

Supporting Information

DFT Studies on Mechanistic Origin of Ligand-Controlled Selectivity in Pd-Catalyzed Non-Decarbonylative and Decarbonylative Reductive Conversion of Acyl Fluoride

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I. CARTESIAN COORDINATES AND ELECTRONIC ENERGIES FOR ALL OF THE CALCULATED STRUCTURES.....	S2-S28
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1. Cartesian coordinates and electronic energies for all of the calculated structures

1				C	-3.011300	-0.572700	2.851000
SCF done: -1158.732935				C	-3.542600	-1.371800	0.525400
C	2.674500	-4.869100	-0.409600	H	-1.614200	-1.384800	1.441800
C	2.835800	-3.773600	-1.209800	C	-3.399600	-1.943100	3.405000
C	1.717700	-2.997000	-1.627300	H	-3.895000	0.083000	2.866100
C	0.400000	-3.398100	-1.203200	H	-2.263400	-0.103700	3.504700
C	0.275800	-4.545100	-0.362900	C	-3.933000	-2.738700	1.078000
C	1.374800	-5.256300	0.024700	H	-4.439100	-0.729700	0.488900
H	2.852000	-1.564700	-2.760100	H	-3.182400	-1.454900	-0.509400
H	3.539600	-5.449200	-0.095800	C	-4.430000	-2.630400	2.515400
H	3.828900	-3.466400	-1.539200	H	-3.780700	-1.842300	4.429800
C	1.855200	-1.864600	-2.434400	H	-2.497300	-2.573100	3.467100
C	-0.710500	-2.680300	-1.639000	H	-4.693900	-3.202600	0.437700
H	-0.722700	-4.840400	-0.040600	H	-3.050000	-3.400400	1.046200
H	1.263100	-6.128200	0.665200	H	-4.681900	-3.621200	2.915100
C	-0.571600	-1.529700	-2.444300	H	-5.362400	-2.042300	2.527100
C	0.752100	-1.098800	-2.820200	C	-3.043600	2.094500	0.232000
H	-1.713800	-3.013300	-1.373000	C	-3.704600	1.872300	-1.131400
H	0.869300	-0.322700	-3.572700	C	-4.098700	2.327800	1.311900
C	-1.781100	-0.936600	-3.017500	H	-2.425900	3.010900	0.153400
O	-2.921400	-1.264500	-2.845200	C	-4.608400	3.045700	-1.494800
F	-1.502100	0.089500	-3.858300	H	-4.306800	0.949700	-1.099500
P	-1.730700	0.785300	0.561200	H	-2.938300	1.707200	-1.900700
C	0.454700	2.382800	1.432900	C	-5.002900	3.503300	0.945500
H	1.015200	2.834600	2.263300	H	-4.717300	1.420500	1.405200
H	0.107200	3.208500	0.793600	H	-3.633900	2.494500	2.294600
P	1.558500	1.337100	0.327900	C	-5.656800	3.288700	-0.414800
Pd	-0.032000	0.185700	-1.080500	H	-5.086900	2.866700	-2.465900
C	-0.736600	1.580600	1.955100	H	-3.992800	3.952700	-1.611200
H	-0.384300	0.760400	2.597800	H	-5.764000	3.651800	1.722900
H	-1.386400	2.210400	2.578600	H	-4.400000	4.425500	0.917200
C	2.901700	2.567200	-0.150100	H	-6.290200	4.146300	-0.675800
C	3.853500	3.061100	0.938900	H	-6.323600	2.412800	-0.358400
C	3.686400	2.063800	-1.366300	2			
H	2.296200	3.429800	-0.488800	SCF done: -1756.841609			
C	4.779800	4.148000	0.396500	C	-6.054100	-3.975200	0.006100
H	4.468400	2.216000	1.290500	C	-4.705600	-4.196400	-0.128100
H	3.296800	3.430800	1.811900	C	-3.851200	-3.188400	-0.634200
C	4.619100	3.144600	-1.902800	C	-4.417600	-1.933300	-1.007200
H	4.282600	1.182200	-1.076000	C	-5.812500	-1.735200	-0.859000
H	2.989200	1.721800	-2.144400	C	-6.614500	-2.732300	-0.363500
C	5.560300	3.650400	-0.815100	H	-2.036500	-4.359800	-0.538800
H	5.464100	4.490400	1.183800	H	-6.698400	-4.759400	0.397300
H	4.175500	5.022200	0.104700	H	-4.270500	-5.154600	0.153700
H	5.188500	2.763800	-2.760400	C	-2.454100	-3.384300	-0.787900
H	4.014600	3.986200	-2.277900	C	-3.564800	-0.923200	-1.509700
H	6.211600	4.443000	-1.205100	H	-6.234100	-0.772700	-1.148600
H	6.223000	2.827200	-0.501500	H	-7.684400	-2.570400	-0.254600
C	2.251500	0.058000	1.529500	C	-2.204800	-1.126800	-1.600900
C	3.394600	-0.736700	0.893600	C	-1.640700	-2.380800	-1.243900
C	2.613500	0.486700	2.950700	H	-3.985700	0.035100	-1.816500
H	1.393900	-0.640000	1.600700	H	-0.569000	-2.511300	-1.406900
C	3.738400	-1.955100	1.744000	C	-1.343300	0.035500	-1.976000
H	4.284300	-0.089400	0.807500	O	-1.703400	0.905400	-2.735200
H	3.117200	-1.043000	-0.126000	F	0.988900	-1.485000	-2.270400
C	2.955900	-0.735100	3.801500	P	-0.234300	1.598400	0.562900
H	3.478800	1.165200	2.927000	C	2.273200	1.022500	1.775500
H	1.791200	1.046000	3.418300	H	2.823000	0.716000	2.675000
C	4.081000	-1.550400	3.173200	H	2.736600	1.955800	1.423700
H	4.568900	-2.513000	1.290700	P	2.453800	-0.207600	0.373000
H	2.872700	-2.638500	1.743600	Pd	0.438000	0.044500	-1.024300
H	3.224500	-0.425200	4.820000	C	0.797700	1.251900	2.097400
H	2.057900	-1.367700	3.893200	H	0.360700	0.347900	2.548100
H	4.301200	-2.435800	3.783300	H	0.673200	2.061400	2.829100
H	5.000500	-0.941900	3.163200	C	4.244000	-0.051300	-0.147400
C	-2.492600	-0.707900	1.418700				

C	5.304200	-0.514600	0.849800	C	-5.999500	3.217200	1.410400
C	4.460800	-0.687400	-1.524800	C	-4.869600	2.366700	1.457200
H	4.347900	1.043700	-0.273600	C	-5.072700	0.964000	1.620400
C	6.706000	-0.211200	0.323600	C	-6.395400	0.467800	1.729500
H	5.206600	-1.602400	0.995000	C	-7.470700	1.318800	1.681700
H	5.148900	-0.050000	1.834600	H	-3.398800	3.940100	1.272500
C	5.863700	-0.385300	-2.040500	H	-8.128500	3.373900	1.485000
H	4.331800	-1.777700	-1.446400	H	-5.840400	4.287900	1.288900
H	3.689900	-0.347000	-2.227400	C	-3.544700	2.863700	1.359300
C	6.925900	-0.842600	-1.046700	C	-3.943900	0.113900	1.669900
H	7.461500	-0.562000	1.038600	H	-6.538700	-0.605100	1.856500
H	6.832300	0.880900	0.244900	H	-8.481500	0.927400	1.770800
H	6.015600	-0.862400	-3.016800	C	-2.466200	2.019700	1.383900
H	5.964600	0.700100	-2.204500	H	-4.081200	-0.959100	1.810700
H	7.931400	-0.607800	-1.418800	H	-1.436200	2.377200	1.358300
H	6.877300	-1.939300	-0.947700	P	-0.682000	-0.977800	-1.506900
C	2.098300	-1.876600	1.153700	C	1.398400	0.314600	-2.911300
C	2.321000	-2.995800	0.129500	H	1.703800	0.953500	-3.750300
C	2.705800	-2.230600	2.509700	H	2.025900	-0.587100	-2.961100
H	1.001800	-1.800400	1.293300	P	1.750800	1.137400	-1.259800
C	1.725100	-4.301300	0.643800	Pd	0.007600	0.299900	0.295400
H	3.406000	-3.136100	-0.015800	C	-0.075600	-0.062600	-3.028600
H	1.892400	-2.705200	-0.843400	H	-0.701000	0.839700	-3.098100
C	2.110600	-3.544200	3.016400	H	-0.259700	-0.652400	-3.936000
H	3.797000	-2.340300	2.415000	C	3.553900	0.756100	-0.960800
H	2.533000	-1.433900	3.248200	C	4.550400	0.928600	-2.105700
C	2.301500	-4.671500	2.006700	C	4.054600	1.458700	0.302100
H	1.899100	-5.106600	-0.081000	H	3.490400	-0.326100	-0.727900
H	0.631000	-4.185400	0.724100	C	5.912700	0.370000	-1.693800
H	2.555700	-3.811500	3.983900	H	4.652100	1.998700	-2.346000
H	1.032900	-3.399400	3.197000	H	4.199300	0.432500	-3.021500
H	1.851100	-5.599200	2.383000	C	5.406900	0.893600	0.720700
H	3.380000	-4.871600	1.895100	H	4.169800	2.534700	0.091300
C	-1.999000	1.506600	1.203700	H	3.311800	1.378500	1.108100
C	-2.249200	2.001100	2.631900	C	6.421800	1.021300	-0.411200
C	-3.009500	2.135300	0.238500	H	6.638500	0.501900	-2.506800
H	-2.167800	0.413000	1.187100	H	5.816500	-0.716600	-1.533300
C	-3.683100	1.691000	3.060400	H	5.768700	1.403200	1.623800
H	-2.081100	3.088700	2.683700	H	5.285500	-0.169900	0.991000
H	-1.549000	1.540600	3.340500	H	7.384900	0.584100	-0.118900
C	-4.434500	1.803500	0.669400	H	6.609700	2.090400	-0.602900
H	-2.881100	3.230400	0.244500	C	1.445400	2.953400	-1.588500
H	-2.829800	1.806000	-0.792500	C	1.469600	3.761200	-0.285200
C	-4.700800	2.281000	2.091600	C	2.257300	3.656000	-2.673800
H	-3.855400	2.063000	4.078700	H	0.388900	2.916200	-1.923900
H	-3.813500	0.597900	3.100000	C	0.895600	5.152800	-0.527100
H	-5.151500	2.248500	-0.033400	H	2.516300	3.868500	0.043100
H	-4.577800	0.711500	0.613800	H	0.953500	3.219100	0.521300
H	-5.720400	2.022300	2.403800	C	1.697700	5.057700	-2.918000
H	-4.632700	3.380800	2.122300	H	3.305800	3.740000	-2.343700
C	0.238500	3.350700	0.096500	H	2.268700	3.081700	-3.611700
C	-0.231200	3.700900	-1.320000	C	1.660800	5.876400	-1.631100
C	-0.129000	4.448100	1.094600	H	0.917500	5.737200	0.401400
H	1.342800	3.277300	0.059900	H	-0.165900	5.062000	-0.812300
C	0.331800	5.050000	-1.752700	H	2.288200	5.573000	-3.686900
H	-1.330900	3.743200	-1.345000	H	0.675200	4.965900	-3.319300
H	0.052600	2.907300	-2.023000	H	1.225500	6.865700	-1.823500
C	0.433900	5.795100	0.645200	H	2.694300	6.051800	-1.290500
H	-1.226200	4.524400	1.162300	C	-2.519200	-1.214100	-1.833900
H	0.232700	4.203600	2.103700	C	-2.932000	-1.400400	-3.297400
C	-0.036800	6.147700	-0.761200	C	-3.132700	-2.313600	-0.960800
H	-0.028200	5.298700	-2.758600	H	-2.928800	-0.247900	-1.483300
H	1.429400	4.978400	-1.823200	C	-4.454100	-1.427500	-3.427800
H	0.148500	6.578100	1.359400	H	-2.516900	-2.345900	-3.683500
H	1.534800	5.745600	0.657900	H	-2.527300	-0.597600	-3.926700
H	0.383800	7.111400	-1.075300	C	-4.652300	-2.318600	-1.092800
H	-1.132000	6.272200	-0.752300	H	-2.742700	-3.291300	-1.288800
				H	-2.834400	-2.195900	0.088400
				C	-5.074500	-2.503000	-2.544700
				H	-4.734500	-1.577000	-4.478400
				H	-4.854200	-0.443900	-3.133800

3
SCF done: -1998.845420
C -7.269500 2.707600 1.519800

H	-5.079900	-3.105700	-0.458300	C	2.545300	1.199000	1.419700
H	-5.047500	-1.360900	-0.715100	H	3.282200	1.030700	2.216700
H	-6.167800	-2.489600	-2.636100	H	2.846500	2.121600	0.901800
H	-4.742100	-3.494200	-2.894700	P	2.600700	-0.146300	0.110100
C	0.247700	-2.602000	-1.590100	Pd	0.531300	-0.001100	-1.148900
C	0.154300	-3.384800	-0.278400	C	1.138700	1.347500	1.995300
C	-0.032800	-3.491200	-2.800700	H	0.870500	0.455400	2.581200
H	1.295600	-2.247000	-1.656800	H	1.080000	2.204400	2.680000
C	1.089800	-4.586400	-0.309000	C	4.332200	0.046600	-0.584000
H	-0.878500	-3.729300	-0.112300	C	5.501400	-0.233900	0.358900
H	0.394800	-2.721800	0.563300	C	4.495000	-0.709400	-1.905600
C	0.900200	-4.700000	-2.809400	H	4.344800	1.126500	-0.826800
H	-1.075900	-3.844700	-2.758200	C	6.830600	0.114500	-0.307600
H	0.070700	-2.926800	-3.738900	H	5.505900	-1.304800	0.618700
C	0.801500	-5.485400	-1.505800	H	5.388400	0.319000	1.302500
H	1.008000	-5.144700	0.633500	C	5.828200	-0.366200	-2.562600
H	2.130400	-4.226200	-0.368200	H	4.454500	-1.793300	-1.713200
H	0.673300	-5.342000	-3.670300	H	3.651800	-0.483400	-2.571100
H	1.936600	-4.350300	-2.943500	C	6.997600	-0.638500	-1.622700
H	1.487000	-6.342100	-1.522900	H	7.663300	-0.103700	0.373500
H	-0.215600	-5.899700	-1.410800	H	6.861400	1.198500	-0.503600
Si	2.461500	-1.208600	2.848400	H	5.943300	-0.929400	-3.497100
H	2.013300	-1.098000	1.418100	H	5.827500	0.700500	-2.839900
C	4.018500	-2.303200	2.850200	H	7.948400	-0.370200	-2.100500
H	4.059200	-2.849200	3.804900	H	7.046700	-1.719500	-1.413000
H	4.903800	-1.648900	2.845400	C	2.436100	-1.734800	1.108700
C	4.080800	-3.281700	1.681500	C	2.677700	-2.966000	0.230100
H	4.081500	-2.747300	0.719300	C	3.184800	-1.853400	2.435700
H	4.973300	-3.919800	1.704100	H	1.351400	-1.719000	1.335800
H	3.203600	-3.943400	1.669400	C	2.276800	-4.241600	0.963700
C	1.125100	-2.019400	3.903400	H	3.749300	-3.024700	-0.024800
H	0.245800	-1.360500	3.916200	H	2.129100	-2.865500	-0.717300
H	1.516300	-2.031600	4.932800	C	2.781200	-3.134500	3.163600
C	0.718500	-3.430300	3.490400	H	4.270000	-1.868700	2.252700
H	1.588500	-4.097100	3.402600	H	2.988200	-0.983500	3.077600
H	0.033000	-3.886700	4.215300	C	3.011700	-4.365100	2.293400
H	0.197300	-3.420600	2.525200	H	2.470900	-5.117300	0.331600
C	2.868000	0.491900	3.552900	H	1.190000	-4.223000	1.147100
H	3.818700	0.828900	3.112500	H	3.331400	-3.219500	4.109800
H	2.086800	1.176100	3.192100	H	1.712800	-3.073900	3.427700
C	2.974400	0.505300	5.075700	H	2.702000	-5.274000	2.824900
H	3.696000	-0.238300	5.445300	H	4.091700	-4.469600	2.098500
H	3.294600	1.482500	5.457500	C	-1.758600	1.071000	1.507500
H	2.009400	0.277200	5.544300	C	-1.949800	1.522600	2.957000
C	-2.669900	0.622300	1.532200	C	-2.979800	1.455400	0.666500
C	-1.526200	-0.333200	1.451800	H	-1.700500	-0.035300	1.505100
O	-1.532500	-1.412100	2.003400	C	-3.219700	0.899400	3.536900
F	0.463500	1.636700	1.805100	C	-2.032700	2.619900	2.998000
				H	-1.084700	1.250700	3.577100
				C	-4.241600	0.819100	1.238700
				H	-3.091200	2.552700	0.674700
				H	-2.844600	1.159700	-0.381400
				C	-4.445700	1.230500	2.692300
				H	-3.362600	1.233300	4.573000
				H	-3.092800	-0.194500	3.575200
				H	-5.112900	1.093300	0.629200
				H	-4.149500	-0.277700	1.167700
				H	-5.338700	0.749000	3.110700
				H	-4.627000	2.317200	2.735400
				C	-0.086400	3.314700	0.183500
				C	-0.767000	3.565200	-1.166500
				C	-0.560200	4.313800	1.238000
				H	1.000400	3.466300	0.032400
				C	-0.538600	5.000700	-1.626200
				H	-1.849500	3.386300	-1.068400
				H	-0.417200	2.842600	-1.915700
				C	-0.331000	5.748400	0.764700
				H	-1.638100	4.166900	1.415100
				H	-0.057600	4.143900	2.201300
				C	-1.011400	5.999700	-0.576200
				H	-1.047000	5.172900	-2.582900

