

Supporting Information

On the Non-Innocent Behavior of Substrate Backbone Esters in Metal-Catalyzed Carbocyclizations and Friedel-Crafts Reactions of Enynes and Arenynes

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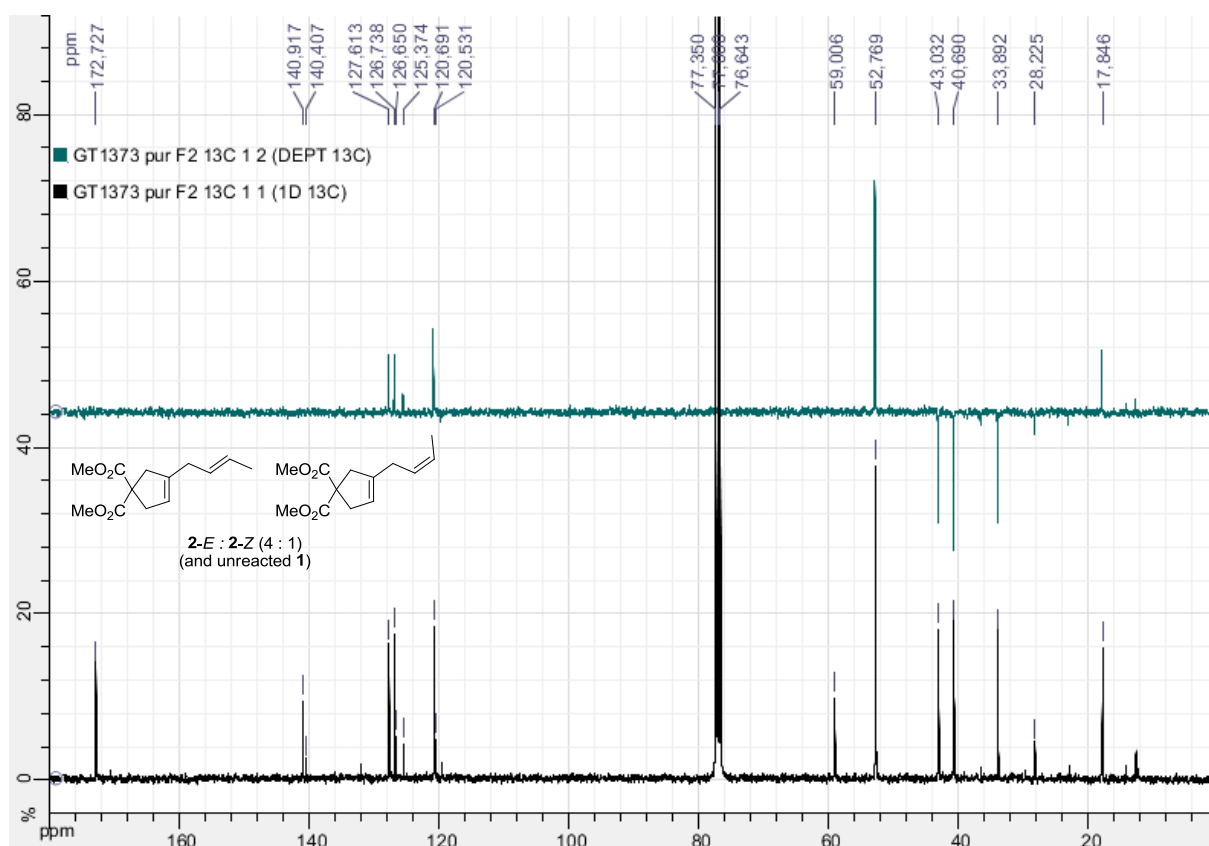
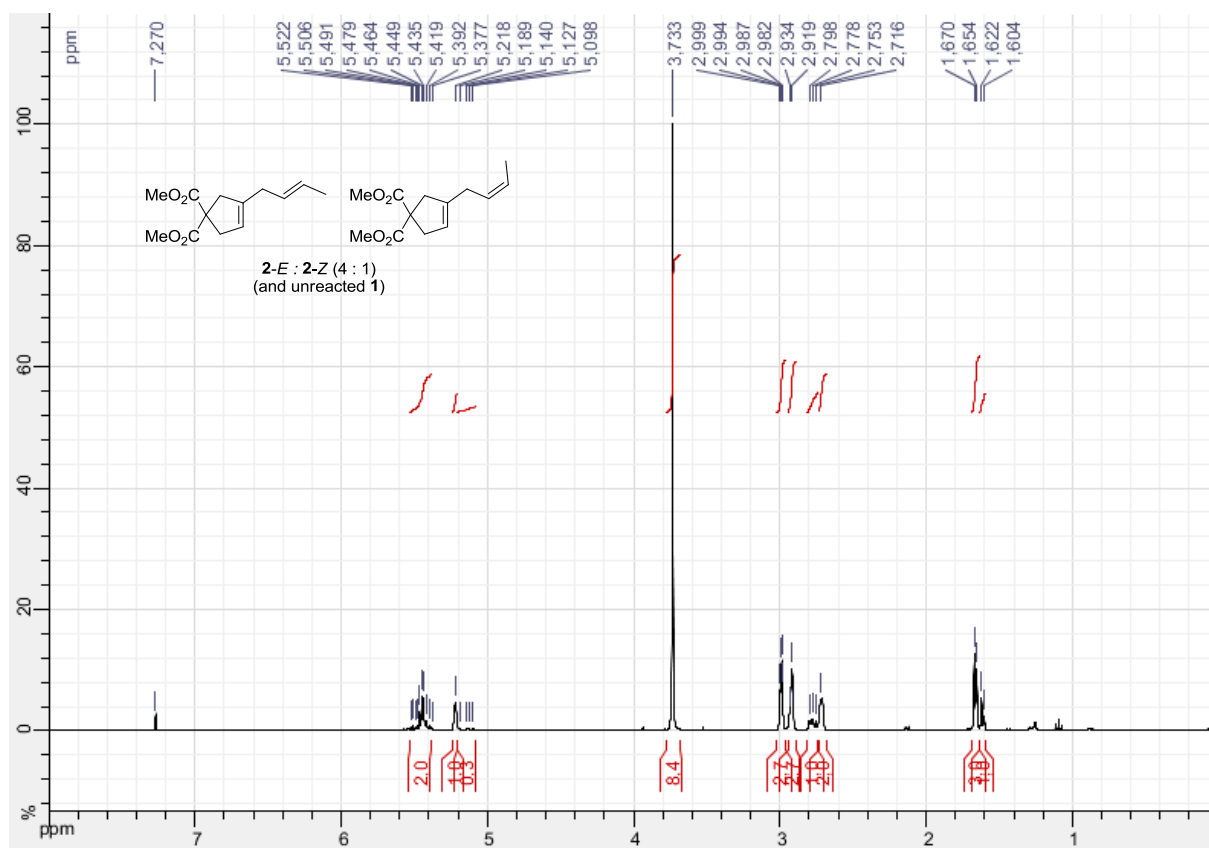
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1. NMR Spectra of 2:



2. Computations:

Table S1. Coordinates (x,y,z) of the Computed Intermediates and Transition States

J E(RM062X) = -2194.72633584 A.U.				TSa'-InCl ₃ E(RM062X) = -2194.70582240 A.U. Frequency -410.5550			
H	3.458950000	-2.646400000	-0.847490000	H	-1.346071000	-2.303807000	1.076865000
C	1.856711000	-1.630996000	-0.116054000	C	-0.716623000	-1.379934000	1.484970000
C	2.487296000	-2.346861000	-1.273698000	C	-2.064281000	-0.956903000	1.356634000
C	-1.378684000	-0.629314000	-1.708035000	C	1.778706000	-0.931975000	-1.373287000
C	-1.970465000	-0.192348000	-0.340983000	C	0.396320000	-1.092979000	0.555226000
C	0.998188000	-2.388747000	0.762258000	C	0.297580000	-0.939737000	-0.945810000
C	0.023346000	-1.489479000	-0.027266000	H	-0.394625000	-1.659597000	2.493346000
H	0.878418000	-3.455991000	0.579658000	C	1.638956000	-0.882547000	0.997275000
H	0.961662000	-2.096014000	1.809098000	H	-0.268482000	-1.743872000	-1.421735000
H	0.074598000	-2.352669000	-2.018709000	H	2.085468000	-1.948557000	-1.629486000
H	-0.874380000	0.216959000	-2.196211000	H	1.974865000	-0.289364000	-2.230995000
H	-2.126234000	-1.021432000	-2.400275000	H	1.956776000	-0.907327000	2.034658000
H	-1.071409000	-0.602050000	1.639103000	Cl	-2.960759000	-1.405505000	-2.288500000
H	-0.188153000	0.568361000	0.660937000	Cl	-5.288847000	0.220573000	0.374139000
Cl	1.974234000	0.756360000	2.598324000	C	-2.905348000	-1.073722000	2.575279000
Cl	4.993285000	0.142718000	0.081987000	C	-2.913059000	0.360914000	3.169362000
Cl	1.663071000	1.786485000	-1.199175000	H	-3.932713000	-1.352644000	2.335206000
C	-0.338178000	-1.630349000	-1.326127000	H	-2.486990000	-1.767959000	3.310971000
C	2.740298000	-1.513711000	-2.527748000	H	-1.902911000	0.688989000	3.420639000
H	1.967378000	-3.285184000	-1.503943000	H	-3.356700000	1.081162000	2.480667000
C	-0.764466000	-0.358921000	0.620980000	H	-3.516100000	0.349944000	4.077189000
H	3.194556000	-2.130847000	-3.303916000	In	-3.100319000	-0.002092000	-0.431476000
H	1.812541000	-1.087932000	-2.918873000	Cl	-1.961828000	2.052382000	-0.528700000
H	3.421585000	-0.684829000	-2.326417000	C	2.575115000	-0.479084000	-0.118150000
In	2.687795000	0.369161000	0.397650000	C	2.852969000	1.019133000	-0.071287000
C	-3.153405000	-1.069880000	0.053207000	C	4.230068000	1.262825000	0.008040000
C	-4.306980000	-0.288926000	0.206544000	C	4.930525000	-0.030915000	0.046962000
C	-3.960194000	1.116198000	-0.051884000	C	3.974693000	-1.053711000	-0.017033000
C	-2.595759000	1.189085000	-0.355884000	H	0.873897000	1.882358000	-0.149484000
H	-2.321692000	-3.061480000	0.155165000	C	1.943357000	2.064243000	-0.104863000
C	-3.205951000	-2.441096000	0.258626000	C	2.431409000	3.370377000	-0.078066000
C	-4.422214000	-3.026504000	0.612307000	H	1.736289000	4.200759000	-0.111776000
H	-4.474901000	-4.095916000	0.777750000	C	3.802482000	3.616918000	-0.007562000
C	-5.568160000	-2.247828000	0.759202000	H	4.161177000	4.639191000	0.013104000
H	-6.504070000	-2.718699000	1.035209000	H	5.778865000	2.763121000	0.100803000
H	-6.410882000	-0.266540000	0.677438000	C	4.714474000	2.565748000	0.039987000
C	-5.519004000	-0.871384000	0.558108000	C	6.284127000	-0.336296000	0.134981000
C	-4.743923000	2.263945000	-0.025217000	H	7.029715000	0.449411000	0.183346000
H	-5.801029000	2.212012000	0.210012000	C	6.667203000	-1.674936000	0.162051000
C	-4.141245000	3.487007000	-0.304673000	H	7.718021000	-1.930623000	0.229711000

H	-4.733834000	4.394052000	-0.287869000	C	5.714678000	-2.691477000	0.103219000
C	-2.780688000	3.559109000	-0.601032000	H	6.033405000	-3.726825000	0.126455000
H	-2.326625000	4.520773000	-0.807768000	H	3.616361000	-3.176988000	-0.034744000
H	-0.934328000	2.471242000	-0.855112000	C	4.357102000	-2.384740000	0.012761000
C	-1.993875000	2.407519000	-0.629624000	H	-0.192955000	0.001287000	-1.214492000
TSb⁺-InCl₃ E(RM062X) = -2194.70943435 A.U. Frequency -534.2510				C-GaCl₃ E(RM062X) = -4112.56825023 A.U.			
H	-3.255082000	-2.333592000	-0.821499000	H	3.295395000	-2.333442000	-0.973183000
C	-2.216058000	-1.758903000	-0.425626000	C	1.655078000	-1.561676000	-0.062725000
C	-2.817434000	-2.654841000	0.453814000	C	2.243436000	-2.214246000	-1.280320000
C	1.458395000	-1.025143000	1.595891000	C	-1.660563000	-0.853308000	-1.325641000
C	2.094023000	-0.414800000	0.312974000	C	-2.076954000	-0.241447000	0.042567000
C	-0.962572000	-2.205439000	-1.142360000	C	1.019268000	-2.420818000	0.928726000
C	0.174390000	-1.644731000	-0.321975000	C	-0.159774000	-1.684755000	0.301136000
H	-0.890153000	-3.299718000	-1.201125000	H	1.037583000	-3.494721000	0.753842000
H	-0.921955000	-1.788248000	-2.149955000	H	1.118791000	-2.127948000	1.971175000
H	-0.463096000	-2.058201000	1.728294000	H	-0.210012000	-2.553977000	-1.684253000
H	0.919531000	-0.234689000	2.121547000	H	-1.234206000	-0.078083000	-1.971649000
H	2.214052000	-1.434396000	2.266477000	H	-2.490188000	-1.307304000	-1.873919000
H	1.078747000	-0.283072000	-1.723295000	H	-1.385613000	-1.090386000	1.943867000
Cl	-1.370281000	1.551511000	-1.932333000	H	-0.380567000	0.224067000	1.353486000
Cl	-4.931477000	0.685961000	-0.526456000	Cl	2.033510000	0.678301000	2.508677000
Cl	-1.899067000	0.732470000	1.943682000	Cl	4.320992000	0.533997000	-0.333515000
C	0.438740000	-2.072683000	1.104957000	Cl	0.858469000	1.657170000	-0.854964000
C	-3.909270000	-2.332371000	1.415287000	C	-0.594288000	-1.833783000	-0.974310000
H	-2.422187000	-3.676976000	0.487898000	C	2.204446000	-1.407658000	-2.575766000
C	1.053218000	-0.733320000	-0.737232000	H	1.857602000	-3.230388000	-1.421611000
H	-4.586384000	-3.174543000	1.553725000	C	-0.963402000	-0.642115000	1.042966000
H	-3.411678000	-2.130314000	2.372586000	H	2.728365000	-1.945282000	-3.367156000
H	-4.465371000	-1.435599000	1.140295000	H	1.176879000	-1.230066000	-2.903420000
In	-2.605311000	0.454954000	-0.293822000	H	2.685119000	-0.436228000	-2.455504000
C	3.444161000	-1.013058000	-0.059330000	Ga	2.235515000	0.379430000	0.339184000
C	4.426777000	-0.016818000	-0.126619000	C	-2.273107000	1.272324000	0.038261000
C	3.794646000	1.278694000	0.167383000	O	-2.304537000	1.914043000	1.050535000
C	2.434383000	1.059773000	0.420874000	O	-2.418882000	1.777038000	-1.182967000
H	2.992105000	-3.105014000	-0.285878000	C	-2.507591000	3.205893000	-1.238266000
C	3.759074000	-2.337120000	-0.318049000	H	-3.363034000	3.550830000	-0.657917000
C	5.078155000	-2.666273000	-0.630152000	H	-1.590897000	3.639248000	-0.837163000
H	5.343388000	-3.697150000	-0.833404000	H	-2.624839000	3.452367000	-2.289786000
C	6.058770000	-1.676615000	-0.689610000	C	-3.391850000	-0.909149000	0.443034000
H	7.078289000	-1.948335000	-0.937098000	O	-3.466005000	-1.928396000	1.072120000
H	6.506328000	0.422671000	-0.499427000	O	-4.442764000	-0.259870000	-0.056741000
C	5.741132000	-0.343515000	-0.441996000	C	-5.723174000	-0.830129000	0.239139000
C	4.323933000	2.563514000	0.206629000	H	-5.795600000	-1.831524000	-0.185500000
H	5.376042000	2.740023000	0.012383000	H	-5.866171000	-0.883848000	1.318049000
C	3.471327000	3.625124000	0.497495000	H	-6.451743000	-0.163915000	-0.213825000

