1.142673000	4.848417000
6	-0.873432000	2.293059000	0.167333000
6	-2.010593000	2.316515000	0.984394000
6	-0.626977000	3.408986000	-0.645842000
6	-2.862233000	3.415338000	0.996345000
1	-2.214135000	1.462930000	1.621660000
6	-1.480971000	4.505870000	-0.633440000
1	0.245625000	3.395364000	-1.289175000
6	-2.605644000	4.519922000	0.187773000
1	-3.731035000	3.409812000	1.648357000
1	-1.269637000	5.353988000	-1.278662000
1	-3.274055000	5.374892000	0.193747000
6	-2.630092000	-0.506357000	-0.258180000
7	-3.772366000	-0.321368000	-0.414070000
6	-5.146331000	-0.035238000	-0.580208000
1	-5.744776000	-0.748863000	-0.010968000
1	-5.356302000	0.975345000	-0.223480000
1	-5.413921000	-0.105824000	-1.636063000
7	2.042140000	0.288342000	0.148640000
6	3.442531000	0.390590000	0.170016000
6	4.243953000	-0.754677000	0.309908000
6	4.099076000	1.629504000	0.037252000
6	5.633220000	-0.660366000	0.325013000
1	3.783317000	-1.728488000	0.412553000
6	5.482668000	1.709528000	0.055165000
1	3.494510000	2.519016000	-0.078303000
6	6.270095000	0.567342000	0.200111000
1	6.218960000	-1.568127000	0.437909000
1	5.954122000	2.682596000	-0.051015000
1	7.352788000	0.636216000	0.211210000
44	-0.679250000	-0.851741000	-0.037208000

5a, TE = - 2482.311213

6	0.264125000	1.323471000	-0.889551000
6	-1.860962000	-0.005667000	-0.486445000
6	0.269730000	-1.328207000	-0.882714000
7	-1.173195000	-1.155443000	-0.610474000
7	-1.177886000	1.146345000	-0.615536000
6	-1.941816000	-2.344996000	-0.494016000
6	-1.668128000	-3.451907000	-1.304851000
6	-2.975593000	-2.445985000	0.443754000
6	-2.417617000	-4.618255000	-1.189576000
1	-0.874117000	-3.393439000	-2.040607000
6	-3.720372000	-3.613134000	0.554702000
1	-3.182114000	-1.592327000	1.077703000

6	-3.449097000	-4.709472000	-0.260885000
1	-2.193607000	-5.459589000	-1.838548000
1	-4.513355000	-3.669829000	1.294638000
1	-4.029685000	-5.621631000	-0.169578000
6	-1.951134000	2.333348000	-0.503981000
6	-1.682389000	3.437618000	-1.320052000
6	-2.984679000	2.434531000	0.434013000
6	-2.436462000	4.601470000	-1.209646000
1	-0.888656000	3.378920000	-2.056088000
6	-3.734057000	3.599192000	0.540099000
1	-3.187517000	1.582943000	1.071919000
6	-3.467689000	4.692838000	-0.280685000
1	-2.216247000	5.440696000	-1.862633000
1	-4.526798000	3.656095000	1.280277000
1	-4.051858000	5.603082000	-0.193182000
1	0.421954000	-1.270430000	-1.967880000
1	0.511098000	-2.352786000	-0.589190000
1	0.501622000	2.350632000	-0.601971000
1	0.415857000	1.260213000	-1.974494000
26	1.516763000	0.002696000	0.049862000
6	0.422239000	0.003698000	1.541593000
7	-0.240723000	0.004360000	2.502936000
6	2.513995000	1.390488000	0.754711000
7	3.120038000	2.295240000	1.183373000
6	2.526868000	0.001401000	-1.499377000
7	3.134746000	0.000656000	-2.496856000
6	2.520636000	-1.376926000	0.761392000
7	3.131214000	-2.276620000	1.194242000
6	3.856861000	3.382098000	1.706176000
1	4.318311000	3.098099000	2.654206000
1	4.639761000	3.672414000	1.002720000
1	3.195569000	4.234654000	1.873486000
6	-1.089126000	0.004776000	3.632470000
1	-0.492208000	0.017644000	4.546534000
1	-1.731371000	0.887719000	3.614032000
1	-1.714066000	-0.890664000	3.627709000
6	3.873560000	-3.357189000	1.722244000
1	4.653676000	-3.651238000	1.017248000
1	4.339020000	-3.064177000	2.665560000
1	3.215391000	-4.210069000	1.899896000
6	3.878966000	-0.000578000	-3.698801000
1	4.434652000	-0.935811000	-3.790190000
1	3.205204000	0.099011000	-4.551773000
1	4.582418000	0.834278000	-3.700228000

5b, TE = - 5629.806655

6	0.106943000	-1.359914000	0.940950000
6	-2.005343000	-0.004140000	0.499314000
6	0.098601000	1.365420000	0.936727000
7	-1.335232000	1.154959000	0.635858000
7	-1.328455000	-1.158823000	0.640823000
6	-2.125441000	2.330527000	0.506208000
6	-1.906395000	3.430098000	1.342433000
6	-3.123177000	2.422728000	-0.469819000
6	-2.675925000	4.581882000	1.214507000
1	-1.139656000	3.377001000	2.107032000
6	-3.887952000	3.575685000	-0.593864000
1	-3.286068000	1.573877000	-1.122792000
6	-3.672211000	4.664838000	0.247376000
1	-2.495748000	5.418127000	1.883318000
1	-4.652366000	3.627031000	-1.363580000
1	-4.268468000	5.565776000	0.146386000
6	-2.112384000	-2.339294000	0.517899000
6	-1.883615000	-3.435243000	1.356312000
6	-3.113944000	-2.440017000	-0.453452000
6	-2.647075000	-4.591805000	1.234914000
1	-1.114125000	-3.375778000	2.117658000
6	-3.872533000	-3.597684000	-0.570964000
1	-3.284788000	-1.593706000	-1.107642000
6	-3.646949000	-4.683291000	0.272321000
1	-2.459194000	-5.425041000	1.905364000
1	-4.639997000	-3.655544000	-1.337183000
1	-4.238434000	-5.587916000	0.176384000
1	0.235269000	1.295008000	2.022988000
1	0.317839000	2.399829000	0.663097000
1	0.332104000	-2.393609000	0.669387000
1	0.244115000	-1.286412000	2.026954000
6	0.294224000	-0.001357000	-1.639305000
7	-0.373301000	-0.005601000	-2.596472000
6	2.529558000	-1.468726000	-0.791174000
7	3.132424000	-2.380872000	-1.210227000
6	2.505708000	0.011487000	1.618809000
7	3.098906000	0.014958000	2.624007000
6	2.519241000	1.484316000	-0.796606000
7	3.115048000	2.399334000	-1.219479000
6	3.872443000	-3.467775000	-1.728056000
1	4.637631000	-3.104208000	-2.417264000
1	4.356088000	-4.009703000	-0.912873000
1	3.207274000	-4.149455000	-2.261938000
6	-1.211818000	-0.011240000	-3.733533000
1	-0.605708000	-0.021445000	-4.641438000

1	-1.848862000	-0.897833000	-3.718677000
1	-1.840965000	0.881085000	-3.733393000
6	3.846236000	3.489869000	-1.742181000
1	4.319206000	4.043889000	-0.928865000
1	4.619324000	3.128932000	-2.423911000
1	3.176794000	4.159733000	-2.285599000
6	3.836567000	0.019669000	3.830075000
1	4.455431000	0.917410000	3.880967000
1	3.152966000	0.007031000	4.680761000
1	4.479017000	-0.861745000	3.873487000
44	1.450392000	0.005451000	-0.044355000

6a, TE = -2630.346356

6	0.174050000	1.403535000	0.407417000
7	-1.239168000	1.165397000	0.133815000
6	-1.908338000	0.000056000	0.023665000
7	-1.239243000	-1.165310000	0.133931000
6	0.173929000	-1.403466000	0.407766000
8	0.424577000	2.528629000	0.812641000
6	-2.080961000	2.334584000	0.086330000
6	-2.003630000	3.194918000	-1.003876000
6	-2.828360000	4.312928000	-1.066129000
6	-3.729280000	4.577193000	-0.038254000
6	-3.800942000	3.716381000	1.052944000
6	-2.975929000	2.598139000	1.116451000
1	-1.302064000	2.981421000	-1.804100000
1	-2.770167000	4.976775000	-1.922905000
1	-4.374026000	5.448568000	-0.089128000
1	-4.500944000	3.914886000	1.858389000
1	-3.027575000	1.917762000	1.960126000
6	-2.081093000	-2.334461000	0.086520000
6	-2.003671000	-3.194935000	-1.003567000
6	-2.828456000	-4.312908000	-1.065786000
6	-3.729515000	-4.576995000	-0.037988000
6	-3.801261000	-3.716046000	1.053098000
6	-2.976198000	-2.597840000	1.116569000
1	-1.302000000	-2.981570000	-1.803735000
1	-2.770198000	-4.976861000	-1.922475000
1	-4.374304000	-5.448339000	-0.088833000
1	-4.501370000	-3.914417000	1.858483000
1	-3.027912000	-1.917355000	1.960152000
8	0.424313000	-2.528437000	0.813429000
26	1.481751000	-0.000084000	0.035369000
6	2.760328000	-1.340710000	-0.322220000
6	1.882278000	0.000176000	1.850009000
6	2.760484000	1.340327000	-0.322563000