4
SCF done: -1657.601724

C	-6.444900	-3.647300	-0.372600
C	-5.113300	-3.829400	-0.094600
C	-4.137400	-2.943300	-0.610700
C	-4.560000	-1.854900	-1.431700
C	-5.942700	-1.692600	-1.697600
C	-6.864700	-2.567200	-1.181400
H	-2.435900	-3.932900	0.283600
H	-7.184300	-4.336100	0.030100
H	-4.785700	-4.660700	0.528700
C	-2.754900	-3.093200	-0.333800
C	-3.588800	-0.963500	-1.938800
H	-6.255600	-0.857100	-2.322600
H	-7.923200	-2.433300	-1.392800
C	-2.251900	-1.119200	-1.643700
C	-1.839300	-2.202300	-0.832100
H	-3.887100	-0.118200	-2.560400
H	-0.772000	-2.305600	-0.624500
C	-1.272400	-0.067100	-2.104600
O	-1.624800	0.781600	-2.901600
P	-0.152300	1.495300	0.633100

H	0.537100	5.154000	-1.812700
H	-0.690400	6.457200	1.522200
H	0.752200	5.923500	0.660600
H	-0.829800	7.029500	-0.909800
H	-2.101700	5.899500	-0.449100
H	0.891000	-1.067500	-2.325400

5

SCF done: -1657.622988

C	-2.848500	4.753400	-0.407300
C	-2.965100	3.666600	-1.226900
C	-1.815600	2.949900	-1.666400
C	-0.514000	3.401100	-1.241800
C	-0.437200	4.537600	-0.382200
C	-1.564800	5.191500	0.024700
H	-2.896800	1.486400	-2.812500
H	-3.736600	5.287600	-0.077000
H	-3.945400	3.319900	-1.555300
C	-1.910900	1.826000	-2.492700
C	0.625000	2.740400	-1.699100
H	0.548600	4.873900	-0.061600
H	-1.488000	6.057000	0.679000
C	0.529800	1.607000	-2.528100
C	-0.772800	1.124700	-2.896700
H	1.618300	3.106100	-1.436100
H	-0.857800	0.348200	-3.659200
C	1.730000	1.007800	-3.124500
O	2.875800	1.380500	-2.933200
P	1.810900	-0.815800	0.380600
C	-0.346000	-2.450400	1.264300
H	-0.879200	-2.932200	2.095900
H	-0.013900	-3.250500	0.585400
P	-1.491000	-1.374300	0.232000
Pd	0.071200	-0.199900	-1.210500
C	0.855100	-1.657900	1.776200
H	0.515800	-0.859700	2.452300
H	1.525200	-2.301400	2.363800
C	-2.854800	-2.597600	-0.207400
C	-3.749500	-3.119500	0.917200
C	-3.699800	-2.072700	-1.372800
H	-2.265400	-3.451200	-0.593900
C	-4.699300	-4.197800	0.399200
H	-4.350100	-2.286000	1.317600
H	-3.148900	-3.505400	1.753300
C	-4.657600	-3.144500	-1.883000
H	-4.279900	-1.196200	-1.037500
H	-3.041400	-1.718100	-2.178700
C	-5.541000	-3.675800	-0.759700
H	-5.342300	-4.558400	1.212800
H	-4.109300	-5.064200	0.058700
H	-5.270700	-2.747900	-2.702600
H	-4.071200	-3.976600	-2.305300
H	-6.210700	-4.461100	-1.133300
H	-6.188000	-2.861300	-0.394700
C	-2.134900	-0.126900	1.493400
C	-3.313400	0.670300	0.928900
C	-2.429600	-0.586700	2.920800
H	-1.280500	0.576800	1.538100
C	-3.624900	1.870300	1.817000
H	-4.201400	0.017200	0.875100
H	-3.090900	0.998800	-0.096700
C	-2.736600	0.616700	3.810800
H	-3.294100	-1.266700	2.921500
H	-1.587100	-1.153900	3.340200
C	-3.895300	1.436200	3.253200
H	-4.479900	2.429600	1.413800
H	-2.765300	2.560800	1.789100
H	-2.954100	0.286100	4.835000
H	-1.838300	1.252900	3.870900
H	-4.090600	2.308400	3.890300
H	-4.810500	0.821700	3.276100

C	2.493700	0.708200	1.255400
C	3.022500	0.585900	2.685800
C	3.498500	1.449700	0.370700
H	1.574400	1.328400	1.290300
C	3.321900	1.970000	3.260300
H	3.949100	-0.007500	2.691700
H	2.309300	0.057000	3.332600
C	3.804800	2.829000	0.946200
H	4.434700	0.867200	0.320600
H	3.133900	1.531100	-0.662300
C	4.308500	2.731300	2.381600
H	3.708100	1.877900	4.284100
H	2.382100	2.541700	3.330700
H	4.533600	3.349900	0.312300
H	2.882000	3.434500	0.926100
H	4.500100	3.729800	2.795700
H	5.274700	2.200400	2.385600
C	3.186200	-2.065300	0.063600
C	3.794900	-1.859700	-1.326100
C	4.274600	-2.186200	1.127700
H	2.623100	-3.019100	0.039800
C	4.791100	-2.966100	-1.659400
H	4.300600	-0.881100	-1.369300
H	2.993700	-1.817100	-2.076400
C	5.257800	-3.303400	0.784500
H	4.828400	-1.235100	1.181000
H	3.837000	-2.351700	2.122900
C	5.872900	-3.081700	-0.592200
H	5.237500	-2.786800	-2.645800
H	4.251900	-3.925400	-1.729200
H	6.038400	-3.370000	1.553600
H	4.725600	-4.268700	0.793700
H	6.571800	-3.891900	-0.836700
H	6.464400	-2.151900	-0.576100
H	1.508900	0.160900	-3.820100

6

SCF done: -1544.309919

C	6.218500	-3.561500	-1.302700
C	5.621500	-2.575400	-2.048100
C	4.277300	-2.199000	-1.813900
C	3.538000	-2.861200	-0.790200
C	4.182600	-3.875700	-0.039200
C	5.489000	-4.217700	-0.286200
H	4.176000	-0.699100	-3.367300
H	7.252600	-3.841500	-1.492300
H	6.174400	-2.064900	-2.836900
C	3.624600	-1.191800	-2.565100
C	2.195800	-2.471200	-0.543300
H	3.616200	-4.381000	0.743000
H	5.968200	-4.999200	0.300300
C	1.580500	-1.455300	-1.247200
C	2.321900	-0.845300	-2.298100
H	1.663300	-2.987900	0.258500
H	1.845800	-0.073600	-2.905500
P	-2.405500	0.000300	0.072000
C	-0.925800	1.722800	1.716700
H	-0.944200	0.986200	2.534000
H	-0.785400	2.708400	2.178600
P	0.543400	1.248600	0.641100
Pd	-0.231900	-0.685500	-0.668200
C	-2.227500	1.666200	0.921800
H	-3.092000	1.895200	1.558100
H	-2.219500	2.415000	0.115800
C	0.774600	2.763300	-0.459000
C	0.530000	4.144700	0.149800
C	2.129300	2.720700	-1.173400
H	-0.000500	2.592000	-1.230400
C	0.626000	5.230100	-0.921200
H	1.279500	4.342400	0.931600
H	-0.452200	4.196600	0.639800

C	2.214700	3.803700	-2.243500	H	0.656000	-4.884400	0.629700
H	2.929600	2.891100	-0.434500	H	5.327200	-3.922400	0.882100
H	2.307900	1.724700	-1.602800	H	3.107600	-4.926500	0.425200
C	1.967200	5.183100	-1.644300	C	0.707600	-3.936400	1.164500
H	0.462500	6.217800	-0.470600	C	0.875500	-1.462300	2.520100
H	-0.184000	5.083200	-1.654100	H	3.421600	-0.663900	2.946100
H	3.192600	3.765900	-2.740000	H	5.481700	-1.790200	2.162800
H	1.460500	3.603500	-3.021600	C	-0.383900	-2.086200	2.327600
H	2.013200	5.957900	-2.420100	C	-0.427100	-3.337700	1.622100
H	2.771100	5.411900	-0.925400	H	0.976500	-0.655500	3.247800
C	1.923100	1.130700	1.911800	H	-1.395300	-3.810600	1.462000
C	3.192000	0.488300	1.340800	P	-2.163400	0.158400	-0.479800
C	2.256400	2.393700	2.704700	C	-0.282800	1.933100	-1.669500
H	1.483800	0.396700	2.615500	H	-0.632000	2.805800	-1.096900
C	4.191900	0.190800	2.453000	H	0.180100	2.319000	-2.588700
H	3.657600	1.170800	0.613100	P	1.003200	1.060700	-0.598600
H	2.939900	-0.425900	0.788900	Pd	-0.195900	-0.505100	0.801400
C	3.259700	2.086600	3.814600	C	-1.456000	1.017400	-2.001600
H	2.697200	3.140700	2.024700	H	-2.245200	1.558200	-2.544200
H	1.347700	2.846800	3.126500	H	-1.125000	0.200100	-2.660100
C	4.524400	1.443900	3.255000	C	2.026600	0.163600	-1.910100
H	5.100600	-0.252200	2.026200	C	2.937500	1.004700	-2.801800
H	3.764300	-0.568200	3.128400	C	2.795500	-1.005100	-1.288200
H	3.501500	3.003600	4.367800	H	1.234300	-0.271200	-2.550300
H	2.793800	1.398200	4.538400	C	3.609600	0.145100	-3.871100
H	5.225700	1.210900	4.066500	H	3.724000	1.463000	-2.180400
H	5.034900	2.167700	2.598900	H	2.381600	1.830600	-3.268600
C	-2.974400	-1.145900	1.455400	C	3.482400	-1.849700	-2.355200
C	-3.951600	-0.596000	2.494300	H	3.553900	-0.619800	-0.585200
C	-3.468300	-2.480000	0.888000	H	2.117400	-1.624700	-0.683700
H	-2.017200	-1.352000	1.970400	C	4.389300	-1.002200	-3.238800
C	-4.185100	-1.617800	3.606000	H	4.266800	0.766300	-4.494200
H	-4.914300	-0.359500	2.015900	H	2.838800	-0.266700	-4.542700
H	-3.578000	0.341900	2.928400	H	4.044000	-2.661700	-1.875200
C	-3.705600	-3.492200	2.004300	H	2.713900	-2.327900	-2.985100
H	-4.418300	-2.314000	0.352100	H	4.863200	-1.618200	-4.014200
H	-2.748800	-2.866200	0.152500	H	5.205700	-0.586800	-2.625500
C	-4.676800	-2.946700	3.044300	C	1.972900	2.523300	0.091700
H	-4.897800	-1.218100	4.339100	C	3.213100	2.030800	0.839800
H	-3.239000	-1.781800	4.146700	C	2.315600	3.699700	-0.824000
H	-4.077200	-4.435300	1.584000	H	1.259400	2.896500	0.852500
H	-2.743800	-3.723900	2.488900	C	3.876800	3.162500	1.618000
H	-4.824900	-3.673900	3.852800	H	3.935600	1.622100	0.112700
H	-5.662900	-2.796300	2.574600	H	2.941000	1.197200	1.503900
C	-3.796500	0.314500	-1.147300	C	2.961300	4.829700	-0.024400
C	-3.865600	-0.767600	-2.229000	H	3.020800	3.373800	-1.601100
C	-5.181400	0.598500	-0.566300	H	1.421000	4.066200	-1.345500
H	-3.439600	1.238700	-1.641200	C	4.206000	4.340500	0.707600
C	-4.850300	-0.371500	-3.324700	H	4.782000	2.797100	2.119900
H	-4.191300	-1.717900	-1.776800	H	3.192400	3.501400	2.412300
H	-2.864400	-0.950200	-2.640100	H	3.207300	5.669400	-0.687500
C	-6.161900	0.991500	-1.669900	H	2.236800	5.214300	0.711900
H	-5.556100	-0.311000	-0.069100	H	4.660700	5.157100	1.283200
H	-5.135200	1.383100	0.202100	H	4.958100	4.024200	-0.034000
C	-6.232200	-0.081800	-2.750000	C	-2.910200	1.627600	0.449400
H	-4.904900	-1.161000	-4.084700	C	-3.763500	2.651000	-0.297100
H	-4.475000	0.529300	-3.837000	C	-3.585100	1.181800	1.748600
H	-7.155400	1.177600	-1.241700	H	-1.974600	2.140200	0.749700
H	-5.832300	1.941000	-2.121900	C	-4.070600	3.848900	0.600900
H	-6.927000	0.219100	-3.544500	H	-4.713600	2.192900	-0.609500
H	-6.640500	-1.006700	-2.310900	H	-3.260200	2.988200	-1.214100
H	-0.755800	-1.914600	-1.540500	C	-3.906600	2.380000	2.636400
				H	-4.520700	0.647900	1.515100
				H	-2.935100	0.468100	2.274700
				C	-4.751300	3.408000	1.892000
				H	-4.694300	4.575000	0.063100
				H	-3.128200	4.365800	0.845700
				H	-4.418000	2.049500	3.549700
				H	-2.963400	2.850000	2.958600
				H	-4.957800	4.274900	2.532800
				H	-5.728600	2.960800	1.646800