H	3.863547000	4.634719000	0.530976000			
C	2.115869000	3.405605000	0.742774000			
H	1.467804000	4.245768000	0.961814000			
H	0.530384000	1.947177000	0.899681000			
C	1.585283000	2.116540000	0.708050000			
H	0.838316000	-3.093976000	1.131020000			
C-InCl ₃ E(RM062X) = -2189.60556523 A.U.				TSb''-GaCl ₃ E(RM062X) = -4112.55512248 A.U. Frequency -565.3289		
H	-3.010680000	2.588924000	-0.952520000	H	0.628513000	1.284463000
C	-1.412321000	1.713645000	-0.054824000	C	1.505329000	0.933587000
C	-1.965489000	2.417028000	-1.259780000	C	1.595571000	2.276266000
C	1.899125000	0.891095000	-1.327764000	C	-2.498212000	0.020891000
C	2.279438000	0.236133000	0.031381000	C	-2.934388000	0.768831000
C	-0.734319000	2.514027000	0.953026000	C	0.860025000	0.554772000
C	0.401275000	1.727499000	0.298251000	C	-0.612175000	0.385434000
H	-0.691208000	3.592255000	0.807980000	H	1.309001000	-0.378285000
H	-0.836296000	2.198765000	1.989252000	H	1.039577000	1.328977000
H	0.510815000	2.648157000	-1.660513000	H	-1.287497000	-1.588914000
H	1.457982000	0.144094000	-1.996992000	H	-3.556098000	1.639851000
H	2.749226000	1.331957000	-1.854907000	H	-3.529695000	0.097372000
H	1.569718000	1.037219000	1.947561000	H	-1.478842000	1.875221000
H	0.545496000	-0.226136000	1.294452000	Cl	2.125651000	-2.408233000
Cl	-1.862469000	-0.720142000	2.600220000	Cl	1.388514000	-0.524451000
Cl	-4.329467000	-0.412306000	-0.474953000	C	-1.145781000	-0.612173000
Cl	-0.626315000	-1.634308000	-1.044734000	C	2.178057000	2.850598000
C	0.860911000	1.896894000	-0.965015000	C	-1.600068000	1.116048000
C	-1.967111000	1.628302000	-2.567360000	H	1.186534000	2.996578000
H	-1.528389000	3.414807000	-1.388123000	H	2.325382000	2.104673000
C	1.155884000	0.634697000	1.021766000	H	1.568487000	3.676130000
H	-2.423578000	2.220143000	-3.361758000	H	3.161555000	3.251265000
H	-0.952274000	1.362746000	-2.874608000	Ga	2.434395000	-0.529025000
H	-2.538237000	0.702462000	-2.479498000	H	-0.516568000	-0.772113000
In	-2.123671000	-0.373985000	0.298353000	Cl	4.532709000	0.100757000
C	2.449602000	-1.279930000	-0.013158000	C	-2.253777000	1.060817000
O	2.424176000	-1.955342000	0.977091000	O	-1.182846000	1.556419000
O	2.642649000	-1.743816000	-1.243538000	O	-3.383333000	1.415085000
C	2.705424000	-3.171406000	-1.347724000	C	-3.263879000	2.396924000
H	3.528269000	-3.555101000	-0.744965000	H	-2.899292000	3.336888000
H	1.763577000	-3.598764000	-1.002351000	H	-2.573274000	2.044637000
H	2.862958000	-3.382214000	-2.401736000	H	-4.264323000	2.517505000
C	3.594652000	0.876857000	0.473194000	C	-3.503838000	-1.012525000
O	3.665035000	1.900547000	1.096134000	O	-4.497775000	-1.336508000
O	4.649800000	0.202251000	0.020300000	O	-3.096912000	-1.554841000
C	5.929388000	0.752110000	0.356401000	C	-3.939711000	-2.577975000
H	6.036663000	1.746041000	-0.078236000	H	-4.015198000	-3.409135000
H	6.033257000	0.817820000	1.439144000	H	-4.935193000	-2.177720000

H	6.660809000	0.066085000	-0.060807000	H	-3.462164000	-2.895074000	-2.414412000
TSb''-InCl₃ E(RM062X) = -2189.59234252 A.U. Frequency -379.5149				9 E(RM062X) = -4187.57749102 A.U.			
H	0.352455000	1.476997000	0.231882000	C	1.486128000	2.713755000	-1.395626000
C	1.252385000	1.102962000	1.039724000	C	-0.282471000	0.491889000	-0.040072000
C	1.256226000	2.435662000	0.681537000	C	-1.054567000	1.219954000	0.541066000
C	-2.704744000	0.026199000	0.665715000	Ga	-2.613443000	-0.477965000	-0.181120000
C	-3.204220000	0.784456000	1.922265000	Cl	-2.167696000	-2.189420000	1.071673000
C	0.585354000	0.720991000	2.362836000	Cl	-4.290443000	0.757779000	0.408385000
C	-0.873190000	0.491460000	2.099420000	Cl	-2.338578000	-0.791029000	-2.310248000
H	1.055167000	-0.193175000	2.737810000	H	-1.637982000	1.953865000	1.053232000
H	0.714209000	1.511055000	3.108546000	C	0.671859000	-0.396794000	-0.705897000
H	-1.457103000	-1.518892000	1.589586000	H	0.270430000	-1.413665000	-0.672911000
H	-3.851397000	1.626718000	1.667362000	H	0.755426000	-0.109076000	-1.755761000
H	-3.791292000	0.104866000	2.547367000	C	2.063378000	-0.369037000	-0.023887000
H	-1.830003000	1.974167000	3.319920000	C	2.887759000	0.906731000	-0.349887000
Cl	1.944717000	-2.405619000	1.108166000	C	2.100445000	2.191132000	-0.255617000
Cl	1.074117000	-0.484625000	-2.192729000	C	1.903491000	-0.559534000	1.488182000
C	-1.340859000	-0.546822000	1.097817000	O	2.442851000	0.099540000	2.330780000
C	1.848445000	3.003961000	-0.565482000	O	1.069213000	-1.566594000	1.729625000
C	-1.901501000	1.194964000	2.570217000	C	0.803724000	-1.851479000	3.107467000
H	0.784577000	3.154942000	1.361148000	H	1.732864000	-2.099995000	3.619903000
H	2.054511000	2.242578000	-1.318293000	H	0.117535000	-2.693084000	3.102869000
H	1.198495000	3.771991000	-0.986017000	H	0.342599000	-0.984101000	3.580709000
H	2.798130000	3.473887000	-0.288122000	C	2.902339000	-1.550956000	-0.511789000
In	2.290921000	-0.478951000	-0.178115000	O	3.719675000	-2.112630000	0.160516000
H	-0.687328000	-0.699335000	0.237558000	O	2.657719000	-1.834563000	-1.793203000
Cl	4.488010000	0.278389000	-0.435098000	C	3.441723000	-2.899061000	-2.348788000
C	-2.466758000	1.052207000	-0.437798000	H	4.501069000	-2.647637000	-2.299976000
O	-1.411681000	1.598321000	-0.661365000	H	3.262352000	-3.820276000	-1.795230000
O	-3.582940000	1.333456000	-1.097871000	H	3.112701000	-2.997248000	-3.379261000
C	-3.464456000	2.293805000	-2.155348000	H	3.268726000	0.798079000	-1.369067000
H	-3.136585000	3.253111000	-1.755068000	H	3.741167000	0.921367000	0.330578000
H	-2.744939000	1.941872000	-2.894253000	C	1.930467000	2.850277000	0.963920000
H	-4.457277000	2.375720000	-2.587875000	H	2.413611000	2.457603000	1.850368000
C	-3.655544000	-1.055071000	0.184571000	C	1.125832000	3.981115000	1.044432000
O	-4.665218000	-1.389956000	0.737312000	H	1.635642000	2.227897000	-2.355354000
O	-3.177432000	-1.622105000	-0.925094000	C	0.678763000	3.842879000	-1.316546000
C	-3.957359000	-2.692322000	-1.467674000	H	0.201439000	4.229204000	-2.209184000
H	-4.060841000	-3.490417000	-0.732643000	C	0.486469000	4.472383000	-0.091352000
H	-4.946244000	-2.328850000	-1.748100000	H	-0.143036000	5.352135000	-0.025807000
H	-3.410500000	-3.039541000	-2.339610000	H	0.998695000	4.481687000	1.997470000
TS₉₋₁₁ E(RM062X) = -4187.52158745 A.U. Frequency -536.9136				11 E(RM062X) = -4187.63986742 A.U.			
C	1.017017000	2.074560000	-0.598711000	C	0.106359000	1.940073000	-0.803063000
C	-0.161701000	0.969057000	-0.379169000	C	-0.179237000	0.586425000	-1.272741000

C	-1.430230000	1.353231000	-0.222669000	C	-1.429276000	0.166724000	-1.694664000
Ga	-2.962960000	0.053615000	0.119127000	Ga	-2.437291000	-0.753493000	0.061425000
Cl	-2.474313000	-1.217938000	1.858635000	Cl	-2.494951000	0.641050000	1.731980000
Cl	-4.788599000	1.243289000	0.389913000	Cl	-4.420078000	-0.925272000	-0.865240000
Cl	-2.994837000	-1.178823000	-1.734618000	Cl	-1.521085000	-2.723942000	0.273039000
H	-1.681600000	2.404689000	-0.357418000	H	-2.207081000	0.886798000	-1.925718000
C	0.285866000	-0.477272000	-0.454805000	C	0.954565000	-0.406013000	-1.374961000
H	-0.170912000	-0.975865000	0.405886000	H	0.577868000	-1.413845000	-1.182931000
H	-0.149679000	-0.925327000	-1.354255000	H	1.298585000	-0.385611000	-2.419832000
C	1.793187000	-0.722774000	-0.453516000	C	2.156615000	-0.089191000	-0.467825000
C	2.472411000	0.213143000	-1.474846000	C	2.595491000	1.365190000	-0.714269000
C	2.306224000	1.618888000	-0.988173000	C	1.446380000	2.331998000	-0.549078000
C	2.380856000	-0.447247000	0.929040000	C	1.741179000	-0.279148000	0.999581000
O	1.823518000	0.165126000	1.794762000	O	0.605800000	-0.457045000	1.375365000
O	3.627758000	-0.918313000	1.019745000	O	2.803925000	-0.181834000	1.817194000
C	4.279792000	-0.694668000	2.276525000	C	2.515119000	-0.333900000	3.223651000
H	4.357364000	0.375111000	2.472398000	H	1.802088000	0.426646000	3.547900000
H	5.264235000	-1.143765000	2.180710000	H	3.471020000	-0.213745000	3.731500000
H	3.713591000	-1.167528000	3.078560000	H	2.093656000	-1.322529000	3.416403000
C	2.054078000	-2.173931000	-0.847637000	C	3.312576000	-1.042691000	-0.803936000
O	2.575117000	-2.514878000	-1.872075000	O	4.348232000	-0.716384000	-1.338155000
O	1.588407000	-2.996556000	0.085400000	O	2.997271000	-2.303281000	-0.461402000
C	1.716121000	-4.397870000	-0.191951000	C	3.997520000	-3.301493000	-0.746381000
H	1.179897000	-4.644533000	-1.107775000	H	4.215680000	-3.326617000	-1.816182000
H	2.768363000	-4.660082000	-0.301485000	H	4.916724000	-3.082854000	-0.198650000
H	1.273906000	-4.903943000	0.660927000	H	3.566843000	-4.245955000	-0.417685000
H	1.990994000	0.054835000	-2.444840000	H	3.008642000	1.422159000	-1.729083000
H	3.527256000	-0.036267000	-1.586624000	H	3.412554000	1.629964000	-0.039253000
C	3.393473000	2.461087000	-0.798727000	C	1.705037000	3.643773000	-0.144556000
H	4.383759000	2.114448000	-1.070083000	H	2.731310000	3.943355000	0.048208000
C	3.218195000	3.735491000	-0.271354000	C	0.671358000	4.561834000	0.025142000
H	0.251248000	1.875233000	-1.467202000	H	-1.488120000	-0.766628000	-2.251989000
C	0.858928000	3.369996000	-0.040079000	C	-0.930336000	2.878317000	-0.603242000
H	-0.119712000	3.693176000	0.289923000	H	-1.962526000	2.584833000	-0.747599000
C	1.951345000	4.192502000	0.107496000	C	-0.653474000	4.174204000	-0.197221000
H	1.833632000	5.178279000	0.538774000	H	-1.464625000	4.877997000	-0.043351000
H	4.079384000	4.380301000	-0.138478000	H	0.896257000	5.574832000	0.345199000
12 E(RM062X) = -4187.65067419 A.U.				TS₉₋₁₃ E(RM062X) = -4187.54184209 A.U. Frequency -247.5346			
C	3.595550000	-0.209671000	-0.301994000	O	-3.866539000	1.087397000	-0.447238000
C	3.325129000	1.232288000	-0.497836000	H	-1.869308000	2.141518000	-1.263704000
C	4.144951000	2.205184000	-0.100067000	C	-1.052330000	2.538445000	-0.673591000
H	5.075303000	1.997572000	0.413604000	C	0.092775000	1.032049000	-0.766491000
C	2.014475000	1.550507000	-1.166534000	C	-0.974859000	2.194821000	0.708184000
H	1.839156000	2.626160000	-1.183624000	C	-0.184154000	2.997377000	1.556781000
H	2.031772000	1.194059000	-2.202485000	C	0.482541000	4.086475000	1.055857000