6	0.903595000	-0.000239000	-1.730835000
7	3.553705000	2.161574000	-0.546244000
7	3.553454000	-2.162115000	-0.545662000
7	2.112124000	0.000375000	2.991105000
7	0.529481000	-0.000324000	-2.833493000
6	0.062328000	-0.000403000	-4.168256000
1	0.426149000	-0.890021000	-4.685053000
1	-1.028962000	-0.001252000	-4.174022000
1	0.424761000	0.890003000	-4.684673000
6	4.500614000	3.180086000	-0.804312000
1	4.588860000	3.334720000	-1.880806000
1	4.177110000	4.108899000	-0.331651000
1	5.471937000	2.889052000	-0.401308000
6	2.379495000	0.000942000	4.379748000
1	2.900596000	-0.917824000	4.653818000
1	3.004405000	0.858914000	4.633105000
1	1.441685000	0.062198000	4.934406000
6	4.500238000	-3.180792000	-0.803534000
1	5.470880000	-2.891135000	-0.397909000
1	4.175101000	-4.110243000	-0.333252000
1	4.590705000	-3.333538000	-1.880113000

6b, TE = - 5777.837831

6	0.026150000	1.450099000	0.439641000
7	-1.381000000	1.173873000	0.161125000
6	-2.037061000	-0.000062000	0.047067000
7	-1.380946000	-1.173942000	0.161172000
6	0.026240000	-1.450092000	0.439835000
8	0.246917000	2.575614000	0.860823000
6	-2.246076000	2.327105000	0.111972000
6	-2.181915000	3.189449000	-0.977397000
6	-3.026660000	4.292413000	-1.040741000
6	-3.934681000	4.539468000	-0.014997000
6	-3.993167000	3.676503000	1.075350000
6	-3.148215000	2.573436000	1.140068000
1	-1.474717000	2.989830000	-1.776226000
1	-2.978487000	4.957785000	-1.896930000
1	-4.595021000	5.399005000	-0.066683000
1	-4.698478000	3.861639000	1.879326000
1	-3.189478000	1.891655000	1.983146000
6	-2.245949000	-2.327224000	0.112006000
6	-2.181610000	-3.189635000	-0.977299000
6	-3.026296000	-4.292643000	-1.040682000
6	-3.934436000	-4.539675000	-0.015039000
6	-3.993099000	-3.676645000	1.075249000
6	-3.148208000	-2.573534000	1.140005000

1	-1.474326000	-2.990026000	-1.776056000
1	-2.977986000	-4.958063000	-1.896826000
1	-4.594733000	-5.399243000	-0.066756000
1	-4.698503000	-3.861764000	1.879146000
1	-3.189613000	-1.891699000	1.983032000
8	0.246981000	-2.575517000	0.861246000
6	2.774152000	-1.445949000	-0.379399000
6	1.921634000	0.000169000	1.941826000
6	2.773973000	1.446062000	-0.379643000
6	0.795596000	-0.000188000	-1.853640000
7	3.533629000	2.297906000	-0.608315000
7	3.534006000	-2.297644000	-0.607970000
7	2.191465000	0.000298000	3.073355000
7	0.399360000	-0.000324000	-2.947715000
6	-0.087530000	-0.000288000	-4.275548000
1	0.267322000	-0.891424000	-4.795743000
1	-1.178646000	0.001432000	-4.264114000
1	0.270127000	0.889142000	-4.796739000
6	4.448033000	3.342740000	-0.878552000
1	4.356113000	3.648526000	-1.921925000
1	4.230987000	4.194898000	-0.232504000
1	5.466140000	2.997468000	-0.691876000
6	2.514789000	0.000164000	4.450193000
1	3.098874000	-0.890072000	4.688713000
1	3.098594000	0.890523000	4.688942000
1	1.597659000	-0.000054000	5.041282000
6	4.448843000	-3.342124000	-0.878137000
1	5.464658000	-3.004774000	-0.666166000
1	4.215651000	-4.203980000	-0.250853000
1	4.375741000	-3.629915000	-1.928100000
44	1.434416000	-0.000003000	0.020749000

Cartesian coordinates for the optimized geometries of protonated complex **1a-6b**, along with their total energies (in hartrees) including zero point vibrational correction in aqueous phase.

[1a-H]⁺, TE = - 1869.934856

6	-2.124009000	0.902136000	-0.000197000
6	-1.166700000	-1.174538000	0.000242000
1	-1.333472000	-2.252710000	0.000451000
7	-2.287520000	-0.486507000	0.000085000
7	-0.930241000	1.334111000	-0.000290000
6	-3.642219000	-1.045898000	0.000151000
1	-4.173820000	-0.715096000	-0.892586000
1	-3.564173000	-2.130521000	0.000435000
1	-4.173925000	-0.714635000	0.892652000
6	-0.693064000	2.766236000	-0.000578000

1	-0.109132000	3.029346000	0.883880000
1	-0.109075000	3.028977000	-0.885107000
1	-1.628462000	3.329556000	-0.000730000
25	0.491262000	-0.141295000	0.000035000
6	0.479202000	-0.164169000	1.857838000
8	0.474114000	-0.199457000	2.991658000
6	1.521355000	-1.635277000	0.000380000
8	2.136261000	-2.594664000	0.000627000
6	1.949933000	1.005099000	-0.000220000
8	2.856365000	1.691072000	-0.000382000
6	0.479229000	-0.165020000	-1.857758000
8	0.474184000	-0.200851000	-2.991561000
1	-3.014922000	1.524004000	-0.000308000

[1b-H]⁺, TE = -2003.730918

6	-0.590997000	2.246015000	-0.107179000
6	-1.272962000	0.034790000	0.096535000
7	-1.632148000	1.364274000	0.034299000
7	0.605561000	1.815834000	-0.157480000
25	0.773274000	-0.205675000	0.013672000
6	0.839117000	-0.039616000	1.860509000
8	0.855229000	0.052103000	2.992554000
6	0.927080000	-2.006806000	0.141939000
8	1.119487000	-3.131784000	0.201056000
6	2.595475000	-0.127466000	-0.153674000
8	3.729978000	-0.097605000	-0.255758000
6	0.527326000	-0.367344000	-1.818007000
8	0.358696000	-0.484690000	-2.935080000
6	1.689499000	2.769166000	-0.307752000
6	-2.922430000	1.936667000	0.450925000
7	-2.243964000	-0.858159000	0.051651000
6	-3.549763000	-0.658497000	-0.585336000
1	-4.352625000	-0.557859000	0.147751000
1	-3.528499000	0.202250000	-1.247301000
1	-3.744794000	-1.544721000	-1.192589000
6	-2.027068000	-2.241963000	0.455032000
1	-2.961802000	-2.616653000	0.875841000
1	-1.756487000	-2.863998000	-0.402890000
1	-1.266899000	-2.297181000	1.227729000
1	-3.405696000	1.258602000	1.150967000
1	-2.725427000	2.872008000	0.973497000
1	-3.581108000	2.134376000	-0.394367000
1	1.315103000	3.795126000	-0.349714000
1	2.376900000	2.675851000	0.536371000
1	2.242206000	2.555334000	-1.225458000
1	-0.847641000	3.301221000	-0.161060000

[1c-H]⁺, TE = -1984.358048

6	1.205365000	-2.030948000	0.020846000
6	1.409519000	0.265572000	-0.013398000
7	2.035732000	-0.933962000	0.009682000
7	-0.052263000	-1.841153000	0.010530000
25	-0.600077000	0.128909000	-0.013724000
6	-0.552927000	0.153465000	1.844601000
8	-0.518194000	0.181851000	2.978148000
6	-1.048173000	1.889091000	-0.026321000
8	-1.406555000	2.972418000	-0.031617000
6	-2.394011000	-0.291933000	-0.014950000
8	-3.505507000	-0.531971000	-0.016846000
6	-0.544256000	0.122490000	-1.871714000
8	-0.503828000	0.133018000	-3.005432000
6	-0.940951000	-2.989300000	0.021445000
8	2.285023000	1.220181000	-0.031756000
6	1.895305000	2.601164000	-0.068336000
1	1.318275000	2.800755000	-0.970346000
1	1.337110000	2.853803000	0.832136000
1	2.829076000	3.157264000	-0.094342000
6	3.491971000	-1.083622000	0.015077000
1	3.912995000	-0.633222000	-0.883495000
1	3.909722000	-0.597087000	0.896092000
1	3.730478000	-2.144868000	0.037121000
1	-0.381039000	-3.927216000	0.039246000
1	-1.585800000	-2.941079000	0.901788000
1	-1.573420000	-2.967542000	-0.868907000
1	1.675018000	-3.010638000	0.037045000