7
SCF done: -1544.351414

C	4.421700	-3.426600	1.225400
C	3.184600	-3.985000	0.969400
C	1.999300	-3.362000	1.404200
C	2.086100	-2.130000	2.107300
C	3.358500	-1.595900	2.382600
C	4.508000	-2.224200	1.945200

C	-3.495500	-0.918300	-1.319400
C	-3.212900	-2.371900	-0.924300
C	-4.963100	-0.574200	-1.075900
H	-3.302800	-0.815900	-2.402100
C	-4.145000	-3.346200	-1.633900
H	-3.336100	-2.463600	0.169800
H	-2.159800	-2.616900	-1.124100
C	-5.892700	-1.557500	-1.785300
H	-5.171800	-0.603400	0.005800
H	-5.181500	0.446400	-1.413400
C	-5.604400	-2.996000	-1.374300
H	-3.929300	-4.375100	-1.318000
H	-3.951700	-3.305600	-2.718500
H	-6.939300	-1.296800	-1.579600
H	-5.754600	-1.458400	-2.874300
H	-6.271100	-3.688600	-1.903900
H	-5.818500	-3.114100	-0.299600
H	-1.246000	-1.786200	2.922300

8

SCF done: -1756.848813

C	-1.911000	-4.435900	0.128500
C	-0.833800	-4.519100	0.981300
C	0.439400	-4.059400	0.584500
C	0.592100	-3.498600	-0.715400
C	-0.531200	-3.412800	-1.567200
C	-1.760700	-3.873700	-1.155200
H	1.435000	-4.556700	2.443900
H	-2.885100	-4.803600	0.446600
H	-0.947500	-4.948800	1.975700
C	1.571400	-4.138400	1.448000
C	1.881000	-3.043400	-1.131400
H	-0.408600	-2.964300	-2.552400
H	-2.620800	-3.801300	-1.818900
C	2.989300	-3.170000	-0.269300
C	2.801600	-3.701500	1.050300
H	2.048300	-2.791800	-2.177800
H	3.660500	-3.772800	1.710800
C	4.324300	-2.878900	-0.816000
O	4.624300	-2.659700	-1.951300
F	5.267600	-2.881900	0.149800
P	-2.754400	0.035400	-1.222900
C	-0.232600	1.224900	-0.779500
H	-0.592300	2.264300	-0.766100
H	-0.085500	0.949400	-1.835100
P	1.472000	1.116600	-0.019000
Pd	2.322200	-1.076200	-0.079200
C	-1.237400	0.278200	-0.133800
H	-0.785900	-0.723400	-0.027400
H	-1.505400	0.615500	0.878000
C	2.443300	2.315900	-1.094400
C	2.115000	3.803900	-0.980300
C	3.952500	2.080800	-0.984200
H	2.139800	1.978000	-2.103800
C	2.868500	4.607400	-2.038100
H	2.417500	4.165700	0.015700
H	1.032500	3.977500	-1.063600
C	4.707000	2.893300	-2.031500
H	4.297900	2.371700	0.021900
H	4.169600	1.008000	-1.090800
C	4.372100	4.377000	-1.932700
H	2.632000	5.675000	-1.940200
H	2.521900	4.300100	-3.038000
H	5.787400	2.732100	-1.927900
H	4.431800	2.525900	-3.033200
H	4.902600	4.944900	-2.707700
H	4.727400	4.763600	-0.963300
C	1.238300	1.804900	1.716500
C	2.580200	1.937600	2.440800
C	0.394100	3.066800	1.897100
H	0.696400	0.968900	2.197200

C	2.374500	2.250000	3.919900
H	3.164200	2.751900	1.979900
H	3.169100	1.017200	2.312900
C	0.183300	3.358600	3.381100
H	0.899900	3.927100	1.434600
H	-0.577500	2.968400	1.392500
C	1.516700	3.496900	4.106800
H	3.344600	2.368800	4.419400
H	1.877500	1.392200	4.400700
H	-0.420900	4.266600	3.505100
H	-0.392500	2.534500	3.832600
H	1.356100	3.697700	5.173800
H	2.055600	4.369100	3.701800
C	-3.773700	-1.086500	-0.086900
C	-4.246400	-0.581600	1.274900
C	-4.937500	-1.724500	-0.852800
H	-3.038300	-1.891700	0.101600
C	-4.866200	-1.720700	2.083100
H	-5.007600	0.203200	1.133400
H	-3.421400	-0.121300	1.836500
C	-5.586900	-2.845200	-0.046400
H	-5.696600	-0.956600	-1.074600
H	-4.586200	-2.098100	-1.825400
C	-6.028000	-2.356100	1.328200
H	-5.197500	-1.356800	3.064700
H	-4.094000	-2.484600	2.274300
H	-6.436300	-3.270000	-0.597400
H	-4.856900	-3.662300	0.079700
H	-6.463000	-3.179700	1.909100
H	-6.826600	-1.606200	1.204100
C	-3.529600	1.768900	-1.183000
C	-4.939700	1.741900	-1.779100
C	-3.515400	2.577200	0.113500
H	-2.891400	2.309500	-1.908400
C	-5.469900	3.153200	-2.013600
H	-5.615200	1.219800	-1.081000
H	-4.949200	1.161300	-2.713100
C	-4.035000	3.993400	-0.127900
H	-4.148900	2.085800	0.865900
H	-2.503400	2.616200	0.541400
C	-5.436600	3.971700	-0.728000
H	-6.488600	3.114900	-2.421100
H	-4.846500	3.648600	-2.775400
H	-4.024600	4.567900	0.807800
H	-3.352700	4.512200	-0.821400
H	-5.793500	4.993300	-0.911600
H	-6.132200	3.524500	0.001100

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SCF done: -1756.821730

C	5.453700	-2.939200	0.830900
C	4.614900	-3.279000	-0.201500
C	3.209400	-3.202000	-0.047400
C	2.680100	-2.778900	1.208900
C	3.571700	-2.418200	2.250800
C	4.928700	-2.493700	2.065800
H	2.732200	-3.851800	-2.052300
H	6.531700	-3.005300	0.699800
H	5.016800	-3.614900	-1.156800
C	2.316100	-3.521000	-1.101500
C	1.278300	-2.713800	1.369000
H	3.155100	-2.067700	3.194100
H	5.606000	-2.213500	2.868900
C	0.439800	-3.010100	0.311900
C	0.958900	-3.417400	-0.944700
H	0.860700	-2.402200	2.326100
H	0.247200	-3.660700	-1.738500
C	-1.012400	-2.786400	0.529500
O	-1.601300	-2.905500	1.567500
F	-1.641600	-3.735500	-2.245700
P	1.997800	1.113000	1.084400

C	-0.747900	0.495900	0.949500	H	1.134400	5.318000	2.326400
H	-0.971400	1.471000	1.406900	H	1.587400	5.551000	-1.426300
H	-0.601900	-0.208800	1.780400	H	0.409000	5.168000	-0.170900
P	-2.234400	-0.110400	0.008600	H	1.987100	6.922400	0.631100
Pd	-1.888900	-2.123300	-1.109800	H	3.355300	5.865200	0.291500
C	0.504100	0.550600	0.082300				
H	0.731400	-0.453300	-0.304000				
H	0.358100	1.199600	-0.793900	10			
C	-3.556800	-0.248300	1.327700	SCF done:	-1643.540808		
C	-4.067100	1.067100	1.914700	C	5.904200	-3.586300	-1.704000
C	-4.715600	-1.148100	0.888300	C	5.017500	-3.028200	-2.592200
H	-3.010700	-0.796100	2.116800	C	3.805900	-2.449800	-2.145100
C	-5.025700	0.804700	3.073600	C	3.510500	-2.460800	-0.751500
H	-4.601600	1.628500	1.130900	C	4.444200	-3.041400	0.140800
H	-3.233100	1.701700	2.246600	C	5.614800	-3.590200	-0.321700
C	-5.672500	-1.395700	2.049900	H	3.079000	-1.876600	-4.098600
H	-5.264000	-0.670700	0.060200	H	6.832600	-4.026000	-2.062000
H	-4.319900	-2.097200	0.501800	H	5.234700	-3.021400	-3.660200
C	-6.183800	-0.085400	2.637800	C	2.867200	-1.860700	-3.028900
H	-5.396300	1.755900	3.477200	C	2.302900	-1.866000	-0.301100
H	-4.475000	0.310100	3.889500	H	4.212600	-3.041500	1.206800
H	-6.508200	-2.025100	1.719600	H	6.324100	-4.031300	0.375800
H	-5.142500	-1.963700	2.830900	C	1.422900	-1.258500	-1.166400
H	-6.858500	-0.277700	3.481600	C	1.710500	-1.290600	-2.556200
H	-6.778200	0.445300	1.876000	H	2.099000	-1.904400	0.772800
C	-2.597600	1.269400	-1.214900	H	0.991400	-0.865300	-3.255900
C	-3.943700	1.060800	-1.914600	F	-1.298200	-1.862200	-1.694000
C	-2.457900	2.705800	-0.705900	P	-2.489600	0.166300	0.341800
H	-1.808500	1.104600	-1.972000	C	-0.929800	2.263800	1.270200
C	-4.127700	2.063600	-3.049700	H	-0.627200	2.961200	2.061100
H	-4.757600	1.192100	-1.182200	H	-1.233300	2.875500	0.406600
H	-4.025000	0.030400	-2.291500	P	0.542200	1.251200	0.659000
C	-2.640500	3.698000	-1.851900	Pd	-0.361500	-0.496500	-0.548200
H	-3.216000	2.902600	0.066400	C	-2.088300	1.376600	1.713400
H	-1.479200	2.863700	-0.230700	H	-1.800700	0.771300	2.587200
C	-3.981200	3.495400	-2.547800	H	-2.963800	1.973500	2.002300
H	-5.105700	1.917400	-3.525100	C	1.475400	2.564400	-0.306800
H	-3.370400	1.870300	-3.826000	C	1.920200	3.783900	0.505300
H	-2.550100	4.724900	-1.475300	C	2.620100	2.014300	-1.161800
H	-1.824100	3.559300	-2.580000	H	0.685300	2.896600	-1.008000
H	-4.097200	4.207100	-3.374700	C	2.498200	4.862200	-0.409200
H	-4.792100	3.711500	-1.832900	H	2.693400	3.479000	1.229100
C	3.401800	0.596200	-0.077900	H	1.086200	4.197500	1.088900
C	3.210200	0.672300	-1.593100	C	3.184600	3.106200	-2.065000
C	4.715500	1.255900	0.349600	H	3.423600	1.632600	-0.513500
H	3.483000	-0.477500	0.175400				

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SCF done: -1643.540808
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C	-3.630200	-2.415500	0.287100
H	-2.450900	-1.580600	1.852900
C	-4.828700	-2.207700	2.978300
H	-5.347500	-0.627100	1.609000
H	-4.214800	-0.128300	2.867300
C	-3.980000	-3.658300	1.098200
H	-4.503100	-2.147200	-0.329000
H	-2.790400	-2.575800	-0.405300
C	-5.136600	-3.382300	2.053900
H	-5.678500	-2.002300	3.642400
H	-3.979900	-2.473800	3.629000
H	-4.226500	-4.489400	0.425800
H	-3.096000	-3.977100	1.673800
H	-5.376600	-4.276000	2.644500
H	-6.038200	-3.146200	1.465100
C	-3.619100	1.133600	-0.822900
C	-2.860000	1.323300	-2.143800
C	-4.991500	0.517300	-1.091800
H	-3.768600	2.120600	-0.348200
C	-3.661100	2.157300	-3.136900
H	-2.640200	0.324800	-2.556400
H	-1.878100	1.783700	-1.953900
C	-5.790400	1.372900	-2.071100
H	-4.850600	-0.484300	-1.526500
H	-5.551500	0.385300	-0.157600
C	-5.037800	1.552000	-3.383400
H	-3.105700	2.252800	-4.078400
H	-3.782600	3.178700	-2.738800
H	-6.774400	0.918800	-2.245900
H	-5.977200	2.361300	-1.619700
H	-5.616200	2.175300	-4.077300
H	-4.917800	0.569400	-3.866300

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SCF done: -1756.829932

C	6.337100	-3.324200	-0.544400
C	5.412400	-3.134900	-1.541200
C	4.101900	-2.690100	-1.242900
C	3.747000	-2.448900	0.116700
C	4.722500	-2.654600	1.123200
C	5.987900	-3.078900	0.802400
H	3.378600	-2.695200	-3.280100
H	7.341500	-3.664200	-0.787300
H	5.673300	-3.324000	-2.582400
C	3.120800	-2.479300	-2.242500
C	2.439600	-1.983700	0.414400
H	4.444300	-2.469900	2.161500
H	6.727500	-3.231700	1.585700
C	1.515200	-1.722200	-0.572100
C	1.867900	-2.018900	-1.916500
H	2.195600	-1.809200	1.466500
H	1.128100	-1.876400	-2.704500
C	-1.016000	-2.642700	-0.273600
O	-1.333100	-3.400100	0.592600
F	-1.245800	-3.025300	-1.580500
P	-2.393300	0.271000	0.264200
C	-0.822200	2.592200	0.455300
H	-0.536100	3.495900	1.007100
H	-1.105100	2.921200	-0.555400
P	0.653600	1.447100	0.221400
Pd	-0.272500	-0.772300	-0.169000
C	-1.992500	1.886000	1.131700
H	-1.732800	1.614600	2.166500
H	-2.872800	2.540900	1.181800
C	1.631900	2.389300	-1.074500
C	2.111500	3.781600	-0.660000
C	2.764400	1.560800	-1.690000
H	0.864900	2.516800	-1.863100
C	2.760000	4.507800	-1.835700
H	2.849100	3.685200	0.153600
H	1.279700	4.379200	-0.260600

C	3.400300	2.306200	-2.859100
H	3.536300	1.356600	-0.932800
H	2.387200	0.580400	-2.008800
C	3.894000	3.684500	-2.435500
H	3.120900	5.493500	-1.514800
H	1.996700	4.690600	-2.609600
H	4.221500	1.710500	-3.276200
H	2.656000	2.419500	-3.664400
H	4.344300	4.213600	-3.284900
H	4.690500	3.566300	-1.682400
C	1.548500	1.486400	1.887000
C	3.034700	1.136700	1.746600
C	1.375700	2.736500	2.752200
H	1.066000	0.644000	2.417400
C	3.670400	0.923700	3.115900
H	3.553800	1.965400	1.237900
H	3.168800	0.244100	1.122700
C	2.024300	2.532400	4.120900
H	1.840400	3.602600	2.253700
H	0.313500	2.983800	2.885800
C	3.495600	2.154700	3.997000
H	4.732600	0.674300	2.998600
H	3.196900	0.052200	3.598200
H	1.906000	3.438500	4.728900
H	1.488500	1.728400	4.650900
H	3.933300	1.989500	4.989600
H	4.047200	2.997100	3.548200
C	-3.576000	-0.604200	1.426000
C	-4.561000	0.263700	2.212200
C	-4.304300	-1.764900	0.739100
H	-2.866400	-1.051700	2.146700
C	-5.312700	-0.585100	3.236300
H	-5.286200	0.722700	1.522000
H	-4.044100	1.088300	2.720500
C	-5.048700	-2.608800	1.768500
H	-5.030500	-1.359500	0.014500
H	-3.600700	-2.391900	0.178000
C	-6.024200	-1.758400	2.573100
H	-6.026000	0.039800	3.789100
H	-4.593500	-0.969600	3.977300
H	-5.572500	-3.432300	1.267700
H	-4.311600	-3.072600	2.442700
H	-6.540000	-2.367500	3.326100
H	-6.804200	-1.369800	1.897600
C	-3.259500	0.831300	-1.301000
C	-3.332100	-0.298100	-2.334900
C	-4.613000	1.519500	-1.128800
H	-2.544900	1.578000	-1.698100
C	-3.863800	0.224600	-3.665100
H	-3.998900	-1.092500	-1.965700
H	-2.345700	-0.764600	-2.456900
C	-5.135700	2.031600	-2.469300
H	-5.337100	0.797300	-0.718200
H	-4.545700	2.344300	-0.404600
C	-5.217500	0.903600	-3.491800
H	-3.931600	-0.596000	-4.389900
H	-3.145300	0.950000	-4.080900
H	-6.115800	2.506900	-2.334100
H	-4.457000	2.814200	-2.845700
H	-5.587000	1.283200	-4.452800
H	-5.952200	0.158500	-3.145600