C	0.851713000	0.827403000	-0.447520000	H	-0.086052000	2.718862000	2.599165000
C	1.083592000	-0.694775000	-0.442967000	C	1.375702000	1.157280000	-0.634697000
C	2.527209000	-1.112546000	-0.263807000	C	0.378140000	4.456410000	-0.311235000
C	0.777369000	1.350012000	0.994739000	H	1.102847000	4.682397000	1.716128000
O	1.426631000	0.916153000	1.895803000	H	0.901693000	5.334115000	-0.668998000
O	-0.070885000	2.381875000	1.085037000	C	-0.408976000	3.723452000	-1.147686000
C	-0.236288000	2.925066000	2.403259000	H	-0.536706000	4.004908000	-2.185627000
H	-0.603376000	2.148026000	3.073144000	C	-1.646139000	0.979562000	1.274064000
H	-0.965335000	3.723878000	2.301403000	H	-1.012446000	0.583365000	2.069465000
H	0.715641000	3.309422000	2.768639000	H	-2.594458000	1.278644000	1.729111000
C	-0.472315000	1.128996000	-1.117348000	C	-1.902212000	-0.141265000	0.242803000
O	-1.507901000	0.487238000	-0.935600000	H	1.853055000	2.112391000	-0.425375000
O	-0.470192000	2.126423000	-1.950535000	C	-0.862356000	-0.097982000	-0.917513000
C	-1.732825000	2.468960000	-2.562198000	H	-0.280407000	-1.020364000	-0.924243000
H	-2.075705000	1.639572000	-3.178767000	H	-1.357373000	-0.038314000	-1.890458000
H	-2.466959000	2.679192000	-1.785896000	Ga	2.425888000	-0.566928000	-0.271621000
H	-1.524757000	3.348102000	-3.163407000	Cl	1.377356000	-1.195675000	1.616389000
H	0.714593000	-1.110114000	-1.387556000	Cl	2.079320000	-2.095044000	-1.817095000
H	0.488351000	-1.150549000	0.351800000	Cl	4.524195000	-0.054586000	0.067102000
C	2.780226000	-2.470348000	-0.060994000	C	-1.884658000	-1.481411000	1.001648000
H	1.942960000	-3.160153000	-0.018573000	O	-2.313124000	-1.579528000	2.118996000
C	4.075309000	-2.939182000	0.092415000	O	-1.383281000	-2.472550000	0.287091000
C	4.901164000	-0.696742000	-0.160590000	C	-1.226453000	-3.720513000	0.974576000
H	5.734054000	-0.007038000	-0.228826000	H	-0.794547000	-4.399346000	0.245114000
C	5.143334000	-2.045332000	0.038215000	H	-0.550155000	-3.581873000	1.818007000
H	6.160395000	-2.403410000	0.142522000	H	-2.194535000	-4.078618000	1.324220000
H	4.254220000	-3.996028000	0.249733000	C	-3.291955000	0.033074000	-0.372626000
Cl	-1.960991000	-2.706932000	-0.795891000	O	-3.759152000	-1.106696000	-0.868885000
Cl	-1.692110000	-0.505276000	2.146027000	C	-5.036710000	-1.032291000	-1.515307000
Cl	-4.521779000	-0.109473000	-0.177268000	H	-4.984416000	-0.356828000	-2.369170000
Ga	-2.514054000	-0.839652000	0.160604000	H	-5.788431000	-0.672477000	-0.813471000
H	3.895524000	3.246667000	-0.267487000	H	-5.259452000	-2.045323000	-1.836948000
13 E(RM062X) = -4187.53786077 A.U.				TS₁₃₋₁₄ E(RM062X) = -4187.53740956 A.U. Frequency -92.0225			
O	-1.811613000	0.192145000	2.157742000	O	1.689199000	-0.001451000	1.992312000
H	-1.697556000	-1.676324000	1.232161000	H	1.786682000	1.530599000	1.006239000
C	-1.604080000	-1.945837000	0.126542000	C	1.629322000	1.918790000	-0.100609000
C	-0.337393000	-1.098771000	-0.175864000	C	0.339751000	1.132140000	-0.362128000
C	-2.904497000	-1.393255000	-0.229396000	C	2.914369000	1.313030000	-0.380391000
C	-3.981660000	-2.246942000	-0.436751000	C	4.055802000	2.113071000	-0.442500000
C	-3.811322000	-3.619515000	-0.358106000	C	3.959950000	3.483064000	-0.291026000
H	-4.956081000	-1.830816000	-0.666200000	H	5.020120000	1.645915000	-0.607538000
C	0.873433000	-1.489814000	0.205798000	C	-0.858821000	1.588249000	-0.003174000
C	-2.561754000	-4.204084000	-0.068374000	C	2.722818000	4.114708000	-0.054725000
H	-4.665995000	-4.265602000	-0.530661000	H	4.859829000	4.086198000	-0.346825000
H	-2.461402000	-5.281168000	-0.038817000	H	2.675723000	5.191168000	0.047726000

C	-1.482931000	-3.395437000	0.135370000	C	1.587445000	3.360014000	0.012608000
H	-0.503848000	-3.818222000	0.326577000	H	0.623543000	3.831037000	0.159123000
C	-3.109790000	0.085860000	-0.307279000	C	3.052093000	-0.175991000	-0.488958000
H	-3.549023000	0.295434000	-1.289731000	H	3.382597000	-0.393585000	-1.511608000
H	-3.870735000	0.380915000	0.422049000	H	3.860897000	-0.517912000	0.162109000
C	-1.837268000	0.921145000	-0.137875000	C	1.756898000	-0.952507000	-0.220568000
H	0.971817000	-2.434522000	0.741514000	H	-0.925613000	2.571613000	0.461739000
C	-0.650820000	0.218055000	-0.837798000	C	0.581784000	-0.240981000	-0.934629000
H	-0.923699000	0.062275000	-1.889663000	H	0.841941000	-0.168956000	-1.998379000
H	0.221552000	0.869119000	-0.819273000	H	-0.314104000	-0.853185000	-0.862612000
Ga	2.569904000	-0.455798000	-0.136517000	Ga	-2.560518000	0.520371000	-0.128256000
Cl	2.684379000	0.053411000	-2.295418000	Cl	-2.856057000	-0.235891000	-2.192982000
Cl	2.404498000	1.453976000	1.020409000	Cl	-2.198462000	-1.249759000	1.213116000
Cl	4.282938000	-1.663995000	0.546041000	Cl	-4.253599000	1.729587000	0.592994000
C	-2.107603000	2.323161000	-0.686849000	C	1.948119000	-2.389184000	-0.711942000
O	-3.188456000	2.846888000	-0.607694000	O	3.025206000	-2.924507000	-0.746239000
O	-1.038815000	2.870246000	-1.235721000	O	0.811397000	-2.946546000	-1.085236000
C	-1.179582000	4.227564000	-1.671962000	C	0.881103000	-4.322688000	-1.476252000
H	-0.207322000	4.506129000	-2.066888000	H	-0.134573000	-4.598051000	-1.743681000
H	-1.949331000	4.296820000	-2.440474000	H	1.555003000	-4.436528000	-2.325172000
H	-1.451593000	4.858504000	-0.825985000	H	1.241240000	-4.924151000	-0.641551000
C	-1.498238000	1.038784000	1.351463000	C	1.478210000	-0.968184000	1.284683000
O	-0.807413000	2.119512000	1.623891000	O	0.995011000	-2.103579000	1.717048000
C	-0.269598000	2.219392000	2.954967000	C	0.556949000	-2.135095000	3.089095000
H	0.350778000	1.348289000	3.157722000	H	-0.205023000	-1.371792000	3.235500000
H	-1.085732000	2.291232000	3.673529000	H	1.408268000	-1.966951000	3.747958000
H	0.339277000	3.117862000	2.949568000	H	0.136283000	-3.125795000	3.229733000
14 E(RM062X) = -4187.59074683 A.U.				TS₁₄₋₁₁ E(RM062X) = -4187.58147051 A.U. Frequency -852.5838			
O	-0.716408000	0.110985000	1.852909000	H	-0.005671000	0.710533000	1.010733000
H	-0.421328000	-0.651353000	1.257130000	C	-0.668060000	1.573312000	0.172240000
C	-1.837096000	-1.902695000	-0.398505000	O	0.558782000	-0.217871000	1.833266000
C	-0.519689000	-1.229270000	-0.556063000	C	1.054116000	-1.145641000	1.194089000
C	-2.977847000	-1.116319000	-0.177071000	O	1.177439000	-2.337606000	1.696666000
C	-4.202034000	-1.744928000	0.059492000	C	0.561017000	-2.564442000	2.985425000
C	-4.306970000	-3.127668000	0.054237000	H	-0.502645000	-2.342853000	2.904677000
H	-5.082518000	-1.137724000	0.244971000	H	1.029820000	-1.924464000	3.731191000
C	0.644130000	-1.713651000	-0.077031000	H	0.736661000	-3.613577000	3.199702000
C	-3.177610000	-3.907642000	-0.187599000	C	1.638974000	-0.979672000	-0.205319000
H	-5.266712000	-3.597734000	0.231908000	C	1.817322000	-2.373137000	-0.824453000
H	-3.254852000	-4.987845000	-0.208062000	O	2.880436000	-2.892849000	-1.019131000
C	-1.953754000	-3.296774000	-0.405432000	O	0.641335000	-2.906482000	-1.117580000
H	-1.072715000	-3.895737000	-0.605182000	C	0.663009000	-4.237627000	-1.646627000
C	-2.953415000	0.398764000	-0.220027000	H	1.235175000	-4.261782000	-2.573683000
H	-3.450581000	0.739985000	-1.131979000	H	-0.377184000	-4.494283000	-1.823492000
H	-3.540427000	0.814487000	0.604455000	H	1.114764000	-4.914787000	-0.921598000

C	-1.541316000	1.036676000	-0.259319000	C	0.674996000	-0.134007000	-1.075668000
H	0.604528000	-2.705034000	0.378386000	H	-0.271386000	-0.652580000	-1.211979000
C	-0.622930000	0.157410000	-1.146834000	H	1.140705000	-0.001965000	-2.057208000
H	-1.109997000	0.103747000	-2.126455000	C	0.509606000	1.217551000	-0.431573000
H	0.345011000	0.635215000	-1.276298000	H	-0.653185000	2.532689000	0.690849000
Ga	2.408533000	-0.734927000	-0.099075000	C	1.769982000	1.968709000	-0.282704000
Cl	3.068561000	-0.306404000	-2.158688000	C	2.954881000	1.243963000	-0.089813000
Cl	1.981944000	1.309260000	0.847528000	C	3.007422000	-0.269917000	-0.114309000
Cl	3.887010000	-1.784710000	1.136367000	H	3.570405000	-0.638835000	0.747744000
C	-1.630024000	2.462491000	-0.828017000	H	3.579150000	-0.584219000	-0.992008000
O	-2.660833000	3.023898000	-1.073055000	Ga	-2.457433000	0.610354000	-0.077657000
O	-0.421030000	2.960252000	-1.022822000	Cl	-3.981589000	1.664586000	1.085508000
C	-0.359914000	4.295741000	-1.540173000	Cl	-2.167780000	-1.497115000	0.651830000
H	0.698407000	4.516870000	-1.639841000	Cl	-2.831266000	0.523599000	-2.251364000
H	-0.862517000	4.343879000	-2.505840000	C	1.784782000	3.367562000	-0.276328000
H	-0.840216000	4.984164000	-0.844685000	H	0.858787000	3.906439000	-0.441818000
C	-1.046025000	1.124949000	1.160710000	C	2.973491000	4.052511000	-0.092728000
O	-1.115668000	2.256979000	1.741655000	H	2.985540000	5.135030000	-0.107246000
C	-0.607390000	2.373070000	3.100844000	C	4.152578000	3.338006000	0.114338000
H	0.432695000	2.049451000	3.100540000	H	5.085627000	3.865997000	0.270846000
H	-1.214473000	1.757197000	3.761340000	C	4.139224000	1.950402000	0.120900000
H	-0.703763000	3.426851000	3.337653000	H	5.060662000	1.402519000	0.288540000
TS₁₁₋₁₅ E(RM062X) = -4534.31011979 A.U. Frequency -319.5919				15 E(RM062X) = -4534.31472036 A.U.			
C	0.149602000	-0.839575000	1.632659000	C	0.625049000	-0.504758000	1.680901000
C	0.041460000	-0.045897000	0.357016000	C	0.177275000	0.144021000	0.371233000
C	1.374749000	0.236183000	-0.320890000	C	1.332406000	0.932580000	-0.286350000
H	1.213050000	0.592773000	-1.338229000	H	1.060686000	1.194671000	-1.312322000
H	1.952240000	0.994433000	0.210374000	H	1.507772000	1.872139000	0.250082000
C	2.259089000	-1.019281000	-0.355357000	C	2.670718000	0.189797000	-0.292482000
C	2.567919000	-1.450449000	1.083879000	C	3.094850000	-0.076231000	1.156650000
C	1.343206000	-1.489701000	1.968375000	C	1.977832000	-0.615960000	2.021971000
C	1.582230000	-2.083564000	-1.220182000	C	2.575888000	-1.060009000	-1.168972000
O	1.477992000	-1.967052000	-2.410847000	O	2.411062000	-0.998905000	-2.357091000
O	1.093445000	-3.099606000	-0.516158000	O	2.678350000	-2.193176000	-0.480471000
C	0.330231000	-4.055235000	-1.268174000	C	2.484226000	-3.392838000	-1.242106000
H	-0.515242000	-3.559000000	-1.746791000	H	1.483242000	-3.397089000	-1.676485000
H	-0.013596000	-4.788858000	-0.544798000	H	2.598125000	-4.209042000	-0.534700000
H	0.958226000	-4.518115000	-2.028816000	H	3.226281000	-3.455631000	-2.037607000
C	3.570556000	-0.654923000	-1.047496000	C	3.723492000	1.087367000	-0.939091000
O	3.915465000	0.459728000	-1.328327000	O	3.572502000	2.246003000	-1.211730000
O	4.311998000	-1.743657000	-1.256386000	O	4.868153000	0.422261000	-1.116521000
C	5.555684000	-1.526968000	-1.932253000	C	5.924938000	1.163127000	-1.734338000
H	5.374183000	-1.068597000	-2.904188000	H	5.607850000	1.513039000	-2.716637000
H	6.197946000	-0.876887000	-1.337945000	H	6.197028000	2.018954000	-1.116320000
H	6.002615000	-2.510242000	-2.047951000	H	6.757220000	0.470557000	-1.822590000