[1'a-H]⁺, TE = - 2252.937150

6	0.629802000	1.090116000	0.055941000
6	1.177909000	-1.138045000	0.022517000
1	1.989589000	-1.866918000	0.037472000
7	1.622558000	0.109901000	0.046576000
7	-0.577519000	0.678640000	0.074913000
25	-0.748234000	-1.380318000	0.004197000
6	-0.734986000	-1.292131000	-1.856005000
8	-0.714567000	-1.257856000	-2.988742000
6	-0.591078000	-3.185323000	-0.097125000
8	-0.453091000	-4.313819000	-0.160891000
6	-2.610075000	-1.437582000	-0.009698000

8	-3.742997000	-1.509916000	-0.030834000
6	-0.725239000	-1.508142000	1.860205000
8	-0.695628000	-1.613235000	2.988805000
6	-1.619189000	1.648846000	0.005490000
6	-2.630566000	1.634624000	0.963202000
6	-1.625705000	2.592937000	-1.019551000
6	-3.638869000	2.586929000	0.903832000
1	-2.614467000	0.902986000	1.763159000
6	-2.646236000	3.534851000	-1.075153000
1	-0.851790000	2.572852000	-1.779671000
6	-3.651144000	3.536089000	-0.114612000
1	-4.418094000	2.586040000	1.658184000
1	-2.655428000	4.264540000	-1.877501000
1	-4.447047000	4.271371000	-0.161513000
6	3.012091000	0.492259000	0.059729000
6	3.467598000	1.371796000	1.034051000
6	3.863245000	-0.035686000	-0.902453000
6	4.811210000	1.725817000	1.041037000
1	2.791159000	1.760854000	1.787599000
6	5.206092000	0.319742000	-0.877641000
1	3.479174000	-0.700797000	-1.668253000
6	5.679509000	1.199950000	0.089802000
1	5.178983000	2.407712000	1.799556000
1	5.878986000	-0.084387000	-1.625650000
1	6.727446000	1.478928000	0.101208000
1	0.936105000	2.131337000	0.041939000

[1'b-H]⁺, TE = - 2386.738023

6	0.268283000	-1.271752000	-0.296066000
6	1.097910000	0.908624000	-0.168747000
7	1.365117000	-0.451593000	-0.301722000
7	-0.901621000	-0.770220000	-0.181679000
25	-0.909495000	1.257986000	0.132313000
6	-0.641640000	0.960799000	1.946386000
8	-0.452964000	0.795420000	3.053578000

6	-0.928148000	3.045612000	0.416565000
8	-1.041212000	4.168375000	0.595086000
6	-2.734470000	1.292303000	0.331713000
8	-3.862145000	1.350349000	0.476808000
6	-0.997558000	1.564196000	-1.697858000
8	-1.026905000	1.778071000	-2.812653000
6	-2.011689000	-1.663245000	-0.145799000
6	-3.024834000	-1.533316000	-1.093176000
6	-2.088862000	-2.650240000	0.834862000
6	-4.105944000	-2.404521000	-1.067135000
1	-2.958473000	-0.765362000	-1.856122000
6	-3.177234000	-3.515961000	0.855202000
1	-1.308483000	-2.727771000	1.584920000
6	-4.185984000	-3.396656000	-0.094007000
1	-4.887722000	-2.307786000	-1.812906000
1	-3.235840000	-4.281466000	1.621624000
1	-5.034853000	-4.071593000	-0.073868000
6	2.642086000	-1.102658000	-0.108281000
6	3.111901000	-1.999301000	-1.060551000
6	3.346348000	-0.868345000	1.067262000
6	4.310717000	-2.664938000	-0.832395000
1	2.553347000	-2.166109000	-1.975734000
6	4.552027000	-1.526968000	1.277236000
1	2.956463000	-0.180891000	1.810232000
6	5.034418000	-2.425253000	0.331024000
1	4.681580000	-3.365710000	-1.572309000
1	5.107840000	-1.344195000	2.190376000
1	5.972722000	-2.941620000	0.502190000
7	2.091641000	1.740014000	-0.392328000
6	3.307332000	1.443291000	-1.157568000
1	4.160723000	1.269764000	-0.498751000
1	3.158225000	0.586769000	-1.807826000
1	3.508719000	2.318045000	-1.778165000
6	2.013707000	3.143239000	0.003338000
1	3.028572000	3.487640000	0.205575000

1	1.592392000	3.753266000	-0.800159000
1	1.436419000	3.251084000	0.915913000
1	0.455384000	-2.338291000	-0.387296000

[1'**c-H**]⁺, TE = - 2367.360210

6	0.399520000	-1.279539000	-0.052414000
6	1.162100000	0.909034000	0.015095000
7	1.470161000	-0.420247000	-0.017562000
7	-0.778936000	-0.786487000	-0.067093000
25	-0.814551000	1.272022000	0.040422000
6	-0.765304000	1.152253000	1.897999000
8	-0.728430000	1.095134000	3.029770000
6	-0.796535000	3.082861000	0.163255000
8	-0.867738000	4.218386000	0.242989000
6	-2.661349000	1.333914000	0.069237000
8	-3.794399000	1.410359000	0.102919000
6	-0.772105000	1.400386000	-1.815180000
8	-0.733653000	1.499419000	-2.944462000
6	-1.882648000	-1.688973000	-0.056087000
6	-2.825308000	-1.628561000	-1.079755000
6	-2.017518000	-2.617058000	0.974082000
6	-3.895535000	-2.513097000	-1.078196000
1	-2.711370000	-0.909626000	-1.883578000
6	-3.095521000	-3.495727000	0.968731000
1	-1.292460000	-2.637423000	1.781085000
6	-4.034483000	-3.446836000	-0.055146000
1	-4.622064000	-2.473059000	-1.882564000
1	-3.200918000	-4.215528000	1.773332000
1	-4.875556000	-4.131661000	-0.055028000
6	2.815926000	-0.946860000	-0.054167000
6	3.400437000	-1.220028000	-1.283633000
6	3.482902000	-1.185016000	1.140037000
6	4.686245000	-1.747495000	-1.313949000
1	2.855789000	-1.022539000	-2.200585000
6	4.768638000	-1.711232000	1.097404000
1	3.000718000	-0.963288000	2.085784000
6	5.368427000	-1.991760000	-0.126360000
1	5.153071000	-1.967736000	-2.267640000
1	5.299967000	-1.904089000	2.022851000
1	6.371587000	-2.403507000	-0.154474000
8	2.242140000	1.614245000	0.016238000
6	2.210880000	3.050871000	0.042022000
1	1.676021000	3.426216000	-0.829097000
1	1.761224000	3.393835000	0.972772000
1	3.253576000	3.354795000	-0.001926000

1 0.619654000 -2.342977000 -0.076379000

[2a-H]⁺, TE = - 1908.615761

6 -2.572871000 -0.958566000 -0.000060000

6 -1.578599000 1.098325000 -0.000192000

1 -1.746439000 2.178812000 -0.000313000

7 -2.723338000 0.423778000 -0.000202000

7 -1.378567000 -1.398394000 0.000069000

6 -4.066770000 1.001996000 -0.000348000

1 -4.609771000 0.684797000 0.891280000

1 -3.972738000 2.085882000 -0.000445000

1 -4.609653000 0.684627000 -0.891986000

6 -1.157952000 -2.830690000 0.000219000

1 -0.573881000 -3.101506000 -0.882245000

1 -0.573960000 -3.101335000 0.882786000

1 -2.097799000 -3.389143000 0.000231000

6 0.129195000 0.119392000 -1.836664000

8 0.211300000 0.190390000 -2.973862000

6 0.129044000 0.119760000 1.836660000

8 0.211048000 0.191044000 2.973848000

6 1.521438000 -1.162699000 0.000182000

7 2.415137000 -1.908039000 0.000234000

6 1.117903000 1.609478000 -0.000102000

7 1.746842000 2.590832000 -0.000104000

6 2.521276000 3.774090000 0.000058000

1 2.296659000 4.359566000 -0.893024000

1 2.287161000 4.365565000 0.886725000

1 3.582375000 3.518952000 0.006583000

6 3.497380000 -2.818653000 0.000233000

1 4.115749000 -2.650478000 -0.882727000

1 4.099402000 -2.669863000 0.897845000

1 3.115045000 -3.840544000 -0.014392000

25 0.044645000 0.069069000 -0.000001000

1 -3.467829000 -1.575372000 -0.000070000

[2b-H]⁺, TE = - 2042.406276

6	-1.333753000	-2.324744000	-0.017973000
6	-1.629805000	-0.019761000	0.065002000
7	-2.215765000	-1.273608000	0.043973000
7	-0.082994000	-2.095433000	-0.051237000
6	0.276241000	0.069611000	-1.778943000
8	0.193287000	0.242938000	-2.907797000
6	0.458424000	-0.142789000	1.874287000
8	0.481074000	-0.109100000	3.018492000
6	2.253513000	-0.532641000	-0.091313000
7	3.391034000	-0.772915000	-0.174799000
6	0.879100000	1.694469000	0.104134000
7	1.270386000	2.794870000	0.125746000
6	1.688673000	4.144253000	0.159299000
1	0.823529000	4.796170000	0.298429000
1	2.387012000	4.293980000	0.984689000
1	2.183791000	4.400804000	-0.779000000
6	4.766896000	-1.082147000	-0.277071000
1	5.186096000	-0.604518000	-1.164208000
1	5.291611000	-0.721256000	0.609067000
1	4.894454000	-2.163287000	-0.355647000
25	0.402789000	-0.118900000	0.039586000
6	0.827913000	-3.219856000	-0.121464000
6	-3.588842000	-1.595737000	0.455019000
7	-2.461637000	1.010542000	-0.045878000
6	-2.045581000	2.358408000	0.309965000
1	-1.274293000	2.325137000	1.072563000
1	-1.684385000	2.906217000	-0.566228000
1	-2.913823000	2.883077000	0.715445000
6	-3.744712000	0.987944000	-0.751181000
1	-3.819081000	0.109961000	-1.387583000
1	-4.596408000	1.031996000	-0.068131000
1	-3.774708000	1.870221000	-1.394789000
1	-3.568015000	-2.529423000	1.016444000
1	-3.957786000	-0.815386000	1.118214000