TS₁

SCF done: -1756.829463

C	-6.015600	-3.681400	0.308100
C	-4.664800	-3.929200	0.300000
C	-3.773900	-3.064900	-0.378200
C	-4.298900	-1.928100	-1.058100
C	-5.697100	-1.701200	-1.035900
C	-6.537200	-2.556700	-0.367300
H	-1.979800	-4.187900	0.067000

	-6.690000	-4.353300	0.834100	H	-4.786900	2.998400	2.085000
H	-4.257400	-4.798300	0.815300	C	0.034100	3.284600	0.231200
C	-2.373800	-3.295600	-0.419200	C	-0.378900	3.668000	-1.193500
C	-3.406000	-1.050900	-1.720700	C	-0.473300	4.299500	1.255200
H	-6.089800	-0.828200	-1.556800	H	1.140700	3.300100	0.255800
H	-7.608800	-2.371500	-0.357000	C	0.082100	5.082500	-1.528700
C	-2.048500	-1.281200	-1.717300	H	-1.473900	3.609800	-1.292800
C	-1.532100	-2.435300	-1.069400	H	0.026200	2.940800	-1.909600
H	-3.798700	-0.175200	-2.238000	C	-0.008500	5.710900	0.900600
H	-0.465000	-2.627700	-1.138300	H	-1.575100	4.283000	1.267700
C	-1.176800	-0.218200	-2.287500	H	-0.143600	4.034200	2.270400
O	-1.492000	0.624800	-3.084800	C	-0.438200	6.091000	-0.511300
F	0.270400	-1.209900	-2.812100	H	-0.240400	5.350600	-2.542400
P	-0.321000	1.473700	0.583900	H	1.184100	5.111100	-1.534100
C	2.224800	1.009500	1.757800	H	-0.398000	6.429600	1.633300
H	2.797700	0.702600	2.643000	H	1.090500	5.757200	0.970500
H	2.625700	1.986200	1.449900	H	-0.093800	7.103600	-0.757200
P	2.519100	-0.132900	0.295300	H	-1.539300	6.114700	-0.557700
Pd	0.481300	0.092900	-1.110700				
C	0.740100	1.131700	2.099400	TS ₂			
H	0.365500	0.187100	2.521500	SCF done:	-1998.832848		
H	0.581000	1.905600	2.862900	C	-7.092500	-2.986400	1.201700
C	4.346700	0.134700	-0.058400	C	-5.833500	-2.999900	1.747900
C	5.359100	-0.369100	0.968700	C	-4.736100	-2.438800	1.052300
C	4.701200	-0.361900	-1.464400	C	-4.960500	-1.862200	-0.233400
H	4.406300	1.239800	-0.080900	C	-6.272800	-1.857000	-0.768000
C	6.777900	0.044700	0.584300	C	-7.316100	-2.407600	-0.068100
H	5.311400	-1.469200	1.008500	H	-3.252500	-2.917100	2.548700
H	5.114700	-0.006000	1.977100	H	-7.926400	-3.424200	1.745600
C	6.121200	0.046800	-1.842400	H	-5.658200	-3.446200	2.725900
H	4.620600	-1.460600	-1.496200	C	-3.421200	-2.441300	1.583400
H	3.972700	0.018600	-2.193100	C	-3.866700	-1.299100	-0.926900
C	7.132300	-0.448200	-0.814300	H	-6.432700	-1.410800	-1.748800
H	7.495200	-0.336200	1.323000	H	-8.319000	-2.402800	-0.488300
H	6.853500	1.143700	0.612600	C	-2.376300	-1.881200	0.896300
H	6.368700	-0.331100	-2.842300	H	-4.017800	-0.846900	-1.907500
H	6.174100	1.146000	-1.901800	H	-1.350000	-1.945000	1.255400
H	8.147300	-0.132600	-1.087400	F	0.446100	-2.409200	0.284800
H	7.136800	-1.550400	-0.815800	P	-0.653500	1.935700	0.482100
C	2.216300	-1.847300	1.013000	C	1.849700	2.325000	1.705500
C	2.532300	-2.929300	-0.024400	H	2.429100	2.527500	2.615500
C	2.788300	-2.213700	2.381700	H	2.166100	3.069900	0.962300
H	1.113200	-1.827500	1.112900	P	2.268300	0.619000	1.027500
C	1.996800	-4.282400	0.432600	Pd	0.200300	-0.144300	-0.104200
H	3.625400	-3.002000	-0.154000	C	0.353800	2.453900	1.976300
H	2.114700	-2.653100	-1.004400	H	0.046400	1.778800	2.788400
C	2.241800	-3.566800	2.834000	H	0.095000	3.475100	2.286200
H	3.885600	-2.270900	2.328600	C	3.713400	0.948000	-0.123100
H	2.550100	-1.443300	3.128800	C	4.829400	1.877900	0.356400
C	2.540900	-4.654500	1.807800	C	4.292800	-0.356700	-0.674200
H	2.242300	-5.056900	-0.304800	H	3.188500	1.449600	-0.961400
H	0.896100	-4.230900	0.477400	C	5.808100	2.160100	-0.782500
H	2.658200	-3.834700	3.813800	H	5.374400	1.401100	1.184200
H	1.150900	-3.485600	2.968400	H	4.423900	2.820000	0.751600
H	2.130000	-5.616900	2.138700	C	5.279900	-0.078400	-1.801800
H	3.632700	-4.789200	1.736600	H	4.810300	-0.893000	0.139600
C	-2.076400	1.245700	1.215700	H	3.486200	-1.013800	-1.027600
C	-2.390100	1.698000	2.644400	C	6.386300	0.866600	-1.346700
C	-3.089300	1.822900	0.222400	H	6.609800	2.823500	-0.433100
H	-2.178200	0.143200	1.180500	H	5.280300	2.701300	-1.584400
C	-3.820700	1.317600	3.022200	H	5.700800	-1.022400	-2.170600
H	-2.277200	2.790000	2.725500	H	4.734500	0.369000	-2.648900
H	-1.684900	1.255200	3.360200	H	7.075000	1.083600	-2.173000
C	-4.512700	1.444300	0.615400	H	6.983200	0.370100	-0.564300
H	-3.002900	2.922200	0.213100	C	2.779000	-0.321200	2.566100
H	-2.861900	1.481400	-0.797300	C	2.806500	-1.829100	2.301000
C	-4.827700	1.897500	2.035900	C	4.045500	0.126500	3.292600
H	-4.039400	1.653200	4.044400	H	1.912800	-0.117800	3.227500
H	-3.910900	0.219600	3.025600	C	2.974200	-2.598600	3.606700
H	-5.226700	1.873200	-0.100800	H	3.662600	-2.056900	1.643500
H	-4.624400	0.350100	0.549700	H	1.907800	-2.143800	1.752100
H	-5.848800	1.609600	2.316300				

SCF done: -1998.832848

C	4.201300	-0.641000	4.605100	TS₃		
H	4.917400	-0.087400	2.653500	SCF done:	-1657.597277	
H	4.048600	1.210400	3.479100	C	-6.318000	-3.418500
C	4.218000	-2.146900	4.363900	C	-4.989100	-3.629800
H	3.014100	-3.675600	3.399800	C	-3.987500	-2.868900
H	2.084900	-2.435400	4.237400	C	-4.380300	-1.879800
H	5.114800	-0.320700	5.123000	C	-5.759700	-1.693800
H	3.359400	-0.387600	5.269900	C	-6.707800	-2.441900
H	4.311400	-2.684100	5.316600	H	-2.310500	-3.804600
H	5.111400	-2.403300	3.771800	H	-7.078300	-4.005400
C	-2.439300	2.056500	1.046500	H	-4.684300	-4.383600
C	-2.769500	3.132100	2.084100	C	-2.607600	-3.036100
C	-3.419900	2.136200	-0.128400	C	-3.384400	-1.089400
H	-2.580100	1.069200	1.524600	H	-6.050400	-0.938000
C	-4.210800	2.974200	2.568300	H	-7.763900	-2.286600
H	-2.639700	4.131000	1.637700	C	-2.053500	-1.243300
H	-2.089000	3.077700	2.943700	C	-1.668200	-2.239900
C	-4.849000	1.944100	0.368400	H	-3.661000	-0.310500
H	-3.333400	3.128100	-0.601400	H	-0.606200	-2.347000
H	-3.176100	1.398300	-0.902600	C	-1.068600	-0.235100
C	-5.204000	2.996900	1.411900	O	-1.372300	0.545700
H	-4.446500	3.759500	3.297900	P	-0.247800	1.420100
H	-4.301100	2.014300	3.101400	C	2.476800	1.306900
H	-5.550100	1.974700	-0.476000	H	3.222200	1.186300
H	-4.940000	0.938000	0.810600	H	2.715300	2.250300
H	-6.224800	2.845400	1.784300	P	2.629000	-0.021700
H	-5.186700	3.993000	0.940100	Pd	0.559700	0.062100
C	-0.232400	3.261500	-0.775100	C	1.064200	1.360300
C	-0.651800	2.891900	-2.200100	H	0.860200	0.453200
C	-0.645500	4.689500	-0.418700	H	0.949700	2.211300
H	0.873000	3.216600	-0.760100	C	4.369700	0.264100
C	-0.072900	3.891600	-3.195800	C	5.535900	0.017500
H	-1.750100	2.898000	-2.279400	C	4.585100	-0.463500
H	-0.336000	1.867200	-2.435700	H	4.339800	1.347400
C	-0.071000	5.680200	-1.429700	C	6.859700	0.430100
H	-1.745300	4.765900	-0.428200	H	5.581500	-1.056600
H	-0.318500	4.955900	0.597000	H	5.386000	0.549200
C	-0.482000	5.319500	-2.852700	C	5.912400	-0.057900
H	-0.389200	3.630800	-4.213100	H	4.587400	-1.551300
H	1.027000	3.815100	-3.183500	H	3.743900	-0.262900
H	-0.388800	6.700300	-1.178400	C	7.076900	-0.296400
H	1.028600	5.668100	-1.355400	H	7.690800	0.236800
H	-0.048000	6.030300	-3.567200	H	6.848400	1.517100
H	-1.576400	5.412800	-2.945000	H	6.064800	-0.602700
Si	1.249200	-2.712700	-1.605500	H	5.873000	1.011700
H	1.272300	-1.173800	-1.432200	H	8.023400	0.017300
C	2.183800	-2.471400	-3.303100	H	7.167100	-1.377500
H	2.028100	-3.354800	-3.943300	C	2.531000	-1.623100
H	3.267900	-2.451700	-3.094000	C	2.832500	-2.837500
C	1.795000	-1.198700	-4.044600	C	3.270300	-1.725300
H	2.011600	-0.309300	-3.430000	H	1.444300	-1.656500
H	2.325200	-1.070600	-4.998800	C	2.470700	-4.134000
H	0.717900	-1.164500	-4.259500	H	3.908900	-2.852700
C	-0.370200	-3.592900	-2.086200	H	2.294900	-2.752800
H	-1.112000	-3.416900	-1.298500	C	2.902200	-3.024200
H	-0.122100	-4.664800	-2.006200	H	4.357000	-1.706200
C	-0.976800	-3.318400	-3.456900	H	3.041900	-0.866000
H	-0.252600	-3.477100	-4.265900	C	3.189200	-4.239900
H	-1.833000	-3.976000	-3.657700	H	2.708500	-4.996900
H	-1.337300	-2.285000	-3.538000	H	1.381200	-4.159600
C	2.462800	-3.872500	-0.703400	H	3.442200	-3.096500
H	3.289200	-3.273000	-0.290300	H	1.828800	-3.003300
H	1.937100	-4.289000	0.164600	H	2.904500	-5.163300
C	3.031400	-4.988300	-1.574900	H	4.274900	-4.304100
H	3.668400	-4.598700	-2.377700	C	-1.791300	0.812000
H	3.638100	-5.694800	-0.993500	C	-2.010700	1.228600
H	2.236800	-5.572500	-2.059400	C	-3.052100	1.074700
C	-2.603500	-1.287500	-0.371700	H	-1.618600	-0.282500
C	-1.521700	-0.566500	-1.109400	C	-3.211300	0.487100
O	-1.645500	-0.216300	-2.261200	H	-2.193300	2.312800
				H	-1.117200	1.032700
						3.606100

C	-4.249100	0.331200	1.298400
H	-3.265300	2.157000	0.714700
H	-2.895100	0.784200	-0.334600
C	-4.470600	0.716900	2.756200
H	-3.371500	0.796100	4.626400
H	-2.986800	-0.591600	3.609500
H	-5.148200	0.534200	0.701800
H	-4.069300	-0.754300	1.219300
H	-5.315300	0.159400	3.180600
H	-4.742000	1.784300	2.807800
C	-0.379800	3.256100	0.280400
C	-1.070200	3.481200	-1.069800
C	-0.971700	4.158100	1.362700
H	0.684300	3.533300	0.149900
C	-1.004700	4.949900	-1.473800
H	-2.126100	3.175000	-0.997000
H	-0.625000	2.834500	-1.838000
C	-0.901300	5.625700	0.944800
H	-2.027900	3.886100	1.521700
H	-0.462300	4.011100	2.326500
C	-1.596300	5.848300	-0.393600
H	-1.522000	5.099500	-2.429700
H	0.047900	5.231100	-1.642000
H	-1.343900	6.260800	1.723300
H	0.155800	5.925600	0.859600
H	-1.532300	6.903700	-0.688000
H	-2.668900	5.619000	-0.282500
H	0.515000	-0.927200	-2.521000

TS₄

SCF done: -1756.792480

C	-2.373400	5.652800	-0.412500
C	-2.895600	4.718700	-1.272100
C	-2.169100	3.548400	-1.599800
C	-0.873200	3.363500	-1.033500
C	-0.359800	4.346400	-0.152000
C	-1.093500	5.464600	0.156200
H	-3.677300	2.697800	-2.895600
H	-2.945400	6.543900	-0.163600
H	-3.883800	4.858700	-1.709000
C	-2.691300	2.546100	-2.456200
C	-0.154100	2.181900	-1.341300
H	0.630900	4.192000	0.278100
H	-0.692100	6.211900	0.837100
C	-0.700000	1.197800	-2.133700
C	-1.979500	1.400200	-2.710500
H	0.839200	2.050900	-0.905700
H	-2.397800	0.627100	-3.355400
C	0.391300	-0.010900	-3.157700
O	0.839100	0.390300	-4.158600
P	1.971600	-0.424200	0.410400
C	0.047500	-2.090100	1.717400
H	-0.434600	-2.387200	2.659300
H	0.438100	-3.006400	1.252900
P	-1.229600	-1.448500	0.510400
Pd	-0.133200	-0.898100	-1.547400
C	1.175200	-1.095100	1.982200
H	0.787100	-0.217400	2.520700
H	1.932200	-1.549400	2.636500
C	-2.453200	-2.865000	0.440100
C	-3.256900	-3.157700	1.706000
C	-3.372300	-2.745100	-0.779100
H	-1.776300	-3.719700	0.249600
C	-4.099000	-4.420300	1.532100
H	-3.930100	-2.308500	1.909400
H	-2.598100	-3.254300	2.581000
C	-4.216900	-4.004500	-0.944300
H	-4.038300	-1.875600	-0.653400
H	-2.767800	-2.552500	-1.676400
C	-5.015000	-4.306900	0.319100
H	-4.681500	-4.613800	2.442200