H	3.287551000	-0.733295000	1.498714000	H	3.443769000	0.874014000	1.580609000
H	3.051110000	-2.428893000	1.085455000	H	3.940194000	-0.765329000	1.176907000
C	1.398138000	-2.238768000	3.146285000	C	2.332403000	-1.251542000	3.215918000
H	2.320845000	-2.752424000	3.396362000	H	3.384964000	-1.339464000	3.466300000
C	0.297076000	-2.352573000	3.980075000	C	1.375157000	-1.777245000	4.067941000
H	-0.729954000	-0.411417000	-1.597975000	H	-0.169767000	-0.661612000	-1.617324000
C	-0.970878000	-0.993898000	2.457549000	C	-0.332974000	-1.060766000	2.537892000
H	-1.910991000	-0.525372000	2.187054000	H	-1.384720000	-1.021572000	2.276686000
C	-0.899934000	-1.733960000	3.626274000	C	0.030367000	-1.685661000	3.720943000
H	-1.777873000	-1.833071000	4.252752000	H	-0.734148000	-2.109696000	4.360521000
H	0.362864000	-2.937398000	4.889827000	H	1.674122000	-2.268811000	4.986026000
C	-1.039547000	-0.529419000	-0.554835000	C	-0.390235000	-0.937140000	-0.579738000
Ga	-3.013146000	0.020707000	-0.696864000	Ga	-2.326590000	-1.532671000	-0.675231000
Cl	-3.169505000	1.569068000	-2.291839000	Cl	-3.218094000	-0.583799000	-2.504950000
Cl	-3.861774000	0.902830000	1.173468000	Cl	-3.631477000	-0.762338000	1.016444000
Cl	-4.075203000	-1.829328000	-1.248766000	Cl	-2.441850000	-3.729793000	-0.758303000
C	-0.449896000	1.711053000	1.035354000	C	-0.927117000	1.244404000	0.683710000
C	-0.409401000	2.516568000	-0.140968000	C	-1.479454000	1.853831000	-0.526592000
C	0.480414000	2.033315000	2.080768000	C	-0.597748000	2.192371000	1.754328000
C	0.592953000	3.430828000	-0.357761000	C	-1.744934000	3.183478000	-0.634512000
C	1.469785000	2.948515000	1.890244000	C	-0.859442000	3.515396000	1.659479000
C	1.553740000	3.637765000	0.651116000	C	-1.437124000	4.028943000	0.460972000
H	-1.164909000	2.365306000	-0.907665000	H	-1.723595000	1.199764000	-1.361002000
H	0.409445000	1.496833000	3.020792000	H	-0.156680000	1.784572000	2.658897000
H	0.629449000	3.982686000	-1.286391000	H	-2.182467000	3.579204000	-1.540064000
H	2.206841000	3.177833000	2.649348000	H	-0.647748000	4.216850000	2.456262000
O	2.575080000	4.468138000	0.538279000	O	-1.653611000	5.317659000	0.461126000
C	2.777507000	5.167921000	-0.689930000	C	-2.232106000	5.957001000	-0.685809000
H	2.914661000	4.459401000	-1.509147000	H	-1.582960000	5.830782000	-1.553116000
H	1.936938000	5.833876000	-0.894145000	H	-3.224836000	5.549329000	-0.880453000
H	3.683525000	5.749074000	-0.545584000	H	-2.303007000	7.007142000	-0.420517000
H	-1.432439000	1.373621000	1.352778000	H	-1.794664000	0.656633000	1.080456000
H	-1.178685000	-1.595884000	-0.352669000	H	0.149304000	-1.867520000	-0.389878000
TS₁₅₋₁₆ E(RM062X) = -4534.28154062 A.U. Frequency -1162.0287				16 E(RM062X) = -4534.36468716 A.U.			
C	0.613709000	-1.647326000	0.759526000	C	-0.630641000	-1.588651000	1.572816000
C	0.283431000	-0.619123000	-0.307846000	C	-0.085238000	-1.017685000	0.261412000
C	1.561853000	-0.405361000	-1.139206000	H	-0.649621000	0.967410000	1.006854000
H	1.785744000	-1.360174000	-1.619549000	C	0.243925000	-1.735531000	2.655797000
H	1.389734000	0.307682000	-1.947775000	H	1.295079000	-1.501652000	2.517198000
C	2.796976000	0.017328000	-0.302751000	C	-0.201630000	-2.189314000	3.886062000
C	2.544922000	-0.140308000	1.214943000	H	0.494706000	-2.296800000	4.708988000
C	1.775841000	-1.397050000	1.507040000	C	-1.548114000	-2.506492000	4.054501000
C	4.006319000	-0.841825000	-0.690338000	H	-1.912513000	-2.859571000	5.011919000
O	3.979924000	-1.825599000	-1.372446000	C	-2.421179000	-2.362827000	2.989385000
O	5.120593000	-0.360072000	-0.124861000	H	-3.472132000	-2.601704000	3.116922000

C	6.317342000	-1.093932000	-0.403067000	C	-1.980539000	-1.905630000	1.742644000
H	6.223717000	-2.116211000	-0.036437000	C	-2.991232000	-1.815861000	0.620250000
H	7.113379000	-0.568745000	0.117488000	H	-3.950348000	-1.477728000	1.015848000
H	6.503032000	-1.112767000	-1.476980000	H	-3.138693000	-2.817359000	0.198721000
C	3.142156000	1.474245000	-0.604712000	C	-2.551046000	-0.886966000	-0.517852000
O	2.958933000	2.403361000	0.131853000	C	-1.095867000	-1.194000000	-0.891806000
O	3.639427000	1.597073000	-1.841581000	H	-1.075498000	-2.233836000	-1.226250000
C	4.002863000	2.923657000	-2.234739000	H	-0.787233000	-0.586915000	-1.746128000
H	3.124868000	3.570443000	-2.238400000	C	-2.767825000	0.571650000	-0.126867000
H	4.743020000	3.328393000	-1.544489000	C	-3.438119000	-1.172456000	-1.729105000
H	4.416357000	2.831662000	-3.235133000	O	-3.228958000	0.955643000	0.910925000
H	1.981046000	0.738185000	1.542443000	O	-3.119061000	-1.829162000	-2.679735000
H	3.493416000	-0.117619000	1.752323000	O	-2.365905000	1.387941000	-1.110868000
C	2.173355000	-2.295709000	2.488963000	C	-2.558582000	2.785001000	-0.863833000
H	3.076647000	-2.098636000	3.056712000	H	-5.757921000	-1.939522000	-2.747808000
C	1.418918000	-3.437416000	2.745686000	O	-4.653256000	-0.633641000	-1.570558000
H	-0.821540000	-0.435317000	-2.169206000	C	-5.576517000	-0.870218000	-2.637517000
C	-0.131621000	-2.793087000	1.014319000	H	-5.177516000	-0.476135000	-3.572261000
H	-1.039968000	-2.998528000	0.463539000	H	-6.489019000	-0.351143000	-2.357759000
C	0.268046000	-3.682988000	2.009829000	H	-1.977578000	3.096718000	0.006276000
H	-0.327000000	-4.566757000	2.205295000	H	-2.212134000	3.295118000	-1.758057000
H	1.732458000	-4.131732000	3.516061000	H	-3.613459000	2.988756000	-0.678338000
C	-0.901448000	-1.001350000	-1.234793000	C	0.196266000	0.483048000	0.517602000
Ga	-3.026104000	-0.890421000	-0.843230000	H	0.380898000	0.974707000	-0.449351000
Cl	-3.626123000	1.248359000	-0.988629000	Ga	1.506558000	3.098401000	0.171605000
Cl	-3.469683000	-1.645585000	1.181402000	Cl	0.289765000	3.833870000	1.761266000
Cl	-3.821325000	-2.123921000	-2.458974000	Cl	3.476454000	2.370564000	0.563261000
C	-0.280899000	0.689813000	0.341754000	Cl	0.926333000	3.443776000	-1.859312000
C	-0.214920000	1.935663000	-0.334753000	H	1.060864000	0.576437000	1.182985000
C	-0.842987000	0.688119000	1.656478000	C	1.194713000	-1.746886000	-0.158357000
C	-0.758373000	3.081412000	0.198843000	C	1.242491000	-3.147643000	-0.091857000
C	-1.396675000	1.822229000	2.187099000	C	2.356753000	-3.852085000	-0.499394000
C	-1.369789000	3.026640000	1.460887000	H	0.389660000	-3.690582000	0.303719000
H	0.224616000	1.983527000	-1.324864000	C	2.309658000	-1.091379000	-0.660582000
H	-0.888841000	-0.245076000	2.206921000	H	2.331372000	-0.011875000	-0.741417000
H	-0.726842000	4.000406000	-0.368093000	C	3.449662000	-1.785741000	-1.076265000
H	-1.878096000	1.816446000	3.156363000	H	4.295263000	-1.226236000	-1.452724000
O	-1.956777000	4.065778000	2.049570000	C	3.475909000	-3.172247000	-0.993232000
C	-2.041496000	5.299082000	1.346586000	O	4.528801000	-3.947914000	-1.357261000
H	-1.045401000	5.710094000	1.164569000	C	5.682881000	-3.296582000	-1.845208000
H	-2.576767000	5.165967000	0.403421000	H	2.394752000	-4.932958000	-0.440346000
H	-2.600814000	5.967807000	1.994996000	H	5.463273000	-2.735703000	-2.759174000
H	-1.326115000	0.199000000	-0.278938000	H	6.101452000	-2.619541000	-1.093821000
H	-0.918118000	-2.066121000	-1.493495000	H	6.402320000	-4.081841000	-2.065989000
17 E(RM062X) = -4534.39507188 A.U.				TS ₁₁₋₁₈ E(RM062X) = -4534.29976843 A.U. Frequency -54.4734			
C	-1.859985000	-2.053112000	-0.514146000	C	-1.878185000	-0.627172000	-0.095112000

C	-1.423941000	-0.596184000	-0.536502000	C	-0.322873000	-0.289267000	-0.057180000
H	-0.099625000	-1.150130000	-2.169050000	H	-2.332345000	0.484599000	-0.069572000
C	-2.898741000	-2.454375000	-1.360786000	C	-2.583925000	-1.129687000	1.060086000
H	-3.425554000	-1.701067000	-1.936945000	H	-2.226669000	-0.842489000	2.041905000
C	-3.288646000	-3.783204000	-1.452337000	C	-3.721302000	-1.877862000	0.953073000
H	-4.096709000	-4.062712000	-2.119704000	H	-4.271070000	-2.214198000	1.822785000
C	-2.638061000	-4.741994000	-0.681908000	C	-4.205934000	-2.238342000	-0.321267000
H	-2.924223000	-5.785790000	-0.741867000	C	-3.543940000	-1.803658000	-1.491246000
C	-1.608071000	-4.353493000	0.163810000	H	-3.911593000	-2.069970000	-2.471955000
H	-1.103648000	-5.101219000	0.768081000	C	-2.408082000	-1.052759000	-1.365719000
C	-1.204550000	-3.019117000	0.252868000	H	-1.895719000	-0.738383000	-2.268179000
C	-0.096056000	-2.667588000	1.225812000	O	-2.604896000	1.976495000	0.098153000
H	0.619575000	-3.492634000	1.269715000	C	-1.618659000	2.687746000	0.213401000
H	-0.540070000	-2.576722000	2.221164000	C	-0.202422000	2.337055000	-0.213735000
C	0.614531000	-1.359709000	0.905224000	O	-1.692380000	3.884248000	0.752211000
C	-0.443833000	-0.282037000	0.632930000	C	-2.998273000	4.344649000	1.130018000
H	-1.023689000	-0.184226000	1.554217000	H	-3.430669000	3.669853000	1.867866000
H	0.023356000	0.689423000	0.470495000	H	-3.637703000	4.390587000	0.249239000
C	1.541540000	-1.409183000	-0.302871000	H	-2.845280000	5.333893000	1.550506000
C	1.507081000	-0.978498000	2.099365000	C	-0.066761000	0.968464000	-0.917130000
O	2.117074000	-0.419754000	-0.762651000	C	0.151118000	3.375688000	-1.283050000
O	2.688469000	-1.217229000	2.149583000	O	-0.665900000	3.830038000	-2.041865000
O	1.646529000	-2.561845000	-0.876295000	O	1.446575000	3.641993000	-1.323697000
C	2.609697000	-2.707616000	-1.936902000	H	-0.701653000	0.957861000	-1.808601000
H	0.826083000	0.274161000	4.963489000	C	1.879735000	4.492070000	-2.393488000
O	0.810086000	-0.465470000	3.081546000	H	1.408904000	5.471007000	-2.304850000
C	1.558184000	-0.112864000	4.260940000	H	1.615669000	4.045984000	-3.352053000
H	2.291625000	0.647136000	4.000423000	H	2.957788000	4.565344000	-2.285773000
H	2.062336000	-0.991117000	4.659338000	C	0.732845000	2.362920000	0.998144000
H	2.604536000	-3.766525000	-2.176414000	H	0.591750000	3.282314000	1.569369000
H	2.291572000	-2.112958000	-2.792657000	H	1.757449000	2.356394000	0.619259000
H	3.581465000	-2.383406000	-1.575175000	C	0.565458000	1.151732000	1.880472000
C	-0.778154000	-0.345339000	-1.920256000	H	0.969341000	0.920953000	-1.263066000
H	-1.559488000	-0.317042000	-2.679201000	C	0.986846000	1.252325000	3.210097000
Ga	2.836215000	1.493853000	-0.527652000	H	1.327025000	2.215062000	3.577351000
Cl	1.890698000	2.382739000	-2.253500000	C	1.020614000	0.146248000	4.042276000
Cl	2.168665000	2.283680000	1.387595000	H	1.370828000	0.243597000	5.062798000
Cl	4.950345000	1.087219000	-0.633610000	C	0.417136000	-1.474764000	-0.717092000
H	-0.245809000	0.607420000	-1.935013000	C	0.139072000	-0.086935000	1.386176000
C	-2.604096000	0.360564000	-0.286486000	C	0.201635000	-1.200465000	2.233894000
C	-3.477070000	0.099899000	0.781555000	C	0.636532000	-1.095465000	3.544038000
C	-4.513602000	0.950660000	1.101433000	H	-0.063796000	-2.179995000	1.850148000
H	-3.336385000	-0.800142000	1.370906000	H	0.008695000	-2.423082000	-0.350470000
C	-2.832919000	1.513899000	-1.024844000	H	0.226999000	-1.457601000	-1.795991000
H	-2.206143000	1.758846000	-1.872645000	H	0.701783000	-1.982868000	4.161400000
C	-3.879365000	2.390051000	-0.718302000	Ga	2.424798000	-1.633477000	-0.503871000

H	-4.025987000	3.274459000	-1.320814000	Cl	2.920082000	-3.035763000	1.152629000
C	-4.713710000	2.116485000	0.358831000	Cl	3.403186000	0.351428000	-0.113939000
O	-5.759862000	2.895497000	0.746415000	Cl	3.200534000	-2.422145000	-2.436298000
C	-6.082493000	4.019365000	-0.049137000	O	-5.301487000	-2.975189000	-0.329514000
H	-5.184767000	0.745590000	1.926022000	C	-5.863466000	-3.395190000	-1.573319000
H	-5.285490000	4.765221000	-0.048001000	H	-6.162268000	-2.529904000	-2.168161000
H	-6.298923000	3.721643000	-1.080921000	H	-5.151548000	-4.011694000	-2.125215000
H	-6.976543000	4.451226000	0.394994000	H	-6.737584000	-3.983982000	-1.311717000
18 E(RM062X) = -4534.31833723 A.U.				19 E(RM062X) = -4534.33017723 A.U.			
C	-1.644837000	-1.052743000	-0.408043000	C	-1.734549000	-0.735366000	-0.437120000
C	-0.207947000	-0.491684000	-0.137093000	C	-0.255662000	-0.576638000	-0.017982000
H	-2.482045000	0.552068000	-0.247080000	H	-0.754777000	3.549772000	-1.192569000
C	-2.540169000	-1.471640000	0.594159000	C	-2.719890000	-1.231861000	0.412508000
H	-2.271267000	-1.341894000	1.635767000	H	-2.477887000	-1.467922000	1.441141000
C	-3.778967000	-2.052582000	0.300547000	C	-4.033033000	-1.444193000	-0.014829000
H	-4.423222000	-2.354435000	1.117486000	H	-4.751609000	-1.850042000	0.685412000
C	-4.160993000	-2.244956000	-1.029694000	C	-4.394396000	-1.133723000	-1.321982000
C	-3.291022000	-1.833611000	-2.054951000	C	-3.428973000	-0.610395000	-2.186693000
O	-5.331260000	-2.798983000	-1.433787000	O	-5.638538000	-1.292004000	-1.841590000
H	-3.593003000	-1.988890000	-3.085220000	H	-3.717572000	-0.375528000	-3.204120000
C	-2.067779000	-1.264525000	-1.747260000	C	-2.128905000	-0.427019000	-1.749723000
C	-6.228411000	-3.287788000	-0.442956000	C	-6.621223000	-1.889780000	-1.021507000
H	-5.762565000	-4.069949000	0.167966000	H	-6.314536000	-2.891286000	-0.704708000
H	-7.073375000	-3.709532000	-0.987540000	H	-7.519768000	-1.959933000	-1.630206000
H	-6.584694000	-2.481367000	0.209835000	H	-6.829400000	-1.276225000	-0.138641000
H	-1.410202000	-0.992361000	-2.566185000	H	-1.402398000	-0.058348000	-2.466255000
O	-2.806334000	1.471346000	0.049216000	O	-1.968595000	2.977602000	-0.747373000
C	-1.876588000	2.320532000	0.263552000	C	-1.616165000	2.326298000	0.237202000
C	-0.409832000	2.161746000	-0.074110000	C	-0.159269000	2.018289000	0.503203000
O	-2.207765000	3.424133000	0.839469000	O	-2.444359000	1.829204000	1.097950000
C	-3.607416000	3.686577000	1.158621000	C	-3.846649000	1.904083000	0.755015000
H	-3.985234000	2.903629000	1.816172000	H	-3.996696000	1.424917000	-0.212622000
H	-4.181535000	3.724739000	0.232621000	H	-4.157153000	2.947562000	0.722853000
H	-3.597132000	4.652841000	1.656224000	H	-4.358110000	1.360027000	1.542227000
C	-0.045694000	0.878248000	-0.868495000	C	0.281966000	0.809567000	-0.397884000
C	-0.133801000	3.346354000	-1.025026000	C	0.699924000	3.081000000	-0.135922000
O	-0.990083000	3.775917000	-1.774810000	O	0.279762000	3.777570000	-1.105911000
O	1.124790000	3.757109000	-0.969344000	O	1.912373000	3.145252000	0.238092000
H	-0.586655000	0.870907000	-1.819073000	H	0.079087000	1.030527000	-1.447901000
C	1.522810000	4.746994000	-1.945875000	C	2.897923000	3.798478000	-0.614869000
H	1.335024000	4.372581000	-2.953490000	H	2.586490000	4.821889000	-0.811889000
H	2.587613000	4.896181000	-1.780176000	H	2.980940000	3.207599000	-1.527192000
H	0.965505000	5.672693000	-1.789155000	H	3.818042000	3.753128000	-0.042956000
C	0.423055000	2.171699000	1.226843000	C	0.205593000	1.713447000	1.958727000
H	0.162912000	3.033429000	1.848698000	H	-0.342771000	2.381367000	2.627478000
H	1.465466000	2.291919000	0.912762000	H	1.272758000	1.920334000	2.076585000