1	-4.266132000	-1.709995000	-0.391857000
1	1.509300000	-3.189726000	0.732231000
1	0.293463000	-4.174491000	-0.119862000
1	1.429202000	-3.149758000	-1.031221000
1	-1.764021000	-3.324195000	-0.026973000

[2c-H]⁺, TE = - 2023.037777

6	1.904885000	-1.983623000	0.000420000
6	1.747782000	0.317871000	0.000015000
7	2.559626000	-0.774901000	0.000328000
7	0.632510000	-1.977841000	0.000355000
6	-0.212650000	-0.029059000	1.836387000
8	-0.240499000	0.062737000	2.975526000
6	-0.212719000	-0.029175000	-1.835884000
8	-0.240732000	0.062483000	-2.975031000
6	-1.957939000	-0.831170000	0.000039000
7	-3.038766000	-1.262795000	-0.000138000
6	-0.932499000	1.622908000	0.000262000
7	-1.474376000	2.656048000	0.000368000
6	-2.087343000	3.929861000	0.000285000
1	-1.320895000	4.707469000	-0.012542000
1	-2.720009000	4.033346000	-0.882843000
1	-2.699989000	4.043044000	0.896244000
6	-4.346911000	-1.800462000	-0.001645000
1	-4.804487000	-1.651608000	0.977520000
1	-4.947315000	-1.299104000	-0.762254000
1	-4.302107000	-2.868313000	-0.221860000
25	-0.190324000	-0.104671000	0.000228000
6	-0.070649000	-3.244819000	0.000369000
6	4.019035000	-0.705873000	0.000228000
8	2.493030000	1.391986000	-0.000488000
6	1.899884000	2.694121000	-0.001210000
1	1.296511000	2.831409000	-0.897785000
1	1.297161000	2.832714000	0.895596000
1	2.737073000	3.388930000	-0.002020000

1	4.413956000	-1.720187000	0.000788000
1	4.369493000	-0.181306000	-0.888948000
1	4.369541000	-0.180321000	0.888798000
1	-0.711105000	-3.305009000	-0.882688000
1	0.621841000	-4.091262000	0.000112000
1	-0.710753000	-3.305254000	0.883636000
1	2.516568000	-2.882487000	0.000511000

[2'a-H]⁺, TE = - 2291.620781

6	0.992633000	-1.308750000	-0.110253000
6	1.298837000	0.960725000	0.016793000
1	2.044655000	1.757817000	0.072696000
7	1.880907000	-0.246284000	-0.048787000
7	-0.251391000	-1.011302000	-0.105596000
6	-0.640563000	0.962922000	1.874487000
8	-0.664396000	0.977769000	3.014886000
6	-0.669715000	1.266858000	-1.794105000
8	-0.706695000	1.476772000	-2.915247000
6	-2.527724000	0.856984000	0.052676000
7	-3.686169000	0.763923000	0.075772000
6	-0.608666000	2.891395000	0.184531000
7	-0.565977000	4.051023000	0.282285000
6	-0.527316000	5.459618000	0.404420000
1	-0.017718000	5.732406000	1.329854000
1	0.011110000	5.885848000	-0.443460000
1	-1.544612000	5.853940000	0.422104000
6	-5.092068000	0.612603000	0.092431000
1	-5.450147000	0.654600000	1.121976000
1	-5.552564000	1.415128000	-0.485482000
1	-5.357404000	-0.351084000	-0.345864000
25	-0.604703000	1.019547000	0.031330000
6	-1.186337000	-2.082963000	-0.120402000
6	-2.169487000	-2.124884000	-1.107278000
6	-1.127896000	-3.077015000	0.855158000
6	-3.076965000	-3.175617000	-1.127296000
1	-2.208230000	-1.347923000	-1.862225000
6	-2.047385000	-4.120029000	0.832759000
1	-0.379081000	-3.019875000	1.638477000
6	-3.021020000	-4.173989000	-0.157916000
1	-3.831833000	-3.213904000	-1.905579000
1	-2.002040000	-4.888548000	1.597107000
1	-3.737927000	-4.987893000	-0.173402000
6	3.297918000	-0.481962000	-0.065094000
6	3.853749000	-1.392032000	0.827241000

6	4.089926000	0.214804000	-0.970235000
6	5.226968000	-1.605717000	0.807433000
1	3.226311000	-1.914582000	1.541474000
6	5.462932000	0.001689000	-0.972347000
1	3.634979000	0.904775000	-1.672625000
6	6.031968000	-0.908830000	-0.087700000
1	5.667338000	-2.311817000	1.502822000
1	6.086128000	0.541121000	-1.677105000
1	7.103487000	-1.076428000	-0.096677000
1	1.393514000	-2.314974000	-0.181979000

[2'b-H]⁺, TE = - 2425.415121

6	-0.801246000	-1.431254000	-0.142338000
6	-1.193758000	0.873988000	-0.118170000
7	-1.721925000	-0.416726000	-0.209234000
7	0.439766000	-1.155203000	-0.013741000
6	0.851711000	0.949091000	-1.802569000
8	0.859901000	1.066001000	-2.940736000
6	0.754753000	0.958072000	1.863695000
8	0.691380000	1.079233000	3.000082000
6	2.710671000	0.538546000	0.046366000
7	3.861742000	0.360226000	0.040394000
6	1.228487000	2.694329000	0.009740000
7	1.573946000	3.809079000	-0.018247000
6	1.942260000	5.173241000	-0.047226000
1	1.048353000	5.798289000	0.005489000
1	2.588887000	5.398415000	0.802711000
1	2.478339000	5.390456000	-0.972763000
6	5.246275000	0.075761000	0.048708000
1	5.650434000	0.185687000	-0.958875000
1	5.759609000	0.765285000	0.720801000
1	5.403691000	-0.948837000	0.391769000
25	0.835498000	0.860640000	0.030483000
6	1.352418000	-2.243970000	-0.000601000
6	2.214396000	-2.410482000	1.082617000
6	1.395016000	-3.138982000	-1.068492000
6	3.100049000	-3.479902000	1.100953000

1	2.177780000	-1.709632000	1.909186000
6	2.288474000	-4.205321000	-1.044720000
1	0.740929000	-2.987949000	-1.921321000
6	3.141759000	-4.379813000	0.038412000
1	3.760064000	-3.611970000	1.952057000
1	2.317845000	-4.896641000	-1.880501000
1	3.839574000	-5.210226000	0.055065000
6	-3.091651000	-0.815560000	0.018036000
6	-3.739347000	-1.613815000	-0.918091000
6	-3.720946000	-0.453498000	1.204078000
6	-5.036901000	-2.044228000	-0.667037000
1	-3.236266000	-1.884894000	-1.840606000
6	-5.024137000	-0.876050000	1.439501000
1	-3.195968000	0.153393000	1.934006000
6	-5.683044000	-1.671082000	0.507109000
1	-5.544805000	-2.665979000	-1.396314000
1	-5.519936000	-0.590785000	2.361063000
1	-6.698138000	-2.002689000	0.697217000
7	-2.047303000	1.868240000	-0.303702000
6	-1.712646000	3.229042000	0.092917000
1	-0.971830000	3.219970000	0.885196000
1	-1.346827000	3.808367000	-0.759890000
1	-2.622889000	3.700249000	0.470792000
6	-3.318448000	1.801676000	-1.027898000
1	-3.346281000	0.939678000	-1.688402000
1	-4.172963000	1.774500000	-0.347577000
1	-3.383754000	2.704370000	-1.639088000
1	-1.192008000	-2.444976000	-0.175099000

[2'c**-H]⁺, TE = - 2406.042443**

6	-0.890241000	-1.443959000	0.068191000
6	-1.262897000	0.846467000	0.035037000
7	-1.800242000	-0.418907000	0.044608000
7	0.353290000	-1.148120000	0.093914000
6	0.687601000	0.874501000	-1.829067000