H	-3.427300	-5.283900	1.400400
H	-4.885400	-3.900800	-1.808300
H	-3.551200	-4.854400	-1.164600
H	-5.601100	-5.226400	0.194900
H	-5.740500	-3.494800	0.491000
C	-1.965000	0.041400	1.392100
C	-3.224500	0.544200	0.682100
C	-2.196400	-0.046900	2.900900
H	-1.178500	0.801700	1.214800
C	-3.650300	1.900800	1.235400
H	-4.040400	-0.181800	0.840600
H	-3.053500	0.607800	-0.401700
C	-2.623700	1.313200	3.451200
H	-2.984000	-0.785200	3.113100
H	-1.295200	-0.394500	3.424500
C	-3.869700	1.832400	2.741800
H	-4.556200	2.250500	0.721900
H	-2.864700	2.640100	1.008700
H	-2.793000	1.245600	4.533800
H	-1.800500	2.032100	3.305500
H	-4.154100	2.815900	3.137000
H	-4.711800	1.153000	2.954300
C	2.829300	1.113100	1.100400
C	3.558100	1.058200	2.443500
C	3.721300	1.754700	0.034200
H	1.953300	1.781500	1.237500
C	3.993100	2.459400	2.870900
H	4.447400	0.416900	2.355500
H	2.923900	0.608800	3.219500
C	4.165400	3.151100	0.456900
H	4.613200	1.122600	-0.111400
H	3.205100	1.784700	-0.937800
C	4.868800	3.115800	1.809300
H	4.520000	2.416400	3.833100
H	3.095700	3.078700	3.033400
H	4.818100	3.591800	-0.307300
H	3.278100	3.803300	0.522500
H	5.157400	4.128200	2.120100
H	5.804400	2.541300	1.711200
C	3.246300	-1.760000	0.033500
C	3.783800	-1.604600	-1.392700
C	4.389800	-2.006000	1.016100
H	2.601900	-2.660500	0.027700
C	4.599400	-2.826000	-1.801900
H	4.422100	-0.707000	-1.448400
H	2.949100	-1.446000	-2.089000
C	5.196900	-3.236700	0.606100
H	5.061400	-1.131500	1.020100
H	4.017400	-2.121100	2.044500
C	5.730300	-3.095500	-0.815300
H	4.995400	-2.694800	-2.817000
H	3.930800	-3.701300	-1.838400
H	6.019400	-3.402900	1.314300
H	4.549200	-4.126400	0.663800
H	6.292600	-3.992700	-1.105100
H	6.444300	-2.256100	-0.847800
H	0.233100	-2.478100	-1.689000

TS₅

SCF done: -1544.305723

C	6.470000	-2.747400	-1.363600
C	5.717300	-1.943700	-2.184200
C	4.322300	-1.809100	-1.990500
C	3.697600	-2.525300	-0.927600
C	4.499300	-3.355800	-0.105200
C	5.852200	-3.462000	-0.313000
H	3.982700	-0.459600	-3.644500
H	7.542600	-2.838800	-1.520200
H	6.185600	-1.392500	-2.999700
C	3.512700	-0.987000	-2.813400
C	2.308300	-2.353300	-0.704100

H	4.016700	-3.903500	0.704800	H	-2.628500	0.364100	-2.499200
H	6.454700	-4.099200	0.331200	C	-5.287100	2.612900	-0.646100
C	1.543000	-1.490100	-1.465300	H	-5.450500	0.568700	0.003300
C	2.168900	-0.847100	-2.570600	H	-4.588100	1.604400	1.145000
H	1.857300	-2.897000	0.129200	C	-5.471500	2.337400	-2.134400
H	1.571700	-0.205400	-3.218400	H	-4.314400	1.659100	-3.839900
P	-2.401700	-0.400200	0.277200	H	-3.433300	2.706400	-2.730400
C	-1.039200	1.548900	1.821900	H	-6.237600	2.915700	-0.187900
H	-0.715800	1.896800	2.810700	H	-4.593600	3.459700	-0.516500
H	-1.544100	2.403200	1.348100	H	-5.862900	3.227400	-2.643700
P	0.433200	1.131600	0.719700	H	-6.229000	1.546800	-2.261300
Pd	-0.236700	-0.772000	-0.717800	H	-0.132300	-2.095500	-1.627900
C	-2.004200	0.372300	1.948400				
H	-1.541600	-0.437500	2.534900	TS ₆			
H	-2.913800	0.677900	2.482900	SCF done:	-1756.811887		
C	0.898800	2.837000	0.077300	C	5.233600	-2.759100	0.979300
C	1.427900	3.846900	1.094500	C	4.491600	-3.101700	-0.125100
C	1.811800	2.750900	-1.149600	C	3.080300	-3.174500	-0.052900
H	-0.082500	3.202700	-0.283500	C	2.440200	-2.883000	1.187800
C	1.627100	5.218100	0.452100	C	3.230400	-2.515300	2.303900
H	2.396500	3.493000	1.482800	C	4.597900	-2.458900	2.204300
H	0.752300	3.924400	1.958900	H	2.779300	-3.755100	-2.113800
C	2.007300	4.126800	-1.778400	H	6.318500	-2.710600	0.911100
H	2.792100	2.342800	-0.857900	H	4.978500	-3.322500	-1.074900
H	1.391400	2.040900	-1.875300	C	2.281800	-3.523100	-1.173000
C	2.544800	5.127800	-0.762100	C	1.031100	-2.969300	1.265600
H	2.026900	5.926300	1.189500	H	2.729500	-2.273000	3.239700
H	0.647900	5.614200	0.137100	H	5.197000	-2.179300	3.067600
H	2.679400	4.054100	-2.642800	C	0.285800	-3.306200	0.155200
H	1.039900	4.488800	-2.164100	C	0.917600	-3.583900	-1.083800
H	2.671800	6.116200	-1.222300	H	0.533900	-2.762700	2.213100
H	3.545800	4.804600	-0.432800	H	0.281500	-3.873900	-1.913600
C	1.759200	0.488400	1.894200	C	-1.184400	-3.250200	0.318000
C	3.119200	0.454600	1.187900	O	-1.843400	-3.522500	1.270900
C	1.888100	1.088200	3.293000	F	-1.756500	-4.190000	-1.421900
H	1.437100	-0.564800	2.008200	P	2.140300	0.929100	1.021200
C	4.131000	-0.337500	2.007200	C	-0.605600	0.374500	0.841300
H	3.488600	1.486700	1.064900	H	-0.748500	1.371300	1.284200
H	3.018100	0.022500	0.184100	H	-0.544800	-0.333100	1.682700
C	2.921900	0.313900	4.112000	P	-2.144500	-0.077200	-0.108700
H	2.197100	2.143200	3.223500	Pd	-2.032700	-2.151600	-1.128400
H	0.922000	1.075500	3.817300	C	0.670700	0.317600	0.011700
C	4.272800	0.250700	3.405400	H	0.884500	-0.719800	-0.284300
H	5.096900	-0.370700	1.485500	H	0.567100	0.896900	-0.916100
H	3.789000	-1.383500	2.077600	C	-3.453300	-0.153400	1.234700
H	3.025700	0.765100	5.107600	C	-3.436800	0.920300	2.324700
H	2.551600	-0.711900	4.271200	C	-4.855500	-0.312200	0.642800
H	4.987100	-0.330200	4.002900	H	-3.187300	-1.118600	1.706600
H	4.686400	1.269900	3.328000	C	-4.459900	0.588900	3.410400
C	-3.503800	-1.847600	0.756400	H	-3.680200	1.902100	1.889800
C	-4.546500	-1.639200	1.855000	H	-2.438500	1.012300	2.772200
C	-4.134300	-2.485200	-0.483700	C	-5.872400	-0.635700	1.732200
H	-2.749100	-2.559500	1.140700	H	-5.150400	0.629400	0.149300
C	-5.242900	-2.955700	2.195800	H	-4.852300	-1.092900	-0.131700
H	-5.299300	-0.910800	1.518200	C	-5.857900	0.426300	2.825700
H	-4.085000	-1.219100	2.758400	H	-4.450500	1.367700	4.183700
C	-4.829000	-3.797100	-0.133500	H	-4.163300	-0.349100	3.906000
H	-4.881300	-1.789600	-0.902000	H	-6.874900	-0.729700	1.295800
H	-3.369600	-2.636500	-1.259100	H	-5.627600	-1.616200	2.169500
C	-5.870700	-3.588000	0.959300	H	-6.578000	0.177600	3.615500
H	-5.999300	-2.791100	2.974400	H	-6.183100	1.388800	2.397400
H	-4.502800	-3.653000	2.620500	C	-2.397200	1.390800	-1.248400
H	-5.288800	-4.232100	-1.030100	C	-3.429100	1.094700	-2.339900
H	-4.075600	-4.521400	0.214900	C	-2.670800	2.743300	-0.591700
H	-6.356900	-4.537500	1.217600	H	-1.412400	1.447900	-1.750200
H	-6.663600	-2.923700	0.578200	C	-3.452100	2.210500	-3.380300
C	-3.404100	0.953000	-0.565100	H	-4.428300	0.999200	-1.886000
C	-3.588400	0.666800	-2.058200	H	-3.209300	0.126300	-2.813600
C	-4.719800	1.391000	0.074100	C	-2.681400	3.854400	-1.639500
H	-2.698200	1.804400	-0.501400	H	-3.653600	2.711300	-0.094000
C	-4.164700	1.883000	-2.776000	H	-1.926500	2.963700	0.188900
H	-4.273100	-0.186200	-2.187800				

C	-3.704700	3.567300	-2.732500	H	-1.425100	-0.575300	2.834400
H	-4.211600	1.999700	-4.143600	H	-2.760000	0.589900	2.880400
H	-2.482000	2.233400	-3.902400	C	0.474100	2.757200	-0.036600
H	-2.883600	4.821700	-1.161100	C	1.012600	3.962800	0.733600
H	-1.676800	3.931300	-2.088900	C	1.101900	2.626300	-1.428200
H	-3.692300	4.362400	-3.488400	H	-0.610500	2.912700	-0.202500
H	-4.713500	3.573700	-2.288800	C	0.816000	5.245500	-0.070900
C	3.515800	0.669000	-0.252900	H	2.091000	3.819300	0.912000
C	3.402600	1.337600	-1.620900	H	0.540000	4.049800	1.724100
C	4.902000	0.923300	0.348500	C	0.916700	3.926200	-2.206400
H	3.435500	-0.424800	-0.409100	H	2.180200	2.417300	-1.331900
C	4.491300	0.824800	-2.560700	H	0.628100	1.780400	-1.959100
H	3.526800	2.426900	-1.503000	C	1.460500	5.131200	-1.447500
H	2.409400	1.177600	-2.061700	H	1.222300	6.102900	0.482000
C	6.007900	0.452900	-0.593400	H	-0.263700	5.432300	-0.190700
H	5.028600	2.001900	0.537900	H	1.393600	3.840000	-3.190800
H	4.984900	0.422700	1.323900	H	-0.159100	4.074200	-2.399500
C	5.874400	1.084100	-1.974300	H	1.304900	6.056400	-2.018000
H	4.395400	1.291200	-3.550100	H	2.550500	5.019200	-1.324100
H	4.354000	-0.260100	-2.708000	C	2.074700	0.876700	1.833800
H	6.993300	0.672500	-0.161100	C	3.256000	0.913000	0.857700
H	5.944000	-0.642300	-0.692800	C	2.362400	1.746100	3.058800
H	6.656700	0.708000	-2.646500	H	1.967300	-0.168000	2.182400
H	6.029400	2.172700	-1.893000	C	4.539800	0.458100	1.543200
C	1.731100	2.786300	1.093600	H	3.387100	1.946800	0.496800
C	2.912700	3.584600	1.651800	H	3.047800	0.294600	-0.025400
C	1.138400	3.509000	-0.116700	C	3.655600	1.295500	3.738700
H	0.954000	2.796800	1.882900	H	2.461400	2.799300	2.757500
C	2.486700	4.997600	2.037900	H	1.536000	1.703700	3.781300
H	3.699800	3.646400	0.881500	C	4.833500	1.311200	2.770400
H	3.357100	3.060100	2.510300	H	5.373700	0.486500	0.829200
C	0.696700	4.919900	0.268500	H	4.431500	-0.598000	1.841600
H	1.889300	3.574100	-0.918300	H	3.860300	1.931200	4.610000
H	0.285400	2.956200	-0.537600	H	3.519500	0.271800	4.123900
C	1.854000	5.722200	0.855300	H	5.746200	0.967700	3.273800
H	3.344500	5.564900	2.422100	H	5.023400	2.349400	2.451900
H	1.756200	4.938200	2.860800	C	-3.406900	-1.857300	0.951700
H	0.270800	5.438100	-0.601500	C	-4.473900	-1.733200	2.040400
H	-0.111500	4.849300	1.017000	C	-4.003900	-2.395400	-0.351900
H	1.516100	6.723300	1.152700	H	-2.655000	-2.590200	1.299700
H	2.617700	5.870500	0.074400	C	-5.159500	-3.079900	2.265100
				H	-5.228500	-0.991900	1.740000
				H	-4.033200	-1.373100	2.980200
				C	-4.694600	-3.734600	-0.117100
				H	-4.741600	-1.671000	-0.736400
				H	-3.224700	-2.486900	-1.121600
				C	-5.756500	-3.620200	0.970500
				H	-5.932500	-2.982000	3.038200
				H	-4.419900	-3.799800	2.651300
				H	-5.134700	-4.099800	-1.053300
				H	-3.940300	-4.478700	0.184700
				H	-6.235700	-4.591800	1.145700
				H	-6.550800	-2.936900	0.627700
				C	-3.283800	1.038200	-0.170000
				C	-3.256800	0.949900	-1.699900
				C	-4.690900	1.299100	0.366700
				H	-2.660800	1.910100	0.106200
				C	-3.854500	2.216300	-2.303800
				H	-3.853700	0.079800	-2.022700
				H	-2.224800	0.785900	-2.061400
				C	-5.269000	2.568700	-0.255400
				H	-5.341900	0.448700	0.105400
				H	-4.693900	1.378000	1.464200
				C	-5.258700	2.491600	-1.777800
				H	-3.857100	2.140600	-3.398000
				H	-3.200600	3.070500	-2.056600
				H	-6.286300	2.740400	0.120600
				H	-4.666700	3.433200	0.069100
				H	-5.664500	3.416800	-2.207700
				H	-5.929000	1.677200	-2.098400