C	0.293339000	0.879557000	2.004105000	C	0.001334000	0.273914000	2.381870000
H	1.012961000	1.007409000	-1.107012000	H	1.360746000	0.801191000	-0.272892000
C	0.508222000	0.926076000	3.389398000	C	0.059626000	0.023229000	3.755270000
H	0.681758000	1.890076000	3.861454000	H	0.150404000	0.861002000	4.439864000
C	0.535840000	-0.232885000	4.155560000	C	0.036028000	-1.268595000	4.253094000
H	0.714128000	-0.176253000	5.225031000	H	0.093430000	-1.442298000	5.320769000
C	0.811616000	-1.466363000	-0.798792000	C	0.629517000	-1.556885000	-0.841286000
C	0.072518000	-0.359100000	1.370830000	C	-0.101184000	-0.793122000	1.486090000
C	0.133521000	-1.521367000	2.159138000	C	-0.113006000	-2.092917000	2.002716000
C	0.358370000	-1.467146000	3.530168000	C	-0.041698000	-2.336772000	3.364995000
H	0.018447000	-2.490160000	1.685785000	H	-0.186715000	-2.933468000	1.324167000
H	0.572534000	-2.497071000	-0.513887000	H	0.376184000	-2.590459000	-0.601778000
H	0.684041000	-1.431904000	-1.887438000	H	0.379661000	-1.433816000	-1.900910000
H	0.414028000	-2.387397000	4.102805000	H	-0.042412000	-3.356167000	3.731376000
Ga	2.789151000	-1.276293000	-0.486795000	Ga	2.629948000	-1.262420000	-0.759132000
Cl	3.492501000	-2.407851000	1.292120000	Cl	3.297251000	-0.256499000	1.151450000
Cl	3.470673000	0.876676000	-0.282841000	Cl	3.072873000	0.376110000	-2.302158000
Cl	3.775829000	-2.095103000	-2.306656000	Cl	3.829680000	-3.054670000	-1.177459000
$^{20}\text{E(RM062X)} = -4534.31827363 \text{ A.U.}$				$^{TS_{20-17}}\text{E(RM062X)} = -4534.31390376 \text{ A.U.}$ Frequency -757.4205			
C	0.227585000	-1.856194000	1.293181000	C	-0.411252000	-1.643409000	-1.494765000
C	0.485843000	-0.692865000	0.318384000	C	-0.672737000	-0.475857000	-0.536506000
H	-2.319558000	-1.451291000	1.756612000	H	1.290064000	0.426458000	-0.962021000
C	1.041969000	-1.964213000	2.427705000	C	-0.975185000	-1.585902000	-2.775169000
H	1.864743000	-1.267151000	2.543475000	H	-1.590780000	-0.730849000	-3.036072000
C	0.827834000	-2.939962000	3.385663000	C	-0.782375000	-2.598740000	-3.698913000
H	1.476764000	-2.995465000	4.251439000	H	-1.235396000	-2.528950000	-4.680524000
C	-0.222249000	-3.846066000	3.238927000	C	-0.000777000	-3.702059000	-3.360049000
H	-0.400109000	-4.608331000	3.987544000	H	0.164377000	-4.497900000	-4.076232000
C	-1.031429000	-3.766444000	2.118494000	C	0.569104000	-3.769435000	-2.100000000
H	-1.839873000	-4.478113000	1.980695000	H	1.182518000	-4.623114000	-1.829526000
C	-0.808656000	-2.787402000	1.137121000	C	0.366894000	-2.754760000	-1.156957000
C	-1.682416000	-2.789314000	-0.100706000	C	0.984739000	-2.912426000	0.213855000
H	-2.667026000	-3.214148000	0.117753000	H	1.888849000	-3.523834000	0.156948000
H	-1.229839000	-3.419988000	-0.873009000	H	0.290043000	-3.420952000	0.886353000
C	-1.813386000	-1.382983000	-0.706619000	C	1.293489000	-1.539542000	0.860273000
C	-0.393523000	-0.816408000	-0.948673000	C	-0.033075000	-0.743293000	0.855102000
H	0.050604000	-1.516060000	-1.659192000	H	-0.720029000	-1.360907000	1.436939000
H	-0.461197000	0.147889000	-1.453808000	H	0.079659000	0.199020000	1.395055000
C	-2.617759000	-0.470421000	0.175564000	C	2.421025000	-0.944320000	0.048715000
C	-2.551720000	-1.516992000	-2.046859000	C	1.732931000	-1.681569000	2.324526000
O	-2.857248000	-0.701911000	1.418950000	O	2.275470000	-0.156937000	-0.907516000
O	-2.016005000	-1.554509000	-3.111036000	O	2.646228000	-1.107839000	2.839200000
O	-3.082674000	0.571916000	-0.349114000	O	3.593262000	-1.410556000	0.301637000
C	-3.803203000	1.581033000	0.427424000	C	4.710149000	-0.821524000	-0.406806000
H	-4.331487000	-2.731003000	-3.576444000	H	0.389783000	-3.304173000	4.758497000

O	-3.864787000	-1.679478000	-1.845090000	O	0.902338000	-2.501679000	2.978740000
C	-4.654651000	-1.843182000	-3.033832000	C	1.148070000	-2.621372000	4.385965000
H	-4.545839000	-0.966798000	-3.672233000	H	1.060793000	-1.645427000	4.863143000
H	-5.679970000	-1.949503000	-2.691962000	H	2.147655000	-3.019652000	4.558572000
H	-3.695101000	2.485953000	-0.162339000	H	5.589536000	-1.280878000	0.031733000
H	-4.837003000	1.248648000	0.505055000	H	4.627183000	-1.046547000	-1.468619000
H	-3.326610000	1.699791000	1.396800000	H	4.697739000	0.255298000	-0.243002000
C	0.186171000	0.618768000	1.093209000	C	-0.092327000	0.833957000	-1.189109000
H	-0.735545000	0.491051000	1.670881000	H	0.141310000	0.667645000	-2.245719000
Ga	-0.029807000	2.501153000	0.365032000	Ga	0.994987000	2.497778000	-0.316855000
Cl	-1.358416000	3.434322000	1.932697000	Cl	-0.547813000	3.913349000	0.351510000
Cl	1.819521000	3.710514000	0.232025000	Cl	2.246035000	1.905623000	1.422293000
Cl	-1.147991000	2.685197000	-1.574635000	Cl	2.208462000	3.227233000	-1.989674000
H	0.945712000	0.740516000	1.874080000	H	-0.886867000	1.583882000	-1.244160000
C	1.945409000	-0.789250000	-0.146302000	C	-2.181688000	-0.342784000	-0.257914000
C	2.414786000	-2.006289000	-0.666997000	C	-3.052886000	-1.431114000	-0.399270000
C	3.713339000	-2.151989000	-1.108091000	C	-4.390076000	-1.332153000	-0.057108000
H	1.749915000	-2.864936000	-0.713107000	H	-2.688061000	-2.373549000	-0.791498000
C	2.838173000	0.268572000	-0.081087000	C	-2.704184000	0.832917000	0.272897000
H	2.538793000	1.228987000	0.313736000	H	-2.072144000	1.698273000	0.438559000
C	4.156561000	0.142925000	-0.529293000	C	-4.048711000	0.949917000	0.622013000
H	4.807333000	1.004613000	-0.467428000	H	-4.403484000	1.890835000	1.020534000
C	4.598329000	-1.068596000	-1.044628000	C	-4.902026000	-0.136129000	0.450199000
O	5.853426000	-1.303665000	-1.503491000	O	-6.226364000	-0.130821000	0.745419000
C	6.778139000	-0.235906000	-1.453960000	C	-6.784987000	1.073881000	1.229085000
H	4.075829000	-3.092638000	-1.504572000	H	-5.064861000	-2.170482000	-0.180016000
H	6.438927000	0.608757000	-2.061223000	H	-6.325896000	1.370440000	2.177275000
H	6.939671000	0.097956000	-0.424179000	H	-6.669965000	1.881645000	0.499775000
H	7.709391000	-0.624822000	-1.859522000	H	-7.842444000	0.874078000	1.386090000
²⁴ E(RM062X) = -4192.69725805 A.U.				^{TS₂₄₋₂₅} E(RM062X) = -4192.64283771 A.U. Frequency -359.3846			
C	-0.006734000	3.499520000	-1.348611000	C	0.024133000	2.346831000	-1.092868000
C	-0.946219000	0.652393000	-0.633597000	C	-0.783673000	0.953840000	-0.709998000
C	-2.010829000	1.001354000	-0.174943000	C	-2.101545000	0.990072000	-0.480990000
Ga	-2.492583000	-1.366636000	-0.281075000	Ga	-3.159905000	-0.611722000	0.218038000
Cl	-0.998956000	-2.424478000	0.875256000	Cl	-2.219448000	-1.209693000	2.125661000
Cl	-4.419703000	-1.057255000	0.661296000	Cl	-5.247186000	0.034955000	0.431851000
Cl	-2.492741000	-1.795516000	-2.406685000	Cl	-2.880288000	-2.169913000	-1.335569000
H	-2.895894000	1.452340000	0.218126000	H	-2.649790000	1.903743000	-0.705143000
C	0.330883000	0.200056000	-1.182969000	C	0.067850000	-0.302131000	-0.690316000
H	0.305355000	-0.893245000	-1.241573000	H	-0.277133000	-0.884756000	0.169801000
H	0.409892000	0.572512000	-2.209675000	H	-0.178796000	-0.889174000	-1.580793000
C	1.587340000	0.611467000	-0.364728000	C	1.582796000	-0.114491000	-0.607728000
C	1.931808000	2.118780000	-0.527194000	C	2.008922000	0.909998000	-1.689841000
C	0.800946000	3.086374000	-0.286660000	C	1.399601000	2.244136000	-1.401017000
H	2.298736000	2.259993000	-1.548126000	H	1.676250000	0.533817000	-2.664378000

H	2.767460000	2.332165000	0.144557000	H	3.096358000	0.995819000	-1.721514000
C	0.523649000	3.576849000	0.990591000	C	2.176723000	3.396597000	-1.321237000
H	1.165829000	3.296061000	1.818626000	H	3.240021000	3.325030000	-1.517042000
C	-0.568427000	4.408716000	1.210257000	C	1.610066000	4.618454000	-0.990503000
H	0.217793000	3.157187000	-2.354660000	H	-0.670139000	1.723105000	-1.854752000
C	-1.097045000	4.335467000	-1.136186000	C	-0.547240000	3.593683000	-0.747338000
H	-1.715273000	4.639322000	-1.972808000	H	-1.595452000	3.657362000	-0.487745000
C	-1.390188000	4.779999000	0.148708000	C	0.243798000	4.719857000	-0.706609000
H	-2.238805000	5.431706000	0.320060000	H	-0.188305000	5.673625000	-0.432250000
H	-0.773478000	4.776473000	2.208967000	H	2.235516000	5.501998000	-0.938461000
C	2.755672000	-0.216228000	-0.888313000	C	2.328498000	-1.416397000	-0.854294000
C	3.314525000	-0.210425000	-2.156493000	C	2.235220000	-2.273508000	-1.938745000
H	2.938382000	0.445952000	-2.935104000	H	1.532470000	-2.089536000	-2.745390000
C	4.379054000	-1.070353000	-2.425290000	C	3.054306000	-3.402023000	-1.972277000
H	4.826463000	-1.080606000	-3.411805000	H	2.986369000	-4.089804000	-2.806322000
C	4.871909000	-1.917927000	-1.434132000	C	3.951660000	-3.657820000	-0.936797000
H	5.700297000	-2.578787000	-1.659885000	H	4.577283000	-4.541477000	-0.977602000
C	4.310687000	-1.924499000	-0.160582000	C	4.043889000	-2.797494000	0.153679000
C	3.247562000	-1.068452000	0.104622000	C	3.223640000	-1.676055000	0.188924000
C	2.461052000	-0.858650000	1.326526000	C	3.071907000	-0.626251000	1.206208000
C	1.493221000	0.127549000	1.081626000	C	2.089119000	0.277991000	0.776731000
C	0.610348000	0.490303000	2.091053000	C	1.696278000	1.322149000	1.603362000
H	-0.158084000	1.233451000	1.926339000	H	0.904379000	2.007250000	1.322275000
C	0.708018000	-0.133970000	3.334386000	C	2.316201000	1.472101000	2.844249000
H	0.016579000	0.138153000	4.122824000	H	2.007775000	2.276295000	3.501133000
C	1.668711000	-1.114369000	3.568746000	C	3.312398000	0.589689000	3.253534000
H	1.721331000	-1.595286000	4.538223000	H	3.779127000	0.719955000	4.222676000
H	3.298768000	-2.253762000	2.738338000	H	4.450386000	-1.175048000	2.770617000
C	2.554476000	-1.485214000	2.562707000	C	3.694292000	-0.472411000	2.439001000
H	4.696042000	-2.587134000	0.606035000	H	4.735364000	-3.006671000	0.961895000
25 E(RM062X) = -4192.76127685 A.U.				TS ₂₅₋₂₆ E(RM062X) = -4539.42832131 A.U. Frequency -265.4581			
C	-0.793067000	2.171564000	-0.574866000	symmetry c1			
C	-0.620261000	0.914819000	-1.311989000	C	-0.403111000	-0.578303000	1.826123000
C	-1.643450000	0.246655000	-1.932496000	C	-0.363908000	0.053382000	0.452708000
Ga	-2.344172000	-1.236376000	-0.343675000	C	1.046946000	0.334469000	-0.077421000
Cl	-3.055512000	-0.065970000	1.352664000	H	1.029017000	0.345823000	-1.168646000
Cl	-3.980950000	-2.043547000	-1.538919000	H	1.394621000	1.318070000	0.244714000
Cl	-0.687667000	-2.611910000	-0.047704000	C	2.138793000	-0.643294000	0.411853000
H	-2.614978000	0.703364000	-2.082807000	C	2.138845000	-0.595169000	1.942928000
C	0.771660000	0.367863000	-1.461687000	C	0.775834000	-0.886271000	2.521627000
H	0.737733000	-0.718448000	-1.573023000	H	2.458430000	0.407935000	2.255318000
H	1.149432000	0.773691000	-2.411480000	H	2.870673000	-1.301935000	2.341579000
C	1.755775000	0.764520000	-0.346802000	C	0.684627000	-1.505621000	3.769568000
C	1.731777000	2.288743000	-0.217814000	H	1.599692000	-1.762421000	4.292977000
C	0.334367000	2.832728000	-0.045230000	C	-0.544339000	-1.809448000	4.336983000