8	0.677998000	0.918292000	-2.970351000
6	0.751125000	1.073561000	1.841682000
8	0.777499000	1.244434000	2.971172000
6	2.605263000	0.614315000	-0.026538000
7	3.758175000	0.466454000	-0.063346000
6	1.015471000	2.738766000	-0.098668000
7	1.297263000	3.867762000	-0.171463000
6	1.597275000	5.246660000	-0.258238000
1	0.670870000	5.822596000	-0.304263000
1	2.169456000	5.553220000	0.618902000
1	2.185847000	5.438060000	-1.156968000
6	5.151425000	0.227406000	-0.092997000
1	5.527116000	0.379040000	-1.105892000
1	5.655381000	0.914979000	0.587776000
1	5.347370000	-0.800787000	0.217127000
25	0.710473000	0.887435000	0.011647000
6	1.285744000	-2.220482000	0.059278000
6	2.236465000	-2.342920000	1.071366000
6	1.257917000	-3.139329000	-0.988471000
6	3.142287000	-3.395210000	1.040551000
1	2.252750000	-1.624070000	1.883032000
6	2.172273000	-4.187270000	-1.014461000
1	0.533525000	-3.020995000	-1.787928000
6	3.114872000	-4.319025000	-0.001483000
1	3.872341000	-3.494579000	1.837064000
1	2.147715000	-4.897780000	-1.834037000
1	3.828719000	-5.135519000	-0.023822000
6	-3.212507000	-0.710938000	0.046543000
6	-3.882510000	-0.830567000	-1.164403000
6	-3.872176000	-0.882752000	1.256681000
6	-5.240455000	-1.128029000	-1.160369000
1	-3.344380000	-0.692036000	-2.095970000
6	-5.230236000	-1.180944000	1.250986000
1	-3.326827000	-0.783087000	2.189032000
6	-5.913217000	-1.303039000	0.045009000

1	-5.771420000	-1.225292000	-2.101100000
1	-5.753383000	-1.318821000	2.191012000
1	-6.972648000	-1.536446000	0.044379000
8	-2.235272000	1.712128000	0.041370000
6	-1.969625000	3.119445000	0.036945000
1	-1.376706000	3.391753000	0.909092000
1	-1.459492000	3.398958000	-0.883980000
1	-2.948109000	3.592447000	0.083624000
1	-1.284287000	-2.456617000	0.072777000

[3a-H]⁺, TE = - 1947.284258

6	2.573542000	0.230124000	-0.992128000
6	1.590929000	0.144777000	1.069670000
1	1.788865000	0.163681000	2.147431000
7	2.740990000	0.246568000	0.378536000
7	1.372767000	0.122125000	-1.413300000
6	4.081135000	0.364321000	0.944680000
1	4.545371000	1.302826000	0.634926000
1	3.997123000	0.348815000	2.029895000
1	4.705899000	-0.471317000	0.622418000
6	1.135585000	0.097034000	-2.840262000
1	0.623289000	-0.832046000	-3.103366000
1	0.474277000	0.924448000	-3.110332000
1	2.062896000	0.173054000	-3.416927000
25	-0.018504000	-0.000077000	0.080517000
6	-1.517191000	-0.132704000	-1.108742000
7	-2.430251000	-0.212928000	-1.834833000
6	-1.021346000	-0.091451000	1.638010000
7	-1.602514000	-0.145474000	2.655734000
6	-0.274688000	1.879386000	0.061402000
7	-0.444775000	3.035719000	0.054368000
6	0.061649000	-1.895345000	0.057090000
7	0.099569000	-3.063427000	0.044955000
6	0.142678000	-4.475858000	0.042440000
1	1.050621000	-4.820712000	0.541078000

1	-0.727082000	-4.873435000	0.569114000
1	0.136874000	-4.845094000	-0.984885000
6	-3.535440000	-0.310776000	-2.709987000
1	-4.455495000	-0.432430000	-2.134695000
1	-3.609662000	0.594771000	-3.315200000
1	-3.410218000	-1.171509000	-3.369751000
6	-2.327793000	-0.214307000	3.865698000
1	-2.013751000	-1.087736000	4.441422000
1	-2.149098000	0.683696000	4.461174000
1	-3.397360000	-0.293768000	3.658153000
6	-0.655542000	4.432997000	0.061867000
1	-1.588198000	4.663529000	0.580523000
1	0.170310000	4.930587000	0.574025000
1	-0.716303000	4.804492000	-0.962865000
1	3.454837000	0.308109000	-1.624888000

[3b-H]⁺, TE = - 2081.068898

6	1.283837000	-1.329820000	-1.956981000
6	1.619102000	-0.261354000	0.082732000
7	2.181452000	-0.938372000	-0.993961000
7	0.052117000	-1.042776000	-1.814447000
25	-0.382076000	-0.048867000	-0.083120000
6	-2.190648000	0.115252000	-0.567869000
7	-3.321366000	0.230247000	-0.858545000
6	-0.774984000	0.859234000	1.481987000
7	-1.123624000	1.450045000	2.438152000
6	-0.006967000	1.609840000	-0.903998000
7	0.225822000	2.648346000	-1.394424000
6	-0.729801000	-1.692477000	0.789233000
7	-0.943303000	-2.705530000	1.337937000
6	-1.194319000	-3.919414000	2.015319000
1	-0.952183000	-3.812402000	3.074913000
1	-2.247344000	-4.191970000	1.917619000
1	-0.580802000	-4.716781000	1.590721000
6	-4.678370000	0.354857000	-1.228886000

1	-5.296497000	-0.303634000	-0.614619000
1	-5.012381000	1.385388000	-1.089461000
1	-4.805764000	0.081067000	-2.278783000
6	-1.418228000	2.141896000	3.632301000
1	-0.513268000	2.258726000	4.235018000
1	-1.819744000	3.132527000	3.406038000
1	-2.159402000	1.589779000	4.215116000
6	0.497275000	3.909441000	-1.970220000
1	-0.364250000	4.250247000	-2.548431000
1	0.709063000	4.639213000	-1.185758000
1	1.363385000	3.839357000	-2.631656000
6	-0.875648000	-1.460977000	-2.842399000
6	3.490617000	-1.599281000	-1.010511000
7	2.509721000	0.255831000	0.937609000
6	2.111727000	0.655980000	2.275298000
1	2.944206000	0.453413000	2.954965000
1	1.876964000	1.725233000	2.322302000
1	1.249950000	0.077672000	2.593177000
6	3.838230000	0.745892000	0.575346000
1	4.641551000	0.114677000	0.965914000
1	3.933214000	0.838674000	-0.504069000
1	3.950519000	1.744691000	1.006236000
1	-0.378227000	-2.017138000	-3.644254000
1	-1.650706000	-2.091279000	-2.398332000
1	-1.369919000	-0.585115000	-3.271156000
1	3.804546000	-1.799312000	0.013044000
1	3.390224000	-2.556109000	-1.523494000
1	4.257853000	-1.010825000	-1.516368000
1	1.684247000	-1.883371000	-2.805022000

[3c-H]⁺, TE = -2061.704141

6	1.907654000	0.009729000	-1.996992000
6	1.750760000	-0.001094000	0.306151000
7	2.568214000	0.003877000	-0.793991000
7	0.634047000	0.010006000	-1.977357000

25	-0.170302000	0.000993000	-0.090652000
6	-1.935236000	0.003536000	-0.781429000
7	-3.029999000	0.004590000	-1.195616000
6	-0.868977000	-0.007340000	1.628882000
7	-1.398816000	-0.012763000	2.677509000
6	-0.198871000	1.894591000	-0.058365000
7	-0.224174000	3.064046000	-0.026743000
6	-0.198142000	-1.892767000	-0.076235000
7	-0.223047000	-3.062480000	-0.055626000
6	-0.253722000	-4.474323000	-0.009284000
1	0.259354000	-4.828581000	0.887187000
1	-1.287951000	-4.823822000	0.009959000
1	0.244241000	-4.885376000	-0.889680000
6	-4.343960000	0.004188000	-1.714763000
1	-4.964340000	-0.700698000	-1.157545000
1	-4.777410000	1.002879000	-1.631547000
1	-4.327873000	-0.290293000	-2.766299000
6	-1.939911000	-0.018581000	3.981331000
1	-2.555306000	-0.908947000	4.128971000
1	-1.136434000	-0.018176000	4.722642000
1	-2.561238000	0.866739000	4.134407000
6	-0.256038000	4.475547000	0.028059000
1	-0.317496000	4.805154000	1.067250000
1	0.650343000	4.885570000	-0.421852000
1	-1.125105000	4.850356000	-0.516407000
6	-0.077102000	0.016483000	-3.236994000
6	4.025767000	0.002634000	-0.735729000
8	2.526862000	-0.006621000	1.374112000
6	1.944081000	-0.013691000	2.675494000
1	1.337203000	-0.908334000	2.814596000
1	2.783662000	-0.017573000	3.368947000
1	1.337317000	0.879431000	2.824503000
1	4.414912000	0.008050000	-1.752895000
1	4.385955000	0.887227000	-0.208832000
1	4.384835000	-0.888223000	-0.218686000

1	-0.719940000	0.899156000	-3.288109000
1	0.604534000	0.020036000	-4.093860000
1	-0.721301000	-0.864706000	-3.296424000
1	2.513298000	0.013876000	-2.900901000