TS₇
SCF done: -1756.793321

C	6.594000	-2.458800	-0.984500
C	5.754300	-1.793100	-1.842700
C	4.356700	-1.764600	-1.617400
C	3.834400	-2.438500	-0.473000
C	4.724600	-3.125800	0.388900
C	6.074300	-3.135200	0.141700
H	3.877600	-0.572500	-3.356600
H	7.665400	-2.471200	-1.171400
H	6.150500	-1.275500	-2.715500
C	3.464500	-1.082000	-2.485800
C	2.440800	-2.376800	-0.223100
H	4.314200	-3.643000	1.255900
H	6.749000	-3.664100	0.811000
C	1.615400	-1.679300	-1.073200
C	2.115900	-1.042400	-2.235600
H	2.038400	-2.882700	0.656500
H	1.391000	-0.486500	-2.838800
C	-0.172700	-2.530300	-1.197200
O	-0.334500	-3.560100	-1.703700
F	-0.400500	0.257500	-2.482500
P	-2.327700	-0.366000	0.617500
C	-0.868700	1.430700	2.212200
H	-0.406900	1.621800	3.187600
H	-1.382000	2.359400	1.930100
P	0.461400	1.128200	0.896600
Pd	-0.248500	-0.802500	-0.411600
C	-1.872000	0.282200	2.311300

TS₇

SCF done: -1756.792480

C	-6.251175	-3.662420	0.764914
C	-5.218361	-3.674955	1.668844
C	-3.890849	-3.414272	1.254100
C	-3.644517	-3.131533	-0.121004
C	-4.728475	-3.137675	-1.033344
C	-6.004380	-3.396385	-0.600336
H	-2.999353	-3.657146	3.208704
H	-7.267263	-3.861424	1.097486
H	-5.405056	-3.884855	2.721071
C	-2.801292	-3.430397	2.161675
C	-2.322328	-2.826717	-0.525452
H	-4.529382	-2.922739	-2.082655
H	-6.831383	-3.394410	-1.306213
C	-1.289812	-2.823104	0.384408
C	-1.524791	-3.161600	1.739738
H	-2.138723	-2.590223	-1.575317
H	-0.698266	-3.168243	2.447214
C	0.364389	-3.235873	-0.601034
O	0.547522	-4.269039	-1.097842
F	-0.042589	0.020322	1.374534
P	2.314913	-0.184225	-0.337701
C	0.830119	2.251129	-0.526935
H	1.396197	3.128006	-0.188309
H	0.419892	1.746555	0.357758
P	-0.609433	2.859655	-1.588919
Pd	0.405096	-1.532761	0.140435
C	1.754781	1.306374	-1.307565
H	1.244956	0.878281	-2.184473
H	2.633186	1.837629	-1.700020
C	-1.922211	1.603059	-1.038419
C	-2.446184	1.655580	0.395380
C	-3.082495	1.560171	-2.036569
H	-1.361768	0.650393	-1.145379
C	-3.377215	0.480344	0.680465
H	-3.005730	2.595265	0.537866
H	-1.616143	1.628299	1.109609
C	-4.010207	0.383013	-1.748487
H	-3.656337	2.499927	-1.968587
H	-2.697934	1.509550	-3.064963
C	-4.528368	0.415092	-0.315039
H	-3.760186	0.544704	1.707885
H	-2.786247	-0.447006	0.629361
H	-4.843752	0.363081	-2.464354
H	-3.442240	-0.550414	-1.899982
H	-5.158526	-0.464687	-0.115669
H	-5.171596	1.302009	-0.187361
C	-0.986479	4.512085	-0.737694
C	-2.317175	5.077186	-1.241935
C	-0.889733	4.641045	0.783999
H	-0.187700	5.149993	-1.164084
C	-2.508346	6.525721	-0.802721
H	-3.142191	4.467185	-0.837089
H	-2.376357	4.991149	-2.336864
C	-1.065377	6.097560	1.210588
H	-1.671127	4.035336	1.262012
H	0.068629	4.251254	1.152688
C	-2.391848	6.659918	0.711413
H	-3.477605	6.905926	-1.151892
H	-1.736515	7.149706	-1.281981
H	-0.997656	6.183320	2.303242
H	-0.239463	6.700410	0.798100
H	-2.506899	7.708578	1.015607
H	-3.217435	6.103847	1.185394
C	3.669545	-0.895795	-1.421581
C	4.965992	-0.083784	-1.455171
C	3.965592	-2.367437	-1.121250
H	3.208300	-0.847303	-2.426324
C	5.941369	-0.660479	-2.477947
H	5.435356	-0.120982	-0.458867

H	4.764761	0.974755	-1.669049
C	4.951892	-2.942190	-2.133480
H	4.390853	-2.455119	-0.108221
H	3.036557	-2.950837	-1.121418
C	6.237940	-2.125972	-2.182634
H	6.866803	-0.070604	-2.487842
H	5.502503	-0.572327	-3.484716
H	5.166470	-3.991200	-1.893873
H	4.482702	-2.939758	-3.130423
H	6.928524	-2.537419	-2.929545
H	6.749478	-2.199974	-1.209076
C	2.968513	0.436490	1.294699
C	3.651340	-0.681343	2.086124
C	3.823788	1.703094	1.280131
H	2.004639	0.650909	1.790093
C	3.950028	-0.220889	3.509975
H	4.597948	-0.960732	1.592491
H	3.018479	-1.581318	2.094393
C	4.106700	2.157685	2.710683
H	4.781520	1.511034	0.773148
H	3.324022	2.504005	0.719483
C	4.787038	1.053291	3.512179
H	4.458279	-1.019102	4.066167
H	2.997022	-0.031601	4.027921
H	4.723144	3.065925	2.702523
H	3.154953	2.426086	3.195806
H	4.977731	1.385844	4.540485
H	5.771953	0.839300	3.064941

TS₈

SCF done: -1885.535279

C	6.379700	3.073700	0.086500
C	5.628900	2.641000	1.151100
C	4.339100	2.092700	0.953400
C	3.833500	1.980000	-0.373600
C	4.624400	2.448100	-1.450900
C	5.868800	2.982600	-1.227300
H	3.897800	1.765600	3.045800
H	7.367800	3.497800	0.251000
H	6.011400	2.721400	2.168300
C	3.522300	1.659400	2.027600
C	2.550400	1.408200	-0.579300
H	4.216800	2.383000	-2.459900
H	6.465900	3.341800	-2.062700
C	1.778900	0.982900	0.474200
C	2.276500	1.127400	1.795700
H	2.190800	1.329600	-1.605700
H	1.656100	0.816500	2.637500
F	-0.931300	2.305800	1.126900
P	0.859700	-1.861100	0.360400
C	-1.766100	-2.825000	0.528000
H	-2.528400	-3.348300	1.119000
H	-1.781600	-3.282800	-0.470200
P	-2.237400	-1.007800	0.348200
Pd	-0.109600	0.227900	0.297000
C	-0.396500	-2.987900	1.171800
H	-0.428300	-2.687500	2.228800
H	-0.065000	-4.033900	1.143400
C	-3.302400	-1.030700	-1.196800
C	-4.400800	-2.089100	-1.300700
C	-3.845700	0.360500	-1.505200
H	-2.535200	-1.258400	-1.964400
C	-5.053300	-2.042500	-2.682200
H	-5.171000	-1.897800	-0.538700
H	-4.006800	-3.095600	-1.102000
C	-4.519400	0.404800	-2.871200
H	-4.578300	0.647000	-0.731000
H	-3.036600	1.097700	-1.454900
C	-5.609100	-0.654500	-2.983900
H	-5.844300	-2.800600	-2.748700
H	-4.302000	-2.305900	-3.444500

	-4.925400	1.409400	-3.048400	H	-3.470800	3.290400	-1.349000
H	-3.759100	0.234900	-3.650800	H	-3.403200	2.622700	0.278800
H	-6.070200	-0.633800	-3.979500	C	-3.301300	4.768500	0.213500
H	-6.411000	-0.425800	-2.263000	H	-2.887400	5.579800	-0.400500
C	-3.215700	-0.738000	1.930900	H	-4.383000	4.941400	0.293300
C	-3.463400	0.739700	2.232600	H	-2.877700	4.880600	1.220100
C	-4.497700	-1.547200	2.122600				
H	-2.472300	-1.096200	2.671700	TS,			
C	-3.982700	0.905100	3.658100	SCF done:	-1756.821276		
H	-4.227500	1.125800	1.537000	C	-6.299400	-2.783600	-1.258200
H	-2.557300	1.334100	2.055900	C	-5.445900	-3.139300	-0.243600
C	-5.014800	-1.386500	3.551400	C	-4.068700	-2.820300	-0.308000
H	-5.263300	-1.171500	1.425300	C	-3.574500	-2.124500	-1.452500
H	-4.353300	-2.611500	1.888300	C	-4.480100	-1.773200	-2.484200
C	-5.244900	0.082200	3.890700	C	-5.811300	-2.092100	-2.390000
H	-4.169800	1.966100	3.864500	H	-3.532100	-3.736600	1.575700
H	-3.201500	0.584400	4.366400	H	-7.356100	-3.033900	-1.195600
H	-5.937800	-1.965800	3.684700	H	-5.816200	-3.675000	0.630100
H	-4.275300	-1.810700	4.250100	C	-3.158400	-3.175200	0.719000
H	-5.593000	0.185100	4.926600	C	-2.201400	-1.784900	-1.507800
H	-6.051500	0.474400	3.250200	H	-4.094700	-1.240800	-3.353700
C	2.467300	-2.194200	1.279100	H	-6.496900	-1.815700	-3.188200
C	2.601400	-3.586700	1.903700	C	-1.349700	-2.069900	-0.463900
C	3.713100	-1.855000	0.452000	C	-1.835400	-2.817600	0.641100
H	2.417000	-1.458200	2.099900	H	-1.821400	-1.274300	-2.395200
C	3.868000	-3.666300	2.755500	H	-1.143100	-3.098800	1.432500
H	2.648100	-4.348900	1.109700	C	0.550600	-2.504200	-1.029700
H	1.730800	-3.829500	2.526100	O	0.771100	-2.669600	-2.195900
C	4.963100	-1.923200	1.323100	F	0.896700	-3.503400	-0.141300
H	3.814900	-2.580700	-0.371800	P	2.386300	0.326000	0.204100
H	3.618700	-0.862200	-0.002500	C	0.806800	2.208500	1.626500
C	5.112400	-3.300700	1.955600	H	0.595100	3.257300	1.874000
H	3.962300	-4.671900	3.185400	H	0.932100	1.676800	2.581400
H	3.767100	-2.971300	3.604200	P	-0.647400	1.372700	0.780800
H	5.846800	-1.665200	0.726300	Pd	0.253300	-0.742900	-0.100000
H	4.887000	-1.157300	2.111400	C	2.075800	2.093000	0.781300
H	6.003000	-3.341300	2.595200	H	1.983200	2.702200	-0.129800
H	5.263400	-4.049400	1.160700	H	2.948200	2.478100	1.327000
C	0.940300	-2.564100	-1.382500	C	-2.014100	1.475400	2.063700
C	1.623900	-1.635400	-2.388500	C	-2.599800	2.847400	2.394400
C	1.458600	-3.999300	-1.484800	C	-3.123800	0.472000	1.730800
H	-0.128700	-2.579300	-1.662800	H	-1.496800	1.098500	2.967000
C	1.471100	-2.183000	-3.804300	C	-3.613800	2.742400	3.532900
H	2.693800	-1.538000	-2.148400	H	-3.113800	3.242900	1.503000
H	1.190100	-0.628300	-2.312400	H	-1.809000	3.567900	2.648200
C	1.313400						

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SCF done: -1756.821276
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C	-4.029100	0.973900	1.099200	SCF done: -1436.632565		
C	-4.286200	2.276600	0.742300	C	-6.650000	0.577800
H	-2.567100	-0.102900	-3.144700	C	-5.870100	-0.428600
H	-4.238400	3.741300	-0.851200	C	-4.665600	-0.808300
H	-3.273800	2.185800	-2.514000	C	-4.278000	-0.128400
C	-2.617300	-0.402400	-2.098500	C	-5.105200	0.903500
C	-3.168200	-1.270700	0.526600	C	-6.264700	1.251100
H	-4.231500	0.623400	2.110700	H	-4.154700	-2.373800
H	-4.698400	2.972100	1.469100	H	-7.572100	0.860800
C	-2.571300	-2.126000	-0.371200	H	-6.164800	-0.951900
C	-2.318500	-1.715900	-1.725300	C	-3.831900	-1.837400
H	-3.352700	-1.613400	1.544300	C	-3.064800	-0.489300
H	-2.051000	-2.462700	-2.468400	H	-4.800500	1.415600
C	-2.145700	-3.444500	0.115200	H	-6.893400	2.045200
O	-2.203800	-3.866300	1.232400	C	-2.249100	-1.448000
F	-1.618800	-4.201300	-0.864400	C	-2.638800	-2.149600
Pd	-0.452400	-0.562600	-1.429800	H	-2.750100	0.029600
P	1.368600	0.360100	-0.211000	H	-1.969300	-2.929800
C	3.182100	-0.004800	-0.617600	C	-0.900000	-1.598100
C	4.156500	-0.066500	0.561700	O	-0.602500	-1.502200
C	3.286500	-1.272200	-1.473000	F	-0.180200	-3.767500
H	3.478600	0.847900	-1.255600	Pd	0.465700	-1.903600
C	5.586000	-0.309000	0.082200	P	1.382800	0.261500
H	3.865000	-0.887200	1.236500	C	3.004300	0.151900
H	4.112500	0.853600	1.159500	C	4.139100	1.073700
C	4.717700	-1.513000	-1.939700	C	3.494200	-1.298400
H	2.942700	-2.138900	-0.883700	H	2.705100	0.461300
H	2.599000	-1.198100	-2.326500	C	5.345800	0.950700
C	5.679700	-1.576000	-0.759100	H	4.449300	0.800400
H	6.265700	-0.362800	0.942700	H	3.804800	2.119300
H	5.914300	0.552300	-0.522000	C	4.709000	-1.416600
H	4.771400	-2.433900	-2.534400	H	3.754700	-1.662700
H	5.020900	-0.690500	-2.608000	H	2.685200	-1.953400
H	6.709100	-1.733600	-1.105400	C	5.832300	-0.490900
H	5.422900	-2.445000	-0.131400	H	6.149700	1.614200
C	1.319100	2.250400	-0.215200	H	5.062800	1.296600
C	-0.107100	2.770300	-0.429600	H	5.051700	-2.458100
C	2.008500	2.955400	0.953300	H	4.411400	-1.151000
H	1.884400	2.493000	-1.134200	H	6.691900	-0.569600
C	-0.134400	4.287700	-0.569600	H	6.186300	-0.809200
H	-0.755400	2.472400	0.410400	C	0.403600	1.519300
H	-0.536200	2.285000	-1.318500	C	-1.090400	1.479200
C	1.956800	4.473700	0.796100	C	0.965400	2.942200
H	1.515400	2.678200	1.899100	H	0.510700	1.120700
H	3.052700	2.625900	1.038000	C	-1.890200	2.436200
C	0.524500	4.965100	0.625800	H	-1.251900	1.740000
H	-1.171200	4.629400	-0.690800	H	-1.463800	0.454700
H	0.401400	4.579000	-1.488100	C	0.134600	3.872700
H	2.435400	4.956500	1.658200	H	0.967100	3.334800
H	2.544100	4.763700	-0.090400	H	2.011600	2.943000
H	0.502300	6.056900	0.515800	C	-1.334800	3.852200
H	-0.050100	4.728700	1.536800	H	-2.947500	2.404600
C	1.134300	-0.197400	1.578000	H	-1.848200	2.089200
C	-0.202700	0.311800	2.123200	H	0.540300	4.891400
C	1.174400	-1.730300	1.638800	H	0.224800	3.549800
H	1.954000	0.206200	2.196300	H	-1.917100	4.533600
C	-0.506700	-0.233500	3.515300	H	-1.430600	4.224000
H	-0.999200	0.004400	1.424700	C	1.847900	1.008700
H	-0.220400	1.409900	2.145900	C	0.669900	1.635700
C	0.888100	-2.257000	3.041600	C	2.503100	-0.092000
H	0.415400	-2.126000	0.941500	H	2.588900	1.801700
H	2.142300	-2.111100	1.283400	C	1.112700	2.154600
C	-0.456800	-1.754900	3.548100	H	-0.117700	0.880900
H	-1.490800	0.130700	3.842800	H	0.229300	2.456000
H	0.229000	0.169100	4.231400	C	2.936700	0.440800
H	0.909900	-3.354200	3.034700	H	1.774600	-0.906500
H	1.686700	-1.926600	3.726600	H	3.361900	-0.529300
H	-0.649100	-2.124700	4.563400	C	1.754600	1.050900
H	-1.251400	-2.170000	2.908000	H	0.254000	2.589900
				H	1.839600	2.971400
				H	3.389500	-0.367000
						4.229000