H	2.168253000	2.725712000	-1.125174000	H	-0.824003000	-0.561656000	-1.541056000
H	2.356505000	2.603168000	0.621301000	C	-1.638372000	-0.904311000	2.398349000
C	0.150496000	4.025433000	0.651103000	H	-2.557597000	-0.677108000	1.870193000
H	1.016306000	4.530113000	1.065453000	C	-1.713476000	-1.508932000	3.643986000
C	-1.116273000	4.561168000	0.835562000	H	-2.681847000	-1.749595000	4.065150000
H	-1.387042000	-0.562533000	-2.612702000	H	-0.591278000	-2.290162000	5.306915000
C	-2.069744000	2.723038000	-0.373335000	C	-1.272257000	-0.625390000	-0.545605000
H	-2.948260000	2.212560000	-0.744993000	Ga	-3.239252000	-0.273245000	-0.986150000
C	-2.233921000	3.905201000	0.323486000	Cl	-3.276341000	0.995511000	-2.828272000
H	-3.226330000	4.309777000	0.477091000	Cl	-4.355041000	0.852920000	0.603201000
H	-1.235234000	5.485834000	1.388132000	Cl	-4.199991000	-2.224030000	-1.325380000
C	3.125457000	0.218295000	-0.712481000	C	-1.042876000	1.755374000	0.799959000
C	3.935532000	0.568713000	-1.780498000	C	-0.950131000	2.434504000	-0.458419000
H	3.645065000	1.352696000	-2.473388000	C	-0.295939000	2.321340000	1.895836000
C	5.144821000	-0.103760000	-1.956691000	C	-0.051840000	3.448966000	-0.672084000
H	5.793262000	0.161863000	-2.782921000	C	0.588400000	3.336392000	1.705757000
C	5.523685000	-1.117260000	-1.077977000	C	0.741664000	3.891722000	0.405840000
H	6.464581000	-1.632438000	-1.230719000	H	-1.576855000	2.102460000	-1.282518000
C	4.708336000	-1.472727000	-0.006451000	H	-0.420691000	1.883908000	2.881011000
C	3.506885000	-0.795588000	0.173034000	H	0.032405000	3.899703000	-1.650924000
C	2.470057000	-0.921298000	1.206908000	H	1.185954000	3.751252000	2.507787000
C	1.464882000	0.025409000	0.957473000	O	1.660880000	4.833877000	0.304986000
C	0.402078000	0.157629000	1.840145000	C	1.910696000	5.441681000	-0.964225000
H	-0.379204000	0.892836000	1.692851000	H	2.236500000	4.689796000	-1.685705000
C	0.331017000	-0.693633000	2.943731000	H	1.017059000	5.955291000	-1.323107000
H	-0.509321000	-0.609585000	3.622605000	H	2.705705000	6.160546000	-0.789720000
C	1.312138000	-1.655370000	3.167347000	H	-2.039825000	1.399656000	1.058950000
H	1.233169000	-2.315322000	4.022950000	H	-1.310558000	-1.685583000	-0.282686000
H	3.170116000	-2.509048000	2.484175000	C	2.028267000	-2.052733000	-0.165873000
C	2.397060000	-1.770681000	2.302834000	C	1.093832000	-3.051697000	0.078942000
H	5.009643000	-2.261092000	0.674032000	H	0.286830000	-2.910148000	0.787410000
				C	1.207831000	-4.267347000	-0.595771000
				H	0.475408000	-5.045333000	-0.416665000
				C	2.246336000	-4.490656000	-1.496676000
				H	2.313487000	-5.439653000	-2.015067000
				C	3.203649000	-3.507259000	-1.724396000
				C	3.090991000	-2.297125000	-1.050495000
				C	3.979350000	-1.126667000	-1.059234000
				C	3.456502000	-0.171719000	-0.180764000
				C	4.110689000	1.033802000	0.022989000
				H	3.713373000	1.779039000	0.706963000
				C	5.304364000	1.276233000	-0.657130000
				H	5.835156000	2.207620000	-0.499162000
				C	5.823590000	0.325150000	-1.534999000
				H	6.751273000	0.528856000	-2.056442000
				H	5.574404000	-1.620160000	-2.426517000

				C	5.165180000	-0.883532000	-1.744218000
				H	4.024979000	-3.686668000	-2.409115000
26 E(RM062X) = -4539.42982421 A.U.				TS₂₆₋₂₇ E(RM062X) = -4539.40103182 A.U. Frequency -1110.9457			
C	-0.159683000	-0.607988000	1.841302000	C	0.215466000	-1.496659000	0.904855000
C	-0.267467000	0.051408000	0.466596000	C	-0.062056000	-0.519401000	-0.223993000
C	1.105257000	0.563737000	-0.047118000	C	1.268289000	-0.256048000	-0.965710000
H	1.088309000	0.602133000	-1.139274000	H	1.476146000	-1.167780000	-1.531669000
H	1.262764000	1.592886000	0.299799000	H	1.138348000	0.534021000	-1.708183000
C	2.355306000	-0.208799000	0.421267000	C	2.494920000	0.066674000	-0.057280000
C	2.351280000	-0.184391000	1.952999000	C	2.076451000	0.065860000	1.437400000
C	1.058476000	-0.717375000	2.527345000	C	1.286127000	-1.169852000	1.753261000
H	2.495501000	0.853512000	2.281473000	H	1.478920000	0.964677000	1.631480000
H	3.195890000	-0.759571000	2.340444000	H	2.969568000	0.131695000	2.062400000
C	1.086221000	-1.356263000	3.770072000	C	1.624713000	-2.018127000	2.800220000
H	2.037357000	-1.455313000	4.283283000	H	2.466478000	-1.765973000	3.436321000
C	-0.065127000	-1.873597000	4.344595000	C	0.906688000	-3.191027000	3.017986000
H	-0.510077000	-0.715182000	-1.544833000	H	-1.057264000	-0.424313000	-2.153156000
C	-1.313274000	-1.143038000	2.425673000	C	-0.488388000	-2.678012000	1.118239000
H	-2.263301000	-1.076209000	1.907769000	H	-1.321243000	-2.951894000	0.484567000
C	-1.274347000	-1.766193000	3.664487000	C	-0.145278000	-3.520974000	2.174390000
H	-2.184287000	-2.174187000	4.087549000	H	-0.708204000	-4.432737000	2.332744000
H	-0.017484000	-2.367838000	5.307663000	H	1.175869000	-3.847318000	3.836989000
C	-0.938414000	-0.898300000	-0.553558000	C	-1.152553000	-0.994087000	-1.222122000
Ga	-2.923031000	-1.027631000	-0.960663000	Ga	-3.297448000	-1.034253000	-0.946516000
Cl	-3.272332000	0.079182000	-2.886223000	Cl	-4.041156000	1.041130000	-1.270361000
Cl	-4.243249000	0.033829000	0.550130000	Cl	-3.817555000	-1.662401000	1.105078000
Cl	-3.567052000	-3.125543000	-1.107753000	Cl	-3.909376000	-2.441729000	-2.498726000
C	-1.156851000	1.386526000	0.650064000	C	-0.753409000	0.776195000	0.330598000
C	-1.358120000	2.077294000	-0.621043000	C	-0.788320000	1.968388000	-0.442573000
C	-0.742959000	2.248021000	1.760701000	C	-1.348622000	0.826061000	1.630539000
C	-1.187268000	3.419147000	-0.773798000	C	-1.440531000	3.100381000	-0.009311000
C	-0.577794000	3.583764000	1.624531000	C	-2.008173000	1.945621000	2.062291000
C	-0.791314000	4.186348000	0.349836000	C	-2.070666000	3.089653000	1.244845000
H	-1.674300000	1.488429000	-1.479520000	H	-0.344743000	1.974471000	-1.431845000
H	-0.583382000	1.773896000	2.724546000	H	-1.331698000	-0.062921000	2.251053000
H	-1.358474000	3.883653000	-1.734740000	H	-1.491486000	3.965551000	-0.654769000
H	-0.290037000	4.228566000	2.445084000	H	-2.512451000	1.971009000	3.019630000
O	-0.595822000	5.479165000	0.309997000	O	-2.760044000	4.113960000	1.738731000
C	-0.783129000	6.202927000	-0.914058000	C	-2.951440000	5.269334000	0.930421000
H	-0.092966000	5.837584000	-1.675520000	H	-1.995615000	5.752872000	0.714384000
H	-1.816259000	6.110258000	-1.251239000	H	-3.463466000	5.004813000	0.002259000
H	-0.559769000	7.237061000	-0.670998000	H	-3.574918000	5.937105000	1.518278000
H	-2.159433000	0.982524000	0.927426000	H	-1.725345000	0.193705000	-0.305870000
H	-0.656973000	-1.922153000	-0.304971000	H	-1.066628000	-2.056763000	-1.474292000
C	2.507067000	-1.613996000	-0.161373000	C	3.175724000	1.386672000	-0.384088000

C	1.801033000	-2.780440000	0.108358000	C	2.652284000	2.669182000	-0.325652000
H	0.995697000	-2.799363000	0.831860000	H	1.622630000	2.839423000	-0.027562000
C	2.146785000	-3.954748000	-0.560157000	C	3.474929000	3.751751000	-0.638702000
H	1.591831000	-4.863110000	-0.358431000	H	3.077911000	4.759213000	-0.597981000
C	3.192505000	-3.973457000	-1.480310000	C	4.807148000	3.549838000	-0.994708000
H	3.440765000	-4.894486000	-1.993980000	H	5.433072000	4.401381000	-1.233856000
C	3.930393000	-2.820849000	-1.727106000	C	5.341611000	2.264975000	-1.036761000
C	3.588229000	-1.652597000	-1.056355000	H	6.381604000	2.111161000	-1.301931000
C	4.244474000	-0.338848000	-1.063949000	C	4.519078000	1.187264000	-0.727708000
C	3.566274000	0.497182000	-0.170614000	C	4.803374000	-0.254034000	-0.669551000
C	3.998548000	1.797807000	0.040154000	C	3.631804000	-0.921986000	-0.290036000
H	3.482109000	2.454524000	0.734112000	H	2.712353000	-2.837275000	0.095512000
C	5.122369000	2.256462000	-0.647502000	C	3.617380000	-2.305940000	-0.181842000
H	5.479032000	3.266782000	-0.485462000	C	4.792724000	-3.011705000	-0.440246000
C	5.794414000	1.423015000	-1.540447000	H	4.796563000	-4.092119000	-0.358077000
H	6.665144000	1.794440000	-2.067736000	H	6.861631000	-2.910667000	-1.008724000
H	5.889088000	-0.528417000	-2.447939000	C	5.960117000	-2.344085000	-0.807937000
C	5.360975000	0.117914000	-1.755906000	C	5.974061000	-0.957589000	-0.928976000
H	4.765430000	-2.838179000	-2.418532000	H	6.879960000	-0.440130000	-1.224504000
27 E(RM062X) = -4539.47657066 A.U.				28 E(RM062X) = -4539.51205588 A.U.			
C	0.712457000	2.027241000	1.672752000	C	-1.561724000	2.113739000	-0.008270000
C	-0.118339000	1.129066000	0.753857000	C	-1.434748000	1.225242000	-1.250995000
H	-0.036343000	-0.534615000	2.183413000	H	-0.993237000	2.995823000	-2.460176000
C	0.249865000	3.259369000	2.137442000	C	-0.448191000	2.724671000	0.570726000
H	-0.725220000	3.617220000	1.827548000	H	0.544550000	2.521775000	0.184122000
C	1.027695000	4.041037000	2.985280000	C	-0.588651000	3.587304000	1.653192000
H	0.651070000	4.995787000	3.333138000	H	0.290367000	4.044484000	2.091724000
C	2.287189000	3.601101000	3.374976000	C	-1.850925000	3.851548000	2.170604000
H	2.904477000	4.211760000	4.023425000	H	-1.967262000	4.515386000	3.018935000
C	2.750851000	2.369593000	2.928394000	C	-2.964304000	3.245369000	1.600719000
H	3.731328000	2.016514000	3.230683000	H	-3.951209000	3.425647000	2.014297000
C	1.971203000	1.570424000	2.093445000	C	-2.834255000	2.385104000	0.512853000
C	2.452793000	0.211662000	1.661144000	C	-4.032978000	1.669115000	-0.049353000
H	1.963079000	-0.558848000	2.263715000	H	-4.352481000	2.117654000	-0.997316000
H	3.523452000	0.108513000	1.852789000	H	-4.877596000	1.743846000	0.639787000
C	2.183047000	-0.073462000	0.161827000	C	-3.695128000	0.187166000	-0.297894000
C	0.806977000	0.484012000	-0.314989000	C	-2.505764000	0.079752000	-1.286599000
H	1.002343000	1.238686000	-1.075693000	H	-2.032019000	-0.891559000	-1.137640000
H	0.243759000	-0.307790000	-0.816163000	H	-2.915541000	0.060602000	-2.299728000
C	-0.769322000	0.036376000	1.617262000	C	-1.685347000	2.151102000	-2.458698000
H	-1.296551000	-0.664873000	0.953936000	H	-2.696722000	2.557345000	-2.406168000
Ga	-2.526096000	-2.619132000	0.220678000	Ga	5.073307000	-0.322106000	0.255375000
Cl	-1.666750000	-3.916060000	1.683676000	Cl	4.584067000	-1.765819000	1.808777000
Cl	-4.401078000	-1.694445000	0.660236000	Cl	6.978174000	-0.627206000	-0.726986000
Cl	-1.644848000	-2.408185000	-1.703596000	Cl	4.362934000	1.699923000	0.515516000
H	-1.492518000	0.453764000	2.320370000	H	-1.589177000	1.603829000	-3.400493000