[3'a-H]⁺, TE = - 2330.292849

6	-1.078780000	-1.366732000	-0.192360000
6	-1.324195000	0.904024000	0.052652000
1	-2.069614000	1.699916000	0.150197000
7	-1.943332000	-0.302899000	-0.080242000
7	0.174288000	-1.087652000	-0.160193000
25	0.546968000	0.933743000	0.091657000
6	2.468844000	0.765655000	0.145901000
7	3.631046000	0.668272000	0.190502000
6	0.536392000	2.773863000	0.327295000
7	0.469468000	3.934435000	0.472634000
6	0.599538000	0.724579000	1.982031000
7	0.640422000	0.609714000	3.142613000
6	0.710323000	1.218484000	-1.782411000
7	0.816230000	1.411993000	-2.928680000
6	0.928914000	1.651158000	-4.317195000
1	-0.063662000	1.788730000	-4.750149000
1	1.523435000	2.550218000	-4.489558000
1	1.416061000	0.801742000	-4.799596000
6	5.034290000	0.506142000	0.231765000
1	5.515729000	1.302108000	-0.339165000
1	5.379354000	0.547979000	1.266324000
1	5.305093000	-0.460298000	-0.198485000
6	0.416445000	5.335314000	0.647923000
1	-0.112985000	5.796347000	-0.188510000
1	-0.108077000	5.575688000	1.575038000
1	1.428055000	5.744111000	0.696269000
6	0.687365000	0.481405000	4.549476000
1	1.155139000	1.366529000	4.984561000
1	-0.324772000	0.379434000	4.945202000

1	1.269566000	-0.401220000	4.820393000
6	1.088609000	-2.168187000	-0.242819000
6	2.101561000	-2.137934000	-1.201697000
6	0.996160000	-3.250176000	0.633655000
6	2.998925000	-3.193367000	-1.294187000
1	2.168354000	-1.292353000	-1.876585000
6	1.904188000	-4.300020000	0.539832000
1	0.225998000	-3.257284000	1.398439000
6	2.905902000	-4.277096000	-0.423890000
1	3.775954000	-3.169264000	-2.051371000
1	1.828559000	-5.134864000	1.228949000
1	3.614256000	-5.095735000	-0.494448000
6	-3.359015000	-0.503706000	-0.117417000
6	-3.943700000	-1.493680000	0.667559000
6	-4.141472000	0.306288000	-0.935357000
6	-5.321377000	-1.675060000	0.624632000
1	-3.331644000	-2.105816000	1.321596000
6	-5.518987000	0.126991000	-0.959238000
1	-3.672433000	1.060697000	-1.557773000
6	-6.111616000	-0.864959000	-0.184019000
1	-5.777291000	-2.445001000	1.237782000
1	-6.128460000	0.757542000	-1.597690000
1	-7.186731000	-1.006130000	-0.210095000
1	-1.490808000	-2.361613000	-0.331977000

[3'b-H]⁺, TE = - 2464.079720

6	-0.871130000	1.491127000	-0.142319000
6	-1.213612000	-0.824621000	-0.104837000
7	-1.772953000	0.460933000	-0.211150000
7	0.374435000	1.230399000	-0.012709000
25	0.794182000	-0.789935000	0.037025000
6	2.650710000	-0.480322000	-0.000811000
7	3.810522000	-0.316347000	-0.041798000
6	1.170446000	-2.602480000	0.028694000
7	1.515991000	-3.726043000	0.008167000
6	0.789157000	-0.841127000	-1.853865000
7	0.790369000	-0.899936000	-3.023275000
6	0.788679000	-0.813112000	1.932473000

7	0.786770000	-0.851737000	3.103065000
6	0.766493000	-0.909228000	4.514425000
1	1.288662000	-1.804807000	4.857556000
1	1.260998000	-0.029020000	4.930673000
1	-0.264944000	-0.940054000	4.872033000
6	5.191274000	-0.021999000	-0.065622000
1	5.730275000	-0.698874000	0.600662000
1	5.581801000	-0.137503000	-1.078938000
1	5.355700000	1.007001000	0.263703000
6	1.827209000	-5.102590000	-0.003454000
1	0.912432000	-5.697217000	0.067665000
1	2.345517000	-5.363921000	-0.928973000
1	2.473934000	-5.349516000	0.841747000
6	0.807100000	-0.987893000	-4.433359000
1	1.836090000	-0.952817000	-4.797203000
1	0.348071000	-1.925762000	-4.753101000
1	0.248802000	-0.154556000	-4.864734000
6	1.267678000	2.329595000	0.002897000
6	2.186733000	2.457919000	1.045456000
6	1.248103000	3.278547000	-1.020187000
6	3.059378000	3.537692000	1.071188000
1	2.201794000	1.711567000	1.831699000
6	2.128971000	4.355393000	-0.990317000
1	0.555456000	3.159911000	-1.847512000
6	3.035678000	4.490335000	0.054477000
1	3.762694000	3.636554000	1.891906000
1	2.108004000	5.085675000	-1.792838000
1	3.724171000	5.328521000	0.075780000
6	-3.147237000	0.830733000	0.015619000
6	-3.801898000	1.649761000	-0.898844000
6	-3.787483000	0.419719000	1.180839000
6	-5.108617000	2.052635000	-0.647887000
1	-3.294969000	1.958880000	-1.807323000
6	-5.099324000	0.813931000	1.416594000
1	-3.261405000	-0.205009000	1.894672000
6	-5.761837000	1.630856000	0.505517000
1	-5.618336000	2.690613000	-1.361988000
1	-5.600132000	0.489495000	2.322572000
1	-6.783975000	1.940269000	0.695723000
7	-2.074199000	-1.822931000	-0.301851000
6	-1.753527000	-3.173921000	0.126812000
1	-2.668657000	-3.633543000	0.510577000
1	-1.384051000	-3.779611000	-0.707178000
1	-1.012865000	-3.147038000	0.919552000
6	-3.305463000	-1.769616000	-1.087716000
1	-4.197788000	-1.766256000	-0.455595000

1	-3.317019000	-0.898033000	-1.736964000
1	-3.326999000	-2.663552000	-1.716561000
1	-1.279222000	2.498615000	-0.171003000

[3'**c-H**]⁺, TE = - 2444.710898

6	-0.975390000	-1.485069000	-0.074876000
6	-1.275253000	0.818559000	-0.038529000
7	-1.858508000	-0.440985000	-0.037931000
7	0.275363000	-1.213734000	-0.111593000
25	0.670307000	0.819017000	0.013031000
6	2.548533000	0.528144000	0.065959000
7	3.705980000	0.369961000	0.111013000
6	0.986481000	2.640306000	0.182917000
7	1.284289000	3.769522000	0.300371000
6	0.641104000	0.697142000	1.906809000
7	0.628708000	0.636968000	3.074128000
6	0.764363000	1.005119000	-1.871876000
7	0.827557000	1.141112000	-3.031725000
6	0.893968000	1.315469000	-4.432426000
1	1.504207000	2.189541000	-4.668282000
1	1.341133000	0.433514000	-4.895316000
1	-0.109665000	1.460924000	-4.837011000
6	5.092179000	0.100347000	0.146788000
1	5.621838000	0.783572000	-0.519892000
1	5.469817000	0.228973000	1.162957000
1	5.274162000	-0.927613000	-0.175121000
6	1.552091000	5.148905000	0.438276000
1	2.193958000	5.489546000	-0.377134000
1	0.618574000	5.717003000	0.414743000
1	2.057709000	5.339318000	1.387517000
6	0.617192000	0.574562000	4.485939000
1	1.126851000	1.447435000	4.898584000
1	-0.412263000	0.557198000	4.848938000
1	1.129807000	-0.329225000	4.821100000
6	1.182154000	-2.302409000	-0.092446000
6	2.157842000	-2.403463000	-1.084923000
6	1.119436000	-3.263363000	0.916982000
6	3.046513000	-3.470527000	-1.075502000
1	2.204069000	-1.648641000	-1.862058000
6	2.016862000	-4.326614000	0.922955000
1	0.380065000	-3.164888000	1.705555000
6	2.980976000	-4.435351000	-0.072446000
1	3.794638000	-3.549701000	-1.857737000
1	1.962952000	-5.067436000	1.714109000
1	3.681730000	-5.263525000	-0.065855000
6	-3.271059000	-0.705765000	-0.070995000

6	-4.041792000	-0.478557000	1.064079000
6	-3.844392000	-1.209868000	-1.232439000
6	-5.402614000	-0.756322000	1.030700000
1	-3.575495000	-0.091135000	1.963242000
6	-5.206026000	-1.494412000	-1.255294000
1	-3.228648000	-1.375279000	-2.110426000
6	-5.985460000	-1.265388000	-0.126740000
1	-6.007636000	-0.581311000	1.913922000
1	-5.656123000	-1.891473000	-2.158851000
1	-7.047665000	-1.485056000	-0.147268000
8	-2.247436000	1.702082000	-0.091933000
6	-1.944734000	3.096139000	-0.129238000
1	-1.284352000	3.317934000	-0.967226000
1	-2.903370000	3.595443000	-0.260028000
1	-1.484258000	3.406611000	0.808562000
1	-1.391790000	-2.489203000	-0.079220000