H	3.718400	1.206900	3.503500
H	2.068500	1.439000	5.359700
H	1.007600	0.264800	4.575300

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SCF done: -1678.469543

C	-7.269500	2.707600	1.519800
C	-5.999500	3.217200	1.410400
C	-4.869600	2.366700	1.457200
C	-5.072700	0.964000	1.620400
C	-6.395400	0.467800	1.729500
C	-7.470700	1.318800	1.681700
H	-3.398800	3.940100	1.272500
H	-8.128500	3.373900	1.485000
H	-5.840400	4.287900	1.288900
C	-3.544700	2.863700	1.359300
C	-3.943900	0.113900	1.669900
H	-6.538700	-0.605100	1.856500
H	-8.481500	0.927400	1.770800
C	-2.466200	2.019700	1.383900
H	-4.081200	-0.959100	1.810700
H	-1.436200	2.377200	1.358300
P	-0.966200	-0.534300	-1.631200
Pd	0.007600	0.299900	0.295400
C	-2.836600	-0.488500	-1.825900
C	-3.369300	-0.352500	-3.255800
C	-3.528900	-1.649900	-1.105100
H	-3.090000	0.438100	-1.276800
C	-4.887000	-0.175800	-3.249900
H	-3.110200	-1.253000	-3.836600
H	-2.906000	0.499000	-3.770100
C	-5.041300	-1.451600	-1.097200
H	-3.294800	-2.589600	-1.632200
H	-3.146700	-1.763100	-0.083000
C	-5.582300	-1.314800	-2.514500
H	-5.255800	-0.095500	-4.280600
H	-5.132600	0.777000	-2.754300
H	-5.524700	-2.286200	-0.573000
H	-5.279800	-0.540100	-0.524300
H	-6.667900	-1.156300	-2.502400
H	-5.408500	-2.256900	-3.060300
C	-0.267200	-2.213400	-2.079900
C	-0.373400	-3.207600	-0.921200
C	-0.744700	-2.825400	-3.395900
H	0.811400	-1.978000	-2.178800
C	0.390900	-4.484600	-1.245300
H	-1.428800	-3.452800	-0.724300
H	0.009500	-2.743800	-0.002500
C	0.017600	-4.113300	-3.699500
H	-1.820100	-3.055500	-3.320800
H	-0.631800	-2.114300	-4.227200
C	-0.094700	-5.107900	-2.548800
H	0.300600	-5.193200	-0.410700
H	1.463500	-4.244700	-1.335300
H	-0.350400	-4.554700	-4.634700
H	1.079500	-3.869300	-3.864500
H	0.468800	-6.021400	-2.776900
H	-1.148800	-5.410000	-2.435300
Si	2.461500	-1.208600	2.848400
H	2.013300	-1.098000	1.418100
C	4.018500	-2.303200	2.850200
H	4.059200	-2.849200	3.804900
H	4.903800	-1.648900	2.845400
C	4.080800	-3.281700	1.681500
H	4.081500	-2.747300	0.719300
H	4.973300	-3.919800	1.704100
H	3.203600	-3.943400	1.669400
C	1.125100	-2.019400	3.903400
H	0.245800	-1.360500	3.916200
H	1.516300	-2.031600	4.932800
C	0.718500	-3.430300	3.490400

H	1.588500	-4.097100	3.402600
H	0.033000	-3.886700	4.215300
H	0.197300	-3.420600	2.525200
C	2.868000	0.491900	3.552900
H	3.818700	0.828900	3.112500
H	2.086800	1.176100	3.192100
C	2.974400	0.505300	5.075700
H	3.696000	-0.238300	5.445300
H	3.294600	1.482500	5.457500
H	2.009400	0.277200	5.544300
C	-2.669900	0.622300	1.532200
C	-1.526200	-0.333200	1.451800
O	-1.532500	-1.412100	2.003400
F	0.463500	1.636700	1.805100
C	-0.075900	0.803400	-2.485800
C	1.397100	0.737100	-2.137100
C	-0.292100	0.683300	-3.981000
H	-0.501400	1.776400	-2.124600
C	2.190800	1.783200	-2.892900
H	1.793100	-0.282500	-2.385600
H	1.529000	0.890200	-1.034400
C	0.501000	1.729900	-4.736700
H	0.019600	-0.339000	-4.321700
H	-1.382600	0.798200	-4.213400
C	1.973900	1.665200	-4.387600
H	3.281400	1.667000	-2.661300
H	1.880700	2.805500	-2.550800
H	0.369500	1.576600	-5.839300
H	0.103900	2.749300	-4.488500
H	2.521000	2.490800	-4.912700
H	2.401000	0.693500	-4.750700

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SCF done: -1337.41146

C	-6.496100	1.074900	-0.248700
C	-5.735300	0.655800	-1.311600
C	-4.587500	-0.146700	-1.107900
C	-4.234000	-0.516900	0.224000
C	-5.039900	-0.070200	1.300000
C	-6.145800	0.708600	1.070200
H	-4.056200	-0.313300	-3.197600
H	-7.375200	1.692100	-0.418800
H	-6.002000	0.935200	-2.329900
C	-3.770600	-0.583100	-2.181900
C	-3.078300	-1.303500	0.430600
H	-4.762900	-0.358200	2.313100
H	-6.758200	1.046400	1.902900
C	-2.278700	-1.673200	-0.629800
C	-2.634500	-1.312300	-1.951200
H	-2.794400	-1.594900	1.441900
H	-1.980700	-1.624800	-2.764000
C	-0.978800	-2.328000	-0.308700
O	-0.779600	-3.006500	0.665100
Pd	0.522800	-1.595300	-1.376600
P	1.413200	0.332500	-0.144200
C	3.089300	0.891200	-0.829700
C	4.140100	1.343400	0.186800
C	3.663100	-0.189900	-1.753300
H	2.833100	1.762600	-1.459600
C	5.410000	1.817900	-0.516300
H	4.395900	0.502100	0.851600
H	3.746400	2.139300	0.833100
C	4.940700	0.279000	-2.441700
H	3.873900	-1.097700	-1.163700
H	2.910600	-0.482000	-2.503300
C	5.978900	0.733200	-1.422400
H	6.154200	2.132800	0.226500
H	5.175200	2.709000	-1.120900
H	5.341700	-0.520000	-3.077800
H	4.698600	1.120900	-3.110400
H	6.885100	1.090300	-1.927900

H	6.282700	-0.129200	-0.807100
C	0.412400	1.930600	-0.176400
C	-1.093500	1.661000	-0.092700
C	0.860200	3.008400	0.811600
H	0.611700	2.305300	-1.197700
C	-1.903200	2.946500	-0.221500
H	-1.343200	1.180500	0.866200
H	-1.381300	0.943800	-0.873500
C	0.026000	4.278800	0.663700
H	0.757900	2.632000	1.842100
H	1.924900	3.240500	0.668600
C	-1.461900	3.982100	0.805700
H	-2.973200	2.720500	-0.116000
H	-1.769500	3.362500	-1.233600
H	0.348700	5.026300	1.400000
H	0.211500	4.717800	-0.330200
H	-2.049000	4.903700	0.705200
H	-1.658200	3.593000	1.818600
C	1.732300	-0.122500	1.652600
C	0.440100	-0.221600	2.469800
C	2.475100	-1.465100	1.683800
H	2.371300	0.654100	2.106500
C	0.727500	-0.677400	3.898300
H	-0.237400	-0.945400	1.989300
H	-0.081500	0.744500	2.488200
C	2.761800	-1.909200	3.114000
H	1.847500	-2.220700	1.182900
H	3.410900	-1.407000	1.109600
C	1.471400	-2.006600	3.917200
H	-0.212300	-0.749700	4.460800
H	1.337700	0.088200	4.405700
H	3.287400	-2.872400	3.106400
H	3.440000	-1.183600	3.593600
H	1.679600	-2.316500	4.949400
H	0.830600	-2.784000	3.472300
H	-0.075800	-2.909000	-2.144200

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SCF done: -1337.453314

C	-4.496800	2.012600	0.226700
C	-4.380700	1.192800	-0.874000
C	-3.738000	-0.060000	-0.781300
C	-3.205200	-0.466100	0.477000
C	-3.363100	0.380800	1.596000
C	-3.989500	1.600300	1.474700
H	-3.984300	-0.582200	-2.870700
H	-4.988000	2.978900	0.135800
H	-4.778700	1.505200	-1.839100
C	-3.578500	-0.911000	-1.915200
C	-2.508400	-1.709600	0.569800
H	-2.964900	0.054400	2.556700
H	-4.096700	2.246900	2.342400
C	-2.394200	-2.548100	-0.556400
C	-2.917600	-2.102500	-1.813900
H	-2.231000	-2.104800	1.547600
H	-2.800400	-2.751600	-2.681600
C	-1.834900	-3.904200	-0.422700
O	-1.557200	-4.449700	0.625800
Pd	-0.486700	-1.421900	-0.456800
P	1.198100	0.226400	-0.225000
C	2.850000	-0.118000	-1.065300
C	4.015900	0.793400	-0.682200
C	3.230900	-1.598500	-0.970900
H	2.604600	0.076000	-2.126100
C	5.262900	0.468000	-1.502100
H	4.249300	0.668100	0.387700
H	3.739900	1.847800	-0.821100
C	4.478900	-1.897600	-1.794500
H	3.419000	-1.872600	0.078500
H	2.381700	-2.215500	-1.298100
C	5.639700	-1.003200	-1.374900

H	6.096300	1.111900	-1.192300
H	5.065700	0.699000	-2.561500
H	4.749600	-2.956700	-1.698100
H	4.258900	-1.726200	-2.860900
H	6.534400	-1.224200	-1.970900
H	5.900800	-1.219400	-0.325700
C	0.700800	1.895800	-0.988700
C	-0.809800	1.932100	-1.243800
C	1.156600	3.156300	-0.248700
H	1.202200	1.886100	-1.974000
C	-1.236000	3.202900	-1.968200
H	-1.347000	1.874400	-0.282400
H	-1.110400	1.036800	-1.806900
C	0.716900	4.421400	-0.983500
H	0.720800	3.169500	0.762900
H	2.246900	3.162200	-0.114700
C	-0.791000	4.441700	-1.202200
H	-2.326100	3.199000	-2.104700
H	-0.789500	3.219200	-2.976100
H	1.041600	5.308700	-0.424300
H	1.223100	4.465700	-1.961600
H	-1.091100	5.356600	-1.729300
C	-1.301200	4.458700	-0.224500
C	1.551600	0.609000	1.585900
C	0.222800	0.873300	2.303600
C	2.291500	-0.533500	2.286100
C	2.177600	1.515400	1.641500
C	0.433100	1.186700	3.780400
H	-0.401800	-0.030700	2.200000
H	-0.339800	1.684000	1.818600
C	2.501200	-0.229900	3.767900
H	1.703700	-1.460600	2.173800
H	3.264000	-0.719800	1.810700
C	1.183100	0.057300	4.475300
H	-0.536300	1.366200	4.265300
H	1.008400	2.122600	3.875300
H	3.024700	-1.065500	4.249900
H	3.160800	0.648300	3.862600
H	1.357700	0.298600	5.531700
H	0.559500	-0.851000	4.459300
H	-1.683900	-4.421100	-1.403400

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SCF done: -1224.098523

C	7.217600	0.024300	-0.162200
C	6.279500	-0.811600	0.391900
C	4.910900	-0.694200	0.052100
C	4.511800	0.310200	-0.876300
C	5.502600	1.158400	-1.428400
C	6.824200	1.020100	-1.083400
H	4.216700	-2.307400	1.311900
H	8.267100	-0.077700	0.105600
H	6.575600	-1.582900	1.102800
C	3.912900	-1.537500	0.601000
C	3.135600	0.433900	-1.204500
H	5.191500	1.925300	-2.137800
H	7.573900	1.678400	-1.517500
C	2.156300	-0.400400	-0.689600
C	2.597100	-1.393700	0.238700
H	2.869400	1.237600	-1.898300
H	1.860600	-2.070100	0.680400
Pd	0.217700	-0.269700	-1.444500
P	-1.451000	0.005500	-0.000900
C	-2.595700	-1.486500	0.054200
C	-3.762600	-1.456200	-0.930400
C	-1.776100	-2.769300	-0.126500
H	-3.015900	-1.482700	1.074600
C	-4.632700	-2.703200	-0.782900
H	-3.366000	-1.406600	-1.957400
H	-4.376600	-0.558100	-0.777700
C	-2.650900	-4.009600	0.023300

H	-1.325900	-2.750700	-1.132600
H	-0.936500	-2.805400	0.581300
C	-3.815900	-3.977600	-0.957000
H	-5.456800	-2.666600	-1.506500
H	-5.095100	-2.703600	0.217600
H	-2.044800	-4.912100	-0.124100
H	-3.041800	-4.059800	1.052500
H	-4.452600	-4.862300	-0.830900
H	-3.422900	-4.017400	-1.985400
C	-0.797600	-0.012400	1.779500
C	0.454900	0.830300	2.023800
C	-1.840700	0.243900	2.874000
H	-0.487500	-1.070600	1.862400
C	1.053200	0.492300	3.384900
H	0.200400	1.900200	2.005300
H	1.184700	0.664800	1.222700
C	-1.243400	-0.074300	4.246100
H	-2.151800	1.300000	2.853800
H	-2.752300	-0.350400	2.721700
C	0.036600	0.713900	4.499200
H	1.953900	1.094400	3.556900
H	1.382300	-0.559800	3.379000
H	-1.984800	0.125800	5.030700
H	-1.020800	-1.152300	4.293500
H	0.460700	0.445000	5.475100
H	-0.208500	1.787500	4.550900
C	-2.527300	1.539400	-0.182300
C	-1.860800	2.801000	0.376400
C	-2.950800	1.797300	-1.631200
H	-3.425300	1.318200	0.425800
C	-2.791500	4.007300	0.272700
H	-0.932600	2.990500	-0.188500
H	-1.567200	2.665100	1.422400
C	-3.899700	2.988000	-1.724900
H	-2.041900	1.999900	-2.219600
H	-3.405300	0.908800	-2.080900
C	-3.255300	4.245000	-1.157300
H	-2.288400	4.896600	0.672800
H	-3.670800	3.831500	0.914200
H	-4.198000	3.141700	-2.769500
H	-4.823100	2.763200	-1.165800
H	-3.949200	5.093900	-1.201700
H	-2.386700	4.515500	-1.778500
H	-1.309200	-0.236200	-2.068400