C	-1.185543000	1.918627000	-0.009358000	C	-0.039641000	0.599679000	-1.308396000
C	-0.797452000	3.001368000	-0.816802000	C	0.326259000	-0.315325000	-0.312577000
C	-1.712758000	3.722735000	-1.554161000	C	1.595287000	-0.868888000	-0.266158000
H	0.247836000	3.292750000	-0.853222000	H	-0.391580000	-0.584061000	0.455203000
C	-2.537834000	1.607682000	0.022721000	C	0.905586000	0.932134000	-2.276030000
H	-2.909345000	0.800088000	0.639191000	H	0.668416000	1.641103000	-3.057677000
C	-3.482745000	2.320299000	-0.723515000	C	2.186608000	0.381480000	-2.252077000
H	-4.522521000	2.027605000	-0.665012000	H	2.935230000	0.655683000	-2.985443000
C	-3.070192000	3.381010000	-1.518247000	C	2.507018000	-0.502655000	-1.244982000
O	-3.893804000	4.141169000	-2.283799000	O	3.823761000	-1.006955000	-1.196821000
C	-5.268147000	3.815940000	-2.286231000	C	3.955555000	-2.390503000	-1.602553000
H	-1.408016000	4.558697000	-2.171917000	H	1.885897000	-1.548170000	0.527373000
H	-5.431396000	2.796396000	-2.649479000	H	3.440641000	-3.028016000	-0.883518000
H	-5.701299000	3.921111000	-1.286486000	H	3.526756000	-2.490976000	-2.598683000
H	-5.743829000	4.522245000	-2.962875000	H	5.021999000	-2.608587000	-1.616937000
C	3.314236000	0.505320000	-0.678467000	C	-3.461534000	-0.571669000	1.012312000
C	3.686647000	1.833446000	-0.823702000	C	-2.525160000	-0.361664000	2.019980000
H	3.146984000	2.621368000	-0.306293000	H	-1.819349000	0.459250000	1.975409000
C	4.771810000	2.140608000	-1.645075000	C	-2.505252000	-1.220286000	3.120717000
H	5.077629000	3.172916000	-1.767506000	H	-1.775713000	-1.059794000	3.905892000
C	5.466705000	1.132316000	-2.312321000	C	-3.412162000	-2.271807000	3.225625000
H	6.305122000	1.390827000	-2.948309000	H	-3.380837000	-2.926435000	4.088548000
C	5.092161000	-0.201037000	-2.169933000	C	-4.364225000	-2.477987000	2.232057000
C	4.012917000	-0.507386000	-1.348275000	C	-4.382959000	-1.625139000	1.134813000
C	3.393557000	-1.798439000	-1.009225000	C	-5.280729000	-1.607873000	-0.028036000
C	2.332919000	-1.558062000	-0.127460000	C	-4.894560000	-0.555450000	-0.863120000
C	1.570506000	-2.608663000	0.356475000	C	-5.584633000	-0.299223000	-2.037911000
H	0.753764000	-2.434095000	1.050010000	H	-5.288479000	0.514803000	-2.692990000
C	1.866043000	-3.907633000	-0.055700000	C	-6.672283000	-1.105132000	-2.371284000
H	1.271071000	-4.735644000	0.312201000	H	-7.223766000	-0.914515000	-3.284253000
C	2.920489000	-4.145435000	-0.936701000	C	-7.055715000	-2.156360000	-1.538785000
H	3.138777000	-5.159847000	-1.248948000	H	-7.902425000	-2.774474000	-1.813103000
H	4.513834000	-3.283192000	-2.103225000	H	-6.664468000	-3.235525000	0.283963000
C	3.694745000	-3.092982000	-1.418533000	C	-6.362436000	-2.417407000	-0.360399000
H	5.632541000	-0.982687000	-2.692570000	H	-5.080620000	-3.287668000	2.315734000
32 E(RB3LYP) = -1885.85585605 A.U.				TS₃₂₋₃₃ E(RB3LYP) = -1885.82893765 A.U. Frequency -344.2658			
C	1.827989000	1.756604000	-0.789245000	C	2.380492000	1.775455000	-0.588825000
C	2.439978000	2.995672000	-1.012910000	C	2.957961000	3.050065000	-0.681446000
C	0.423763000	1.674926000	-0.995129000	C	0.967856000	1.634522000	-0.624469000
C	1.712193000	4.102558000	-1.435794000	C	2.140796000	4.155251000	-0.840013000
H	3.511633000	3.075749000	-0.875153000	H	4.035465000	3.162769000	-0.664936000
C	-0.309096000	2.803948000	-1.425053000	C	0.146043000	2.772498000	-0.820122000
C	0.334394000	4.007176000	-1.650340000	C	0.739768000	4.014083000	-0.907522000
H	2.222333000	5.043812000	-1.607227000	H	2.581908000	5.141477000	-0.928386000
H	-1.381451000	2.712474000	-1.548014000	H	-0.929761000	2.656100000	-0.862267000

H	-0.231491000	4.869725000	-1.980671000	H	0.118764000	4.894097000	-1.026732000
C	-0.296554000	0.482653000	-0.727975000	C	0.464693000	0.319062000	-0.523023000
C	-0.828976000	-0.669150000	-0.723997000	C	-0.630989000	-0.420044000	-0.533602000
Cl	-0.352703000	-0.594885000	2.480494000	Cl	-0.932929000	-0.765761000	2.619941000
Cl	-3.564061000	0.995463000	-0.506372000	Cl	-3.306560000	1.296533000	-0.846583000
C	-0.903332000	-1.963273000	-1.415578000	C	-0.862673000	-1.568812000	-1.462327000
O	-0.180618000	-2.236104000	-2.344894000	O	-0.217709000	-1.725138000	-2.478887000
O	-1.839473000	-2.752599000	-0.896409000	O	-1.867300000	-2.350551000	-1.077753000
C	-1.999191000	-4.043398000	-1.524019000	C	-2.238902000	-3.407763000	-1.985221000
H	-2.797378000	-4.530550000	-0.970530000	H	-3.084893000	-3.901068000	-1.513846000
H	-2.273132000	-3.919294000	-2.571982000	H	-2.523572000	-2.988694000	-2.950765000
H	-1.072716000	-4.613528000	-1.451282000	H	-1.410404000	-4.104429000	-2.118815000
Pt	-1.819799000	0.159629000	0.829701000	Pt	-1.963917000	0.185509000	0.740892000
C	2.647100000	0.594608000	-0.368642000	C	3.060208000	0.511397000	-0.436329000
C	2.608008000	-0.608991000	-1.082846000	C	2.303473000	-0.630645000	-0.848497000
C	3.502840000	0.709455000	0.733841000	C	4.251484000	0.352960000	0.276939000
H	1.970178000	-0.702896000	-1.954415000	H	1.786688000	-0.599378000	-1.814414000
H	3.519322000	1.632999000	1.302834000	H	4.799810000	1.228463000	0.605435000
C	4.295966000	-0.363590000	1.141621000	C	4.671654000	-0.911606000	0.667905000
C	4.240229000	-1.550917000	0.405520000	C	3.868540000	-2.027185000	0.343124000
H	4.859703000	-2.389873000	0.710333000	H	4.194921000	-3.010406000	0.667806000
C	3.409784000	-1.690048000	-0.709439000	C	2.700466000	-1.928305000	-0.389920000
C	3.401185000	-2.967234000	-1.515117000	C	1.908203000	-3.159859000	-0.716450000
H	3.531702000	-3.841494000	-0.872300000	H	0.980296000	-3.173302000	-0.132994000
H	2.466066000	-3.080421000	-2.066413000	H	1.625738000	-3.191536000	-1.770143000
H	4.219231000	-2.973319000	-2.243864000	H	2.470414000	-4.060755000	-0.466852000
C	5.160617000	-0.259294000	2.374722000	C	5.926561000	-1.105098000	1.475359000
H	5.459051000	0.773613000	2.567639000	H	6.455953000	-0.163855000	1.629395000
H	4.619537000	-0.615244000	3.257927000	H	5.696137000	-1.531066000	2.456763000
H	6.066072000	-0.863265000	2.279051000	H	6.605645000	-1.801640000	0.973859000
33 E(RB3LYP) = -1885.85805878 A.U.				TS₃₃₋₃₄ E(RB3LYP) = -1885.83153455 A.U. Frequency -1007.2100			
C	2.412096000	1.822767000	-0.384223000	C	2.401345000	1.855874000	-0.355964000
C	2.905311000	3.141940000	-0.497364000	C	2.897830000	3.155979000	-0.506547000
C	1.017274000	1.564498000	-0.190284000	C	1.009561000	1.614822000	-0.335191000
C	2.014998000	4.187143000	-0.417604000	C	1.997893000	4.204993000	-0.623709000
H	3.962840000	3.324018000	-0.649158000	H	3.965374000	3.341834000	-0.533343000
C	0.127889000	2.655061000	-0.133987000	C	0.110683000	2.675442000	-0.486540000
C	0.632975000	3.935875000	-0.234373000	C	0.615698000	3.963113000	-0.613601000
H	2.364552000	5.209655000	-0.498142000	H	2.363277000	5.219852000	-0.730449000
H	-0.932386000	2.479838000	-0.006734000	H	-0.956171000	2.498596000	-0.495042000
H	-0.049062000	4.776505000	-0.173517000	H	-0.073080000	4.794399000	-0.708689000
C	0.765138000	0.140909000	-0.208969000	C	0.753113000	0.166443000	-0.276157000
C	-0.449350000	-0.491417000	-0.304937000	C	-0.477481000	-0.497832000	-0.300046000
Cl	-1.598909000	-0.189996000	2.623057000	Cl	-1.506607000	-0.094427000	2.699833000
Cl	-3.046663000	0.883134000	-1.684105000	Cl	-3.174518000	0.788014000	-1.532987000

C	-0.550102000	-1.814536000	-1.020175000	C	-0.595109000	-1.772212000	-1.101261000
O	0.235596000	-2.165014000	-1.880877000	O	0.149445000	-1.997348000	-2.035262000
O	-1.603671000	-2.539923000	-0.651062000	O	-1.589024000	-2.559274000	-0.719551000
C	-1.848183000	-3.747501000	-1.398507000	C	-1.847436000	-3.718919000	-1.541554000
H	-2.754329000	-4.167333000	-0.969375000	H	-2.707981000	-4.201055000	-1.085839000
H	-1.993496000	-3.511157000	-2.452955000	H	-2.072104000	-3.406919000	-2.561495000
H	-1.013159000	-4.441701000	-1.292551000	H	-0.984220000	-4.385261000	-1.541620000
Pt	-2.100199000	0.225134000	0.362694000	Pt	-2.058393000	0.210572000	0.447975000
C	3.116123000	0.597405000	-0.387982000	C	3.106852000	0.602517000	-0.217040000
C	2.137601000	-0.528030000	-0.373765000	C	2.169004000	-0.478084000	-0.158712000
C	4.486699000	0.355994000	-0.276988000	C	4.465368000	0.363070000	-0.033270000
H	2.092006000	-0.914745000	-1.417627000	H	1.430507000	-0.430772000	-1.242992000
H	5.199511000	1.163263000	-0.401575000	H	5.170549000	1.185395000	-0.076925000
C	4.921697000	-0.887571000	0.152220000	C	4.910561000	-0.922219000	0.263744000
C	3.966883000	-1.880627000	0.543298000	C	3.960560000	-1.949109000	0.429992000
H	4.341882000	-2.779854000	1.021601000	H	4.309860000	-2.927798000	0.743388000
C	2.619004000	-1.735007000	0.389027000	C	2.594872000	-1.778490000	0.246001000
C	1.671029000	-2.774605000	0.882886000	C	1.661078000	-2.916758000	0.533330000
H	0.825949000	-2.311318000	1.405755000	H	0.765179000	-2.569456000	1.058966000
H	1.259429000	-3.355828000	0.053108000	H	1.340191000	-3.417077000	-0.383887000
H	2.177443000	-3.462013000	1.561903000	H	2.156838000	-3.656349000	1.163319000
C	6.381921000	-1.187105000	0.318481000	C	6.376325000	-1.218438000	0.443292000
H	7.003701000	-0.316447000	0.108234000	H	6.552403000	-1.821429000	1.338092000
H	6.595236000	-1.534807000	1.334132000	H	6.762631000	-1.785655000	-0.410394000
H	6.680721000	-1.993504000	-0.360428000	H	6.962852000	-0.302026000	0.526364000
34 E(RB3LYP) = -1885.88212072 A.U.				TS₃₄₋₃₅ E(RB3LYP) = -1885.84345257 A.U. Frequency -647.4593			
C	-2.092826000	1.764608000	0.218115000	C	-3.111234000	0.670446000	0.029982000
C	-2.693021000	2.894209000	-0.335014000	C	-2.232655000	-0.433888000	-0.125248000
C	-0.859934000	1.887557000	0.885797000	C	-2.767704000	-1.711266000	-0.344421000
C	-2.051692000	4.126768000	-0.215188000	C	-4.165239000	-1.844350000	-0.246342000
H	-3.645479000	2.820904000	-0.847711000	C	-5.026214000	-0.781934000	0.015700000
C	-0.215982000	3.110449000	1.003424000	C	-4.479142000	0.506253000	0.121052000
C	-0.830365000	4.237772000	0.452508000	H	-4.590591000	-2.829393000	-0.408676000
H	-2.508564000	5.011406000	-0.644229000	H	-5.130176000	1.364998000	0.244036000
H	0.732877000	3.192159000	1.518995000	C	-2.343000000	1.918031000	-0.047812000
H	-0.349595000	5.205145000	0.538950000	C	-2.771984000	3.237565000	-0.049680000
C	-0.430171000	0.509801000	1.418139000	C	-0.981549000	1.605315000	-0.220051000
C	0.879344000	0.138880000	0.785073000	C	-1.828011000	4.249403000	-0.248659000
Cl	1.249886000	-2.746093000	-0.884458000	H	-3.818028000	3.484968000	0.088649000
Cl	1.055306000	1.527031000	-2.168551000	C	-0.047942000	2.611029000	-0.434855000
C	2.125547000	0.395517000	1.611060000	C	-0.484837000	3.938279000	-0.451229000
O	2.147241000	1.273386000	2.443318000	H	-2.146958000	5.285477000	-0.257707000
O	3.128855000	-0.422781000	1.324689000	H	0.995265000	2.374119000	-0.598955000
C	4.349281000	-0.229296000	2.076314000	H	0.233024000	4.730723000	-0.625121000
H	5.020472000	-1.010093000	1.729975000	C	-0.829814000	0.116110000	-0.102240000