[4'a-H]⁺, TE = - 2443.624063

6	1.079945000	-1.213034000	-0.271893000
6	1.312254000	1.162355000	-0.209742000
1	1.543061000	1.656113000	-1.160305000
7	-0.202500000	-1.023986000	-0.197303000
1	1.801215000	1.740433000	0.581568000
6	-0.842739000	2.744542000	0.289494000
6	-0.320123000	0.704393000	1.892976000
6	-0.917194000	1.112701000	-1.787322000
7	-0.897943000	3.899304000	0.422891000
7	-1.020109000	1.236387000	-2.938660000
7	-0.061521000	0.566164000	3.017536000
6	0.249005000	0.396915000	4.387640000
1	1.058453000	-0.327102000	4.491192000
1	0.562245000	1.352503000	4.810615000
1	-0.631688000	0.035404000	4.920422000
6	-0.967019000	5.302600000	0.587067000
1	-0.505535000	5.583124000	1.535140000
1	-0.437831000	5.793713000	-0.231023000
1	-2.010592000	5.621274000	0.585102000
6	-1.145354000	1.377920000	-4.340978000
1	-0.155071000	1.468628000	-4.789517000
1	-1.650857000	0.502659000	-4.751800000
1	-1.729002000	2.271681000	-4.566198000
6	-1.041186000	-2.158902000	-0.221339000
6	-2.162674000	-2.179273000	-1.054866000
6	-0.779900000	-3.266724000	0.591539000
6	-2.992601000	-3.292313000	-1.086525000
1	-2.370074000	-1.322047000	-1.685263000

6	-1.612460000	-4.379953000	0.552206000
1	0.066306000	-3.245731000	1.271244000
6	-2.721681000	-4.399554000	-0.286259000
1	-3.854789000	-3.296343000	-1.745939000
1	-1.396843000	-5.230236000	1.191434000
1	-3.373979000	-5.266048000	-0.311544000
26	-0.691469000	0.922086000	0.066182000
6	-2.529550000	0.641551000	0.357016000
7	-3.666510000	0.500179000	0.559469000
6	-5.045583000	0.285073000	0.786921000
1	-5.625520000	1.060060000	0.283489000
1	-5.329485000	-0.692873000	0.393847000
1	-5.250309000	0.318151000	1.858049000
7	1.923055000	-0.178469000	-0.221922000
6	3.323026000	-0.364761000	-0.229543000
6	4.152157000	0.644769000	-0.726197000
6	3.906214000	-1.530151000	0.282921000
6	5.531653000	0.476343000	-0.736790000
1	3.717184000	1.559231000	-1.110432000
6	5.285011000	-1.692379000	0.255966000
1	3.292062000	-2.303816000	0.729802000
6	6.108258000	-0.693468000	-0.254800000
1	6.158137000	1.270242000	-1.130628000
1	5.717769000	-2.602631000	0.658386000
1	7.185271000	-0.821040000	-0.264587000
1	1.498072000	-2.207159000	-0.409564000

[4'b-H]⁺, TE = -5591.117290

6	-1.301345000	1.203741000	-0.255021000
6	-1.346649000	-1.202918000	-0.229731000
1	-1.549894000	-1.692875000	-1.187879000
7	-0.003219000	1.153634000	-0.179876000
1	-1.800467000	-1.821463000	0.551142000
6	1.111992000	-2.716963000	0.257070000
6	0.353744000	-0.683783000	1.995826000
6	0.974248000	-0.985988000	-1.910138000
7	1.299849000	-3.861311000	0.373402000
7	1.077742000	-1.085577000	-3.063721000
7	0.097046000	-0.598955000	3.126077000
6	-0.207845000	-0.498694000	4.504028000
1	-1.146519000	0.042518000	4.630804000
1	-0.306129000	-1.499147000	4.927864000
1	0.592584000	0.036345000	5.017067000
6	1.528214000	-5.249359000	0.516447000
1	0.761627000	-5.683631000	1.160490000
1	1.490073000	-5.730379000	-0.462423000

1	2.510326000	-5.417208000	0.961872000
6	1.213066000	-1.206290000	-4.466870000
1	0.770037000	-2.147450000	-4.795726000
1	0.701462000	-0.375099000	-4.954239000
1	2.270624000	-1.188899000	-4.734362000
6	0.710558000	2.372905000	-0.198834000
6	1.837926000	2.500320000	-1.013478000
6	0.321663000	3.453459000	0.598934000
6	2.548837000	3.692788000	-1.044327000
1	2.142604000	1.661859000	-1.629425000
6	1.035578000	4.646429000	0.559988000
1	-0.528290000	3.351123000	1.266357000
6	2.150902000	4.773200000	-0.260848000
1	3.417625000	3.779620000	-1.689094000
1	0.723078000	5.475301000	1.187114000
1	2.710473000	5.702256000	-0.284603000
6	2.658085000	-0.357810000	0.340934000
7	3.775712000	-0.088015000	0.526567000
6	5.128758000	0.262149000	0.742112000
1	5.778130000	-0.508232000	0.323185000
1	5.340696000	1.216634000	0.256963000
1	5.318314000	0.351305000	1.812957000
7	-2.046790000	0.097514000	-0.220629000
6	-3.459714000	0.175761000	-0.223678000
6	-4.210428000	-0.855877000	-0.792183000
6	-4.125174000	1.257538000	0.364083000
6	-5.598444000	-0.787865000	-0.798364000
1	-3.709983000	-1.707542000	-1.236193000
6	-5.512200000	1.321441000	0.340549000
1	-3.565741000	2.039914000	0.864888000
6	-6.258792000	0.301783000	-0.241291000
1	-6.165626000	-1.595849000	-1.249085000
1	-6.010693000	2.168335000	0.800819000
1	-7.342234000	0.350772000	-0.249029000
44	0.743045000	-0.835863000	0.055638000
1	-1.816333000	2.152938000	-0.381529000

[5a-H]⁺, TE = -2482.816831

6	0.293388000	1.369628000	-0.870968000
6	-1.729950000	0.001777000	-0.544166000
6	0.294313000	-1.363383000	-0.875871000
7	-1.145626000	-1.177534000	-0.626171000
7	-1.147037000	1.182138000	-0.623850000
6	-1.976783000	-2.331299000	-0.482257000
6	-1.833935000	-3.392700000	-1.375309000
6	-2.909450000	-2.410586000	0.550297000

6	-2.635104000	-4.518783000	-1.241362000
1	-1.104784000	-3.328135000	-2.174821000
6	-3.714304000	-3.538434000	0.670978000
1	-2.992485000	-1.604027000	1.271090000
6	-3.580259000	-4.595540000	-0.221795000
1	-2.524504000	-5.338190000	-1.943922000
1	-4.435886000	-3.594077000	1.479261000
1	-4.203273000	-5.477706000	-0.120504000
6	-1.979855000	2.334816000	-0.480913000
6	-1.827080000	3.402440000	-1.364944000
6	-2.924407000	2.407701000	0.541481000
6	-2.629146000	4.528063000	-1.232109000
1	-1.089366000	3.343369000	-2.156938000
6	-3.729921000	3.535118000	0.660969000
1	-3.017343000	1.596295000	1.255535000
6	-3.585417000	4.598565000	-0.222627000
1	-2.510127000	5.352163000	-1.927775000
1	-4.460499000	3.585311000	1.461496000
1	-4.208951000	5.480427000	-0.121968000
1	0.436048000	-1.331464000	-1.961797000
1	0.506083000	-2.384829000	-0.555031000
1	0.504335000	2.389552000	-0.544804000
1	0.436387000	1.343252000	-1.956882000
26	1.532270000	0.001831000	0.023877000
6	0.487301000	0.001194000	1.559413000
7	-0.136751000	0.002210000	2.544727000
6	2.564837000	1.375096000	0.720144000
7	3.195917000	2.261001000	1.144372000
6	2.535490000	0.004441000	-1.540667000
7	3.142480000	0.006374000	-2.535837000
6	2.563713000	-1.374342000	0.715956000
7	3.193394000	-2.262749000	1.137030000
6	3.967005000	3.327469000	1.661516000
1	4.422598000	3.029794000	2.607738000
1	4.753982000	3.591065000	0.952642000
1	3.329797000	4.197730000	1.828703000
6	-0.867168000	0.004429000	3.755557000
1	-0.176881000	0.034172000	4.600562000
1	-1.517672000	0.880027000	3.793480000
1	-1.475931000	-0.899040000	3.822014000
6	3.962176000	-3.332988000	1.649825000
1	4.748694000	-3.595268000	0.939954000
1	4.418254000	-3.040265000	2.597349000
1	3.323094000	-4.202593000	1.813253000
6	3.888756000	0.008845000	-3.737313000
1	4.470725000	-0.911408000	-3.811285000

1	3.211973000	0.075565000	-4.590699000
1	4.566169000	0.864447000	-3.748109000
1	-2.807025000	0.000687000	-0.426246000