H	4.760381000	0.758634000	1.868137000	C	0.410877000	-0.557308000	0.083003000
H	4.152284000	-0.328239000	3.144102000	Pt	2.163724000	0.236572000	0.026269000
Pt	1.085902000	-0.434559000	-0.953680000	Cl	2.754553000	-0.124682000	-2.201043000
C	-2.552914000	0.376282000	0.307626000	Cl	1.985802000	0.912113000	2.274679000
C	-1.607646000	-0.372143000	1.027322000	H	-0.281444000	-0.028379000	1.096299000
C	-3.731371000	-0.216831000	-0.139476000	C	0.496010000	-2.004231000	0.542869000
H	-0.283390000	0.552330000	2.502970000	O	0.017572000	-2.374132000	1.587284000
H	-4.463520000	0.358442000	-0.696194000	O	1.197042000	-2.750212000	-0.302262000
C	-3.971196000	-1.562828000	0.146356000	C	1.500195000	-4.096749000	0.123906000
C	-3.029637000	-2.276266000	0.902516000	H	2.036592000	-4.073171000	1.072568000
H	-3.237695000	-3.312598000	1.151108000	H	0.584077000	-4.677848000	0.234542000
C	-1.835257000	-1.707118000	1.359052000	H	2.125166000	-4.507275000	-0.664503000
C	-0.865301000	-2.499801000	2.197998000	C	-1.989688000	-2.933818000	-0.754822000
H	0.059579000	-2.704283000	1.650777000	H	-1.116977000	-2.686145000	-1.359188000
H	-0.603227000	-1.962392000	3.115770000	H	-1.656670000	-3.501554000	0.117594000
H	-1.293586000	-3.460794000	2.487536000	H	-2.627432000	-3.588442000	-1.351413000
C	-5.220882000	-2.247131000	-0.353046000	C	-6.511386000	-0.996741000	0.150398000
H	-6.020924000	-1.528174000	-0.542132000	H	-6.808599000	-1.983062000	-0.209564000
H	-5.025092000	-2.776816000	-1.291571000	H	-6.816936000	-0.918295000	1.199180000
H	-5.587746000	-2.983375000	0.366166000	H	-7.073796000	-0.243761000	-0.408019000
35 E(RB3LYP) = -1885.89217763 A.U.				TS₃₃₋₃₆ E(RB3LYP) = -1885.84704203 A.U. Frequency -1177.2662			
C	2.677571000	-1.139072000	0.613437000	C	2.336061000	1.878548000	-0.350050000
C	3.656175000	-2.095181000	0.837312000	C	2.793781000	3.177981000	-0.599779000
C	1.319892000	-1.435666000	0.812589000	C	0.977081000	1.639735000	-0.007290000
C	3.261511000	-3.369598000	1.259090000	C	1.897906000	4.231667000	-0.494483000
H	4.706811000	-1.867094000	0.699764000	H	3.826453000	3.359850000	-0.875175000
C	0.931707000	-2.702623000	1.241998000	C	0.080047000	2.710508000	0.071661000
C	1.913765000	-3.669191000	1.460673000	C	0.554920000	3.995641000	-0.154850000
H	4.011785000	-4.132300000	1.433942000	H	2.233209000	5.246040000	-0.676915000
H	-0.110405000	-2.964402000	1.374153000	H	-0.959310000	2.531348000	0.315113000
H	1.624433000	-4.663176000	1.779729000	H	-0.126789000	4.834223000	-0.071417000
C	0.521042000	-0.206229000	0.596313000	C	0.748514000	0.199753000	0.039719000
C	-0.857890000	-0.220804000	1.063091000	C	-0.423277000	-0.469411000	-0.188702000
Cl	-0.426707000	-2.346845000	-1.781145000	Cl	-1.822643000	-0.471480000	2.616419000
Cl	-3.004612000	1.295653000	-0.803386000	Cl	-2.917459000	0.874142000	-1.730152000
C	-1.454190000	0.864327000	1.927712000	C	-0.322689000	-1.675275000	-1.048049000
O	-0.907159000	1.887816000	2.257099000	O	0.728246000	-1.973923000	-1.660965000
O	-2.643096000	0.458710000	2.393366000	O	-1.416004000	-2.375002000	-1.205789000
C	-3.358315000	1.400482000	3.215762000	C	-1.400882000	-3.450018000	-2.174937000
H	-4.272469000	0.889933000	3.508410000	H	-2.409545000	-3.852491000	-2.156449000
H	-2.766115000	1.670004000	4.090991000	H	-1.158481000	-3.053636000	-3.160499000
H	-3.589032000	2.295839000	2.637362000	H	-0.672214000	-4.207407000	-1.886418000
Pt	-1.426518000	-0.423800000	-0.908137000	Pt	-2.171775000	0.115597000	0.364924000
C	2.776234000	0.268401000	0.211873000	C	3.055954000	0.626375000	-0.330199000
C	1.468439000	0.850315000	0.194260000	C	2.112870000	-0.451042000	-0.091305000

C	3.909781000	0.977905000	-0.104426000	C	4.426019000	0.402492000	-0.292619000
H	-1.135981000	-1.177051000	1.500312000	H	1.703672000	-1.142658000	-1.103987000
H	4.885660000	0.505480000	-0.068277000	H	5.121885000	1.203234000	-0.516904000
C	3.793240000	2.328693000	-0.485934000	C	4.907708000	-0.822586000	0.171500000
C	2.523817000	2.890097000	-0.538038000	C	3.996956000	-1.780903000	0.670910000
H	2.428352000	3.923587000	-0.852613000	H	4.393960000	-2.675248000	1.140181000
C	1.338975000	2.200016000	-0.212880000	C	2.625304000	-1.616056000	0.623379000
C	0.059359000	2.962546000	-0.357869000	C	1.714380000	-2.652670000	1.209147000
H	-0.723021000	2.372939000	-0.834938000	H	0.830009000	-2.196741000	1.664974000
H	-0.324450000	3.256827000	0.619918000	H	1.368230000	-3.352827000	0.442823000
H	0.224054000	3.861148000	-0.954292000	H	2.244228000	-3.232910000	1.966208000
C	5.019723000	3.127864000	-0.834574000	C	6.383622000	-1.104828000	0.220007000
H	5.696943000	3.194107000	0.023084000	H	6.657219000	-1.819316000	-0.564347000
H	5.576940000	2.652671000	-1.648000000	H	6.973139000	-0.199865000	0.066386000
H	4.764319000	4.142230000	-1.143880000	H	6.670948000	-1.551511000	1.175505000
36 E(RB3LYP) = -1885.87656603 A.U.				TS₃₆₋₃₇ E(RB3LYP) = -1885.87582224 A.U. Frequency -40.1865			
O	0.430822000	-2.238608000	-1.669870000	O	0.144749000	-2.292277000	-1.447171000
C	-0.484415000	-1.782365000	-0.832174000	C	-0.479503000	-1.852004000	-0.379643000
C	-0.407049000	-0.518151000	-0.176455000	C	-0.355840000	-0.484403000	0.061526000
C	0.800122000	0.157664000	-0.083268000	C	0.839116000	0.176296000	0.130780000
C	0.985942000	1.612731000	-0.215045000	C	1.025961000	1.639474000	0.001213000
C	2.364169000	1.874704000	-0.402343000	C	2.391296000	1.893904000	-0.256120000
C	3.101926000	0.618467000	-0.237852000	C	3.129122000	0.631939000	-0.151649000
C	2.162337000	-0.423479000	0.013073000	C	2.212387000	-0.406080000	0.172241000
C	4.463041000	0.393315000	-0.186618000	C	4.490828000	0.402211000	-0.231401000
C	4.939810000	-0.878103000	0.178605000	C	4.994972000	-0.873682000	0.062179000
C	4.016274000	-1.856687000	0.545892000	C	4.101577000	-1.856148000	0.488390000
C	2.624769000	-1.661781000	0.503100000	C	2.713160000	-1.654454000	0.577997000
C	2.813954000	3.157941000	-0.678057000	C	2.839695000	3.182191000	-0.519633000
C	1.879061000	4.195377000	-0.754653000	C	1.917071000	4.230883000	-0.503379000
C	0.518991000	3.942004000	-0.571103000	C	0.570390000	3.986122000	-0.229973000
C	0.059608000	2.650258000	-0.309843000	C	0.112932000	2.690524000	0.016548000
C	1.737732000	-2.751040000	1.053737000	C	1.883136000	-2.759945000	1.184778000
C	6.420464000	-1.155358000	0.211868000	C	6.471804000	-1.158161000	-0.045170000
Pt	-2.124272000	0.215595000	0.392297000	Pt	-2.174722000	0.248004000	0.110563000
Cl	-1.579553000	0.164353000	2.672054000	Cl	-2.234040000	0.715444000	2.394492000
O	-1.536198000	-2.525145000	-0.717968000	O	-1.261016000	-2.696681000	0.197487000
C	-1.764646000	-3.630567000	-1.631636000	C	-1.655079000	-3.921122000	-0.488759000
Cl	-3.005542000	0.396675000	-1.791240000	Cl	-2.493074000	-0.124000000	-2.213701000
H	3.867537000	3.359779000	-0.835528000	H	3.885198000	3.377322000	-0.730643000
H	2.214769000	5.205365000	-0.961101000	H	2.251211000	5.243668000	-0.698563000
H	-0.996442000	2.452315000	-0.174069000	H	-0.930928000	2.508265000	0.236145000
H	-0.192820000	4.756740000	-0.632038000	H	-0.132089000	4.810947000	-0.205359000
H	-2.723963000	-4.036894000	-1.326399000	H	-2.362102000	-4.391522000	0.187387000
H	-1.814504000	-3.248167000	-2.650398000	H	-2.130322000	-3.655281000	-1.432243000

H	-0.974363000	-4.373311000	-1.532923000	H	-0.785622000	-4.555644000	-0.652236000
H	1.184496000	-1.622886000	-1.703190000	H	0.624095000	-1.559988000	-1.868327000
H	5.164331000	1.197991000	-0.381148000	H	5.171424000	1.208489000	-0.484487000
H	4.386217000	-2.808403000	0.914180000	H	4.497395000	-2.818441000	0.798485000
H	0.812481000	-2.346868000	1.471357000	H	1.013794000	-2.371418000	1.718620000
H	1.473223000	-3.491043000	0.291804000	H	1.536144000	-3.476231000	0.432973000
H	2.261081000	-3.284993000	1.848898000	H	2.484947000	-3.323235000	1.900527000
H	6.816268000	-1.264523000	-0.803753000	H	6.773927000	-1.254728000	-1.093634000
H	6.966920000	-0.334560000	0.684150000	H	7.064839000	-0.348461000	0.388464000
H	6.645099000	-2.073968000	0.756508000	H	6.739327000	-2.086224000	0.463444000
37 E(RB3LYP) = -1885.88969795 A.U.				TS₃₇₋₃₈ E(RB3LYP) = -1885.84740264 A.U. Frequency -984.6876			
O	1.244098000	-2.776177000	0.094539000	O	1.040710000	2.926461000	-0.219441000
C	0.464759000	-1.881567000	-0.419552000	C	0.467181000	2.022082000	0.336569000
C	0.367784000	-0.506766000	0.034912000	C	0.371650000	0.601820000	-0.161530000
C	-0.786057000	0.187260000	0.219830000	C	-0.773383000	-0.174932000	-0.154456000
C	-0.904475000	1.664725000	0.276615000	C	-0.830754000	-1.652130000	-0.055665000
C	-2.250722000	2.009784000	0.026744000	C	-2.171745000	-2.031001000	0.174908000
C	-3.046640000	0.779046000	-0.019261000	C	-3.012682000	-0.831346000	0.104354000
C	-2.188043000	-0.326418000	0.219750000	C	-2.186641000	0.289198000	-0.180049000
C	-4.416227000	0.624396000	-0.141181000	C	-4.385120000	-0.724679000	0.201924000
C	-4.985982000	-0.645067000	0.033647000	C	-4.996624000	0.518012000	-0.032292000
C	-4.149223000	-1.699426000	0.398138000	C	-4.191592000	1.589142000	-0.412938000
C	-2.754601000	-1.571980000	0.523283000	C	-2.790672000	1.512387000	-0.516380000
C	-2.640168000	3.339614000	-0.069303000	C	-2.510853000	-3.356180000	0.400603000
C	-1.679705000	4.336486000	0.118904000	C	-1.500516000	-4.323266000	0.371274000
C	-0.355810000	3.999997000	0.402534000	C	-0.176685000	-3.958651000	0.131452000
C	0.042143000	2.663769000	0.477817000	C	0.169762000	-2.620838000	-0.070520000
C	-1.991013000	-2.750015000	1.078756000	C	-2.068202000	2.718613000	-1.055252000
C	-6.471256000	-0.849689000	-0.128997000	C	-6.489757000	0.672570000	0.098881000
Pt	2.227375000	0.160271000	0.057484000	Pt	2.260007000	-0.085466000	-0.165997000
Cl	2.220560000	1.297400000	-1.964641000	Cl	2.728639000	-0.489980000	2.039033000
O	-0.225333000	-2.235831000	-1.457790000	O	-0.117881000	2.129419000	1.543278000
C	-0.016322000	-3.551533000	-2.046199000	C	0.070757000	3.384778000	2.226926000
Cl	2.642641000	-1.092586000	2.065666000	Cl	1.791555000	0.293817000	-2.585194000
H	-3.670693000	3.605350000	-0.276661000	H	-3.537327000	-3.644795000	0.595881000
H	-1.967984000	5.379789000	0.055918000	H	-1.749747000	-5.364881000	0.539808000
H	1.071542000	2.415159000	0.700484000	H	1.204566000	-2.344880000	-0.231902000
H	0.375807000	4.782813000	0.564749000	H	0.596830000	-4.717077000	0.111293000
H	-0.726848000	-3.597813000	-2.865887000	H	-0.465344000	3.281425000	3.167287000
H	1.007795000	-3.618658000	-2.411049000	H	1.133074000	3.554574000	2.405384000
H	-0.208847000	-4.330743000	-1.310793000	H	-0.332963000	4.210518000	1.639221000
H	1.770756000	-2.378764000	0.866678000	H	0.641357000	0.570042000	-1.623206000
H	-5.052422000	1.481845000	-0.334855000	H	-4.992564000	-1.593806000	0.431436000
H	-4.596687000	-2.661378000	0.630189000	H	-4.667315000	2.531064000	-0.667006000
H	-1.691939000	-3.460125000	0.302649000	H	-1.694715000	3.363722000	-0.256664000

H	-1.097594000	-2.437091000	1.622041000	H	-1.215366000	2.449060000	-1.678938000
H	-2.621205000	-3.301470000	1.779604000	H	-2.749761000	3.318188000	-1.661326000
H	-6.745058000	-0.883151000	-1.189199000	H	-6.785770000	0.681434000	1.153446000
H	-6.799233000	-1.785908000	0.326979000	H	-6.837947000	1.603469000	-0.351894000
H	-7.037829000	-0.032491000	0.325324000	H	-7.018244000	-0.157467000	-0.377895000
38 E(RB3LYP) = -1885.89777687 A.U.							
O	2.439458000	-0.518092000	-2.786974000				
C	1.790257000	0.186097000	-2.054802000				
C	0.702908000	-0.396606000	-1.176503000				
C	-0.345745000	0.322926000	-0.468518000				
C	-0.303459000	1.662451000	0.173446000				
C	-1.624360000	2.039966000	0.494672000				
C	-2.537063000	0.984309000	0.040058000				
C	-1.774143000	-0.058661000	-0.546827000				
C	-3.914522000	0.951214000	0.081821000				
C	-4.590615000	-0.148309000	-0.474408000				
C	-3.840492000	-1.156572000	-1.077852000				
C	-2.437512000	-1.149920000	-1.145264000				
C	-1.891281000	3.240228000	1.134640000				
C	-0.820085000	4.076999000	1.465102000				
C	0.489323000	3.703395000	1.164811000				
C	0.760529000	2.492255000	0.525821000				
C	-1.771269000	-2.303794000	-1.850029000				
C	-6.093597000	-0.223223000	-0.419928000				
Pt	1.196500000	-0.985501000	0.742093000				
Cl	3.289042000	0.070529000	0.690926000				
O	1.877189000	1.519853000	-2.012693000				
C	2.913663000	2.105673000	-2.828519000				
Cl	-0.467369000	-2.477056000	1.437142000				
H	-2.906581000	3.528909000	1.380946000				
H	-1.009664000	5.017724000	1.969595000				
H	1.781126000	2.198818000	0.335927000				
H	1.311657000	4.352274000	1.442064000				
H	2.821322000	3.179329000	-2.682847000				
H	3.889597000	1.751041000	-2.496024000				
H	2.765600000	1.842245000	-3.876002000				
H	0.371299000	-1.301729000	-1.665163000				
H	-4.476563000	1.765908000	0.525911000				
H	-4.365109000	-1.996853000	-1.519763000				
H	-1.256022000	-1.978868000	-2.759374000				
H	-1.051146000	-2.809275000	-1.203209000				
H	-2.518706000	-3.039610000	-2.149117000				
H	-6.547741000	0.702377000	-0.785450000				
H	-6.477059000	-1.051491000	-1.017491000				
H	-6.435809000	-0.365418000	0.610581000				