[5b-H]⁺, TE = - 5630.312530

6	0.132102000	1.412413000	-0.926055000
6	-1.872007000	0.003628000	-0.574643000
6	0.133655000	-1.401423000	-0.931459000
7	-1.298721000	-1.181759000	-0.662769000
7	-1.300569000	1.190245000	-0.660114000
6	-2.145966000	-2.322829000	-0.498685000
6	-2.052488000	-3.380802000	-1.401727000
6	-3.043056000	-2.390377000	0.565190000
6	-2.868930000	-4.493008000	-1.245420000
1	-1.349996000	-3.324587000	-2.225418000
6	-3.863659000	-3.504146000	0.708322000
1	-3.085435000	-1.585806000	1.291752000
6	-3.779506000	-4.558149000	-0.193997000
1	-2.797892000	-5.310399000	-1.955339000
1	-4.557802000	-3.551538000	1.540738000
1	-4.414568000	-5.429523000	-0.075771000
6	-2.150002000	2.329885000	-0.497128000
6	-2.048591000	3.393048000	-1.393244000
6	-3.057311000	2.391583000	0.558575000
6	-2.866480000	4.504414000	-1.238245000
1	-1.338636000	3.341772000	-2.210791000
6	-3.879191000	3.504537000	0.700320000
1	-3.107499000	1.582981000	1.280097000
6	-3.786669000	4.563832000	-0.194976000
1	-2.788701000	5.325763000	-1.942868000
1	-4.581063000	3.547031000	1.526502000
1	-4.422717000	5.434588000	-0.077556000
1	0.266761000	-1.362047000	-2.017984000
1	0.326014000	-2.429688000	-0.622397000
1	0.323110000	2.439297000	-0.611600000
1	0.266506000	1.378732000	-2.012611000
6	0.357131000	0.002462000	1.652102000
7	-0.272577000	0.002508000	2.633248000
6	2.566619000	1.465780000	0.757685000
7	3.190928000	2.359819000	1.176977000
6	2.516624000	0.007658000	-1.652486000
7	3.114087000	0.009855000	-2.652756000
6	2.566888000	-1.459770000	0.752005000
7	3.191084000	-2.355852000	1.167085000
6	3.958905000	3.429563000	1.691455000
1	4.443325000	3.124514000	2.620993000

1	4.723343000	3.716229000	0.966948000
1	3.313589000	4.287611000	1.888482000
6	-1.006861000	0.003517000	3.841612000
1	-0.318679000	0.021107000	4.688635000
1	-1.649103000	0.885063000	3.882058000
1	-1.624127000	-0.894784000	3.898791000
6	3.958435000	-3.428795000	1.675856000
1	4.718551000	-3.716262000	0.947131000
1	4.448169000	-3.126948000	2.603650000
1	3.311537000	-4.285328000	1.874302000
6	3.857058000	0.012331000	-3.856206000
1	4.490856000	-0.875046000	-3.898066000
1	3.175461000	0.008922000	-4.708259000
1	4.483205000	0.905078000	-3.899097000
44	1.465948000	0.004332000	0.019597000
1	-2.947265000	0.002357000	-0.440695000

[6a-H]⁺, TE = - 2630.837073

6	0.227903000	1.413161000	0.461605000
7	-1.236687000	1.188140000	0.150857000
6	-1.797612000	0.000467000	0.034619000
7	-1.237424000	-1.187534000	0.151209000
6	0.227064000	-1.413410000	0.461781000
8	0.433744000	2.520230000	0.895684000
6	-2.112965000	2.327640000	0.096402000
6	-1.988801000	3.228989000	-0.955165000
6	-2.837952000	4.326403000	-1.014052000
6	-3.803191000	4.520050000	-0.029096000
6	-3.916738000	3.615546000	1.020361000
6	-3.064856000	2.517718000	1.090586000
1	-1.239177000	3.064618000	-1.721640000
1	-2.749274000	5.029275000	-1.835493000
1	-4.465971000	5.377279000	-0.080834000
1	-4.664435000	3.764057000	1.791997000
1	-3.135066000	1.815252000	1.914796000
6	-2.114445000	-2.326479000	0.097064000
6	-1.990722000	-3.228286000	-0.954163000
6	-2.840617000	-4.325133000	-1.012820000
6	-3.806163000	-4.517773000	-0.027968000
6	-3.919266000	-3.612828000	1.021154000
6	-3.066635000	-2.515561000	1.091153000
1	-1.240860000	-3.064703000	-1.720571000
1	-2.752282000	-5.028350000	-1.834002000
1	-4.469536000	-5.374554000	-0.079526000
1	-4.667204000	-3.760545000	1.792710000
1	-3.136518000	-1.812769000	1.915115000

8	0.432331000	-2.520613000	0.895803000
26	1.497530000	-0.000524000	0.045018000
6	2.772357000	-1.341852000	-0.353094000
6	2.002399000	-0.000336000	1.844727000
6	2.773042000	1.340045000	-0.353453000
6	0.904086000	-0.000640000	-1.727791000
7	3.557494000	2.159879000	-0.597940000
7	3.556465000	-2.162061000	-0.597420000
7	2.304652000	-0.000043000	2.965677000
7	0.536782000	-0.000816000	-2.829877000
6	0.092169000	-0.001211000	-4.173289000
1	0.473353000	-0.887428000	-4.682550000
1	-0.998526000	-0.010666000	-4.194877000
1	0.457819000	0.894115000	-4.677982000
6	4.503558000	3.172023000	-0.886116000
1	4.453609000	3.425547000	-1.945892000
1	4.280702000	4.057726000	-0.289576000
1	5.505200000	2.813516000	-0.645202000
6	2.666148000	0.000637000	4.333630000
1	3.208002000	-0.916820000	4.567456000
1	3.302992000	0.861633000	4.541358000
1	1.766514000	0.057706000	4.947967000
6	4.502477000	-3.174050000	-0.886345000
1	5.484124000	-2.869874000	-0.520651000
1	4.203063000	-4.101541000	-0.396343000
1	4.549190000	-3.331244000	-1.964747000
1	-2.866513000	0.000771000	-0.159826000

[6b-H]⁺, TE = - 5778.328802

6	0.079730000	1.467766000	0.471794000
7	-1.381049000	1.195336000	0.175673000
6	-1.929623000	-0.000061000	0.060596000
7	-1.381031000	-1.195460000	0.175524000
6	0.079806000	-1.467883000	0.471570000
8	0.257256000	2.583919000	0.895094000
6	-2.279969000	2.318695000	0.117425000
6	-2.198444000	3.196725000	-0.957496000
6	-3.066014000	4.279600000	-1.018139000
6	-4.007209000	4.481075000	-0.011882000
6	-4.078515000	3.599106000	1.060269000
6	-3.207941000	2.516115000	1.132219000
1	-1.466634000	3.026422000	-1.739709000
1	-3.010542000	4.964650000	-1.857322000
1	-4.684565000	5.326750000	-0.064763000
1	-4.807856000	3.753831000	1.848058000
1	-3.245066000	1.830965000	1.972937000

6	-2.279922000	-2.318824000	0.117232000
6	-2.198118000	-3.197050000	-0.957513000
6	-3.065679000	-4.279926000	-1.018198000
6	-4.007159000	-4.481217000	-0.012167000
6	-4.078748000	-3.599057000	1.059806000
6	-3.208177000	-2.516067000	1.131804000
1	-1.466103000	-3.026894000	-1.739564000
1	-3.009980000	-4.965125000	-1.857244000
1	-4.684505000	-5.326895000	-0.065087000
1	-4.808303000	-3.753631000	1.847427000
1	-3.245517000	-1.830789000	1.972410000
8	0.257372000	-2.584075000	0.894729000
6	2.790414000	-1.440510000	-0.392381000
6	2.004099000	-0.000181000	1.939512000
6	2.790359000	1.440646000	-0.392147000
6	0.814358000	0.000229000	-1.852825000
7	3.553012000	2.282683000	-0.632669000
7	3.553111000	-2.282479000	-0.633019000
7	2.321417000	-0.000288000	3.055991000
7	0.434946000	0.000385000	-2.950451000
6	-0.022918000	0.000750000	-4.289378000
1	0.338502000	-0.894544000	-4.797071000
1	-1.113732000	0.009788000	-4.299557000
1	0.353313000	0.887311000	-4.801622000
6	4.476661000	3.315377000	-0.920712000
1	4.392363000	3.595112000	-1.971690000
1	4.258451000	4.182148000	-0.295366000
1	5.489621000	2.965386000	-0.717524000
6	2.708556000	-0.000416000	4.416943000
1	3.305185000	-0.889726000	4.624484000
1	3.299955000	0.891998000	4.626141000
1	1.818662000	-0.003610000	5.047700000
6	4.476762000	-3.315115000	-0.921158000
1	5.489813000	-2.964782000	-0.718987000
1	4.259263000	-4.181573000	-0.295124000
1	4.391721000	-3.595527000	-1.971901000
44	1.449342000	0.000003000	0.029979000
1	-2.998840000	-0.000052000	-0.132674000