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SCF done: -1224.182010

C	4.866700	1.145700	0.704800
C	4.623300	0.801800	-0.605300
C	3.821900	-0.315600	-0.927300
C	3.257500	-1.083600	0.132100
C	3.537600	-0.718900	1.467300
C	4.320300	0.376600	1.751600
H	3.976700	-0.085700	-3.075500
H	5.484600	2.010300	0.936300
H	5.047300	1.389700	-1.419000
C	3.549700	-0.687400	-2.274400
C	2.433200	-2.210200	-0.184800
H	3.110600	-1.319100	2.272200
H	4.523400	0.647300	2.785500
C	2.215300	-2.580200	-1.520200
C	2.771800	-1.777200	-2.563700
H	2.128500	-2.869400	0.628900
H	2.587800	-2.057900	-3.598300
Pd	0.451600	-1.353100	-0.969500
P	-1.166400	0.172800	-0.185100
C	-0.740500	1.952300	-0.661300
C	-1.424900	3.064500	0.132800
C	0.774300	2.171200	-0.740300
H	-1.119200	1.998200	-1.699800
C	-1.067200	4.443200	-0.419700

H	-1.113800	3.011600	1.189000
H	-2.515100	2.931900	0.121000
C	1.106900	3.550900	-1.296300
H	1.217100	2.080600	0.263600
H	1.231700	1.374400	-1.345800
C	0.441800	4.648400	-0.473700
H	-1.544900	5.225600	0.184700
H	-1.480200	4.539700	-1.437200
H	2.196100	3.688300	-1.322000
H	0.756200	3.618900	-2.339400
H	0.679700	5.639500	-0.881200
H	0.846400	4.625100	0.551700
C	-2.976000	0.039700	-0.739300
C	-3.263000	-1.368000	-1.273000
C	-4.050600	0.462200	0.265500
H	-3.028100	0.733700	-1.598500
C	-4.660800	-1.464500	-1.874300
H	-3.166200	-2.094900	-0.449200
H	-2.495800	-1.646900	-2.008500
C	-5.444300	0.370300	-0.352300
H	-4.011600	-0.199200	1.145700
H	-3.870000	1.479100	0.638000
C	-5.725300	-1.034200	-0.872200
H	-4.851200	-2.485900	-2.228400
H	-4.715800	-0.811600	-2.760900
H	-6.202400	0.670700	0.382800
H	-5.516300	1.086700	-1.186900
H	-6.724900	-1.085600	-1.323100
H	-5.728300	-1.737700	-0.023500
C	-1.220200	0.091900	1.701400
C	-1.563900	-1.344800	2.114300
C	0.135300	0.498400	2.287100
H	-1.999500	0.774400	2.080500
C	-1.491500	-1.544500	3.623700
H	-0.846300	-2.022600	1.619100
H	-2.558000	-1.629400	1.741900
C	0.223200	0.263900	3.791500
H	0.920200	-0.086000	1.778000
H	0.350400	1.553200	2.070900
C	-0.110800	-1.176600	4.150700
H	-1.741700	-2.583500	3.875300
H	-2.247900	-0.911400	4.116400
H	1.229600	0.531200	4.143100
H	-0.479100	0.936700	4.310500
H	-0.051400	-1.331700	5.235800
H	0.637700	-1.845900	3.693100
H	1.766400	-3.543000	-1.760400

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SCF done: -1323.347500

C	6.263800	-0.085500	0.679700
C	5.428900	-1.174700	0.681700
C	4.143300	-1.104100	0.093300
C	3.723700	0.117800	-0.508500
C	4.607900	1.224400	-0.495800
C	5.847200	1.126000	0.085300
H	3.593200	-3.155400	0.503800
H	7.249800	-0.152000	1.133800
H	5.743700	-2.114200	1.134500
C	3.260100	-2.211400	0.072800
C	2.425500	0.200700	-1.081300
H	4.282900	2.156200	-0.957400
H	6.515900	1.984000	0.088000
C	1.585200	-0.881300	-1.040300
C	2.010600	-2.112900	-0.489000
H	2.118300	1.144600	-1.528800
H	1.350200	-2.976700	-0.516300
F	0.369800	-1.785300	-3.465900
Pd	-0.216800	-0.876900	-1.844800
P	-1.245600	0.208600	-0.051400
C	-1.474900	2.041200	-0.429100

C	-2.086900	2.881000	0.694000	O	-1.826800	-1.733000	1.793100
C	-0.202100	2.680500	-0.991000	F	-1.664300	-2.831000	-0.181800
H	-2.201800	2.007000	-1.261900	Pd	-0.655300	-0.262100	-0.412900
C	-2.314800	4.322000	0.242400	P	1.711700	0.240400	-0.270200
H	-1.413300	2.881900	1.566000	C	2.856700	-0.960900	-1.223100
H	-3.036500	2.444100	1.030200	C	4.345400	-0.888300	-0.852500
C	-0.452900	4.122000	-1.421400	C	2.330600	-2.405600	-1.137000
H	0.596200	2.661700	-0.232400	H	2.744500	-0.629600	-2.271800
H	0.156300	2.079600	-1.839000	C	5.164700	-1.822800	-1.761000
C	-1.027400	4.947900	-0.276800	H	4.475300	-1.202000	0.195000
H	-2.729800	4.910900	1.070300	H	4.716200	0.143300	-0.945100
H	-3.071100	4.332200	-0.558900	C	3.156500	-3.320800	-2.053300
H	0.477300	4.566900	-1.796400	H	2.413900	-2.768400	-0.101500
H	-1.163400	4.128400	-2.263500	H	1.264500	-2.433900	-1.404400
H	-1.204300	5.982400	-0.596700	C	4.642000	-3.263700	-1.667900
H	-0.291800	4.993800	0.543100	H	6.226300	-1.779300	-1.480400
C	-3.039500	-0.414400	-0.006100	H	5.078700	-1.475300	-2.803100
C	-3.156400	-1.822800	-0.603500	H	2.782400	-4.351700	-1.986100
C	-3.757300	-0.344800	1.345500	H	3.039800	-2.988800	-3.097700
H	-3.556100	0.277400	-0.696100	H	5.231700	-3.924300	-2.318400
C	-4.612500	-2.265300	-0.710700	H	4.757500	-3.621900	-0.631900
H	-2.597600	-2.536700	0.023700	C	2.237900	1.951000	-0.974800
H	-2.678700	-1.860900	-1.594700	C	1.004400	2.864100	-1.112400
C	-5.215400	-0.777300	1.212900	C	3.351900	2.671100	-0.199100
H	-3.256900	-1.012900	2.064500	H	2.611700	1.726600	-1.990000
H	-3.705400	0.664500	1.773700	C	1.383700	4.182800	-1.804100
C	-5.320400	-2.182600	0.636100	H	0.598400	3.079500	-0.110300
H	-4.663700	-3.282700	-1.117500	H	0.217200	2.345200	-1.681900
H	-5.132300	-1.614200	-1.432100	C	3.727700	3.987800	-0.901300
H	-5.711000	-0.719000	2.190500	H	3.000400	2.902100	0.818600
H	-5.743200	-0.071300	0.551500	H	4.239100	2.028400	-0.110400
H	-6.371200	-2.482800	0.538400	C	2.498800	4.898300	-1.029000
H	-4.854500	-2.895100	1.336000	H	0.499200	4.828800	-1.888600
C	-0.627700	0.046800	1.714900	H	1.736700	3.962700	-2.824500
C	-0.445100	-1.433100	2.071400	H	4.523800	4.494500	-0.338000
C	0.662400	0.826600	1.989400	H	4.118000	3.762000	-1.906500
H	-1.420900	0.465800	2.357900	H	2.770100	5.837200	-1.531000
C	-0.000700	-1.596600	3.521600	H	2.132100	5.150900	-0.021000
H	0.320100	-1.863900	1.408400	C	2.219200	0.256700	1.577600
H	-1.370300	-1.998000	1.890600	C	1.164200	1.091500	2.335700
C	1.106700	0.649400	3.438900	C	2.266900	-1.169400	2.154300
H	1.456800	0.470100	1.317200	H	3.210400	0.725600	1.682800
H	0.524500	1.894700	1.773400	C	1.454700	1.109100	3.844200
C	1.285300	-0.823000	3.785000	H	0.175800	0.632800	2.162200
H	0.131300	-2.661200	3.752700	H	1.130800	2.119300	1.943100
H	-0.795300	-1.226000	4.190800	C	2.557200	-1.136300	3.663900
H	2.038200	1.203400	3.609500	H	1.292800	-1.655200	1.996000
H	0.350000	1.090600	4.108500	H	3.036000	-1.763800	1.643100
H	1.599200	-0.938600	4.830100	C	1.480600	-0.323100	4.393400
H	2.092200	-1.243400	3.162600	H	0.688100	1.705300	4.358500

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SCF done: -1436.690140

C	-5.416200	4.151500	-2.840700
C	-4.959400	2.979200	-3.389000
C	-4.148400	2.092400	-2.636700
C	-3.815100	2.439100	-1.289500
C	-4.305300	3.657200	-0.752000
C	-5.085200	4.494600	-1.508700
H	-3.961700	0.600100	-4.191900
H	-6.037400	4.823000	-3.427300
H	-5.214100	2.709500	-4.412200
C	-3.678500	0.863900	-3.174200
C	-3.010100	1.546700	-0.533700
H	-4.048700	3.913100	0.274400
H	-5.455200	5.426100	-1.088800
C	-2.533500	0.390000	-1.105700
C	-2.900500	0.018800	-2.423500
H	-2.782200	1.781300	0.507100
H	-2.564600	-0.935400	-2.819800
C	-1.661000	-1.683600	0.600100

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SCF done: -1436.649383

C	-6.393000	1.110800	-0.506000
C	-5.699100	0.311600	-1.381200
C	-4.551800	-0.399000	-0.958200
C	-4.131400	-0.278700	0.399200
C	-4.866600	0.552600	1.279000
C	-5.972500	1.234500	0.836700
H	-4.145400	-1.329000	-2.867700
H	-7.272600	1.653400	-0.844600
H	-6.020200	0.214200	-2.417200
C	-3.801300	-1.220100	-1.840200
C	-2.975700	-0.975100	0.820100
H	-4.536300	0.638200	2.313400
H	-6.531300	1.870700	1.518900

C	-2.244100	-1.722900	-0.076600	H	5.403200	3.258800	-2.177000
C	-2.665600	-1.858800	-1.424100	C	3.073000	2.791400	-0.885300
H	-2.641400	-0.884900	1.853500	C	3.331300	1.046500	1.291400
H	-2.065100	-2.495200	-2.067000	H	5.864000	0.202700	1.724800
C	-0.942600	-2.226000	0.409700	H	7.843500	0.790900	0.360800
O	-0.649200	-2.657400	1.479400	C	2.091700	1.510200	0.909300
F	-0.443900	-3.512700	-1.184600	C	1.963200	2.415000	-0.179300
Pd	0.533600	-1.725900	-0.850500	H	3.418100	0.368700	2.140300
P	1.383400	0.345900	-0.177700	H	0.977400	2.812700	-0.402700
C	3.015500	0.711800	-1.069500	C	0.892700	0.898900	1.545300
C	4.078700	1.472000	-0.273000	O	0.797900	0.572200	2.722300
C	3.603200	-0.573800	-1.663000	F	-0.999700	2.927800	0.424600
H	2.703300	1.351900	-1.914700	Pd	-0.711700	0.781600	0.323700
C	5.306600	1.759700	-1.134100	P	-0.380800	-1.534500	-0.216500
H	4.388600	0.869100	0.596100	C	-1.949600	-2.318100	-1.031500
H	3.674200	2.410300	0.130000	C	-2.051600	-3.850700	-0.912700
C	4.836900	-0.283000	-2.511100	C	-3.250500	-1.689700	-0.511600
H	3.872200	-1.264000	-0.846300	H	-1.842000	-2.049500	-2.098600
H	2.840800	-1.094100	-2.264200	C	-3.251400	-4.357200	-1.736700
C	5.888900	0.475400	-1.710900	H	-2.204900	-4.123800	0.143400
H	6.059400	2.296500	-0.542800	H	-1.135900	-4.346200	-1.257800
H	5.020000	2.431500	-1.959400	C	-4.452100	-2.184700	-1.329400
H	5.248800	-1.219400	-2.907900	H	-3.394500	-1.971300	0.544200
H	4.539400	0.322300	-3.382700	H	-3.178000	-0.597700	-0.554100
H	6.764600	0.695500	-2.334400	C	-4.559400	-3.713400	-1.256700
H	6.243900	-0.162000	-0.884900	H	-3.312500	-5.451900	-1.662400
C	0.338000	1.850400	-0.620500	H	-3.090100	-4.101300	-2.796200
C	-1.152900	1.604300	-0.378400	H	-5.371400	-1.712000	-0.953200
C	0.805200	3.175600	-0.016400	H	-4.325000	-1.876100	-2.380000
H	0.477300	1.907800	-1.716100	H	-5.402900	-4.072000	-1.862500
C	-2.004800	2.782700	-0.834200	H	-4.744300	-4.011400	-0.212300
H	-1.336500	1.431400	0.693500	C	0.955000	-1.803000	-1.579100
H	-1.461900	0.686100	-0.894400	C	2.170400	-0.889200	-1.354500
C	-0.068700	4.336200	-0.488300	C	1.397900	-3.261800	-1.781600
H	0.758400	3.118900	1.083200	H	0.440400	-1.463000	-2.495900
H	1.855300	3.368100	-0.276100	C	3.172500	-1.006200	-2.511600
C	-1.540100	4.080100	-0.185000	H	2.677200	-1.165100	-0.416400
H	-3.059800	2.578400	-0.602800	H	1.838100	0.150900	-1.253500
H	-1.935900	2.879700	-1.929900	C	2.402300	-3.359800	-2.944500
H	0.270000	5.271300	-0.024000	H	1.879000	-3.630600	-0.862700
H	0.058600	4.462800	-1.575700	H	0.535500	-3.905500	-1.992400
H	-2.154300	4.925500	-0.520000	C	3.620700	-2.462000	-2.691200
H	-1.675900	4.007000	0.906900	H	4.034000	-0.352700	-2.308200
C	1.778900	0.407400	1.658300	H	2.694300	-0.655900	-3.440900
C	0.520000	0.517700	2.525900	H	2.712700	-4.406400	-3.072700
C	2.568900	-0.854400	2.030700	H	1.905100	-3.041300	-3.874700
H	2.406900	1.294600	1.846800	H	4.334500	-2.545900	-3.522200
C	0.867400	0.474800	4.011900	H	4.131700	-2.797100	-1.774000
H	-0.152800	-0.322500	2.290400	C	-0.009600	-2.629400	1.306400
H	-0.027600	1.443400	2.302100	C	1.449600	-2.473000	1.777500
C	2.909700	-0.881200	3.516900	C	-1.025200	-2.195200	2.390000
H	1.957900	-1.736300	1.778800	H	-0.186200	-3.682400	1.037200
H	3.485700	-0.930200	1.428700	C	1.667000	-3.111000	3.159100
C	1.645000	-0.786700	4.360900	H	1.694900	-1.408400	1.854400
H	-0.051200	0.543300	4.608600	H	2.130200	-2.926200	1.043300
H	1.473600	1.359300	4.268000	C	-0.748500	-2.880500	3.733500
H	3.468700	-1.795300	3.753700	H	-0.930800	-1.108700	2.536000
H	3.574200	-0.034200	3.756100	H	-2.048600	-2.408700	2.051000
H	1.888800	-0.807400	5.430600	C	0.675500	-2.523200	4.171900
H	1.013600	-1.666300	4.158600	H	2.703900	-2.933600	3.478100
				H	1.517900	-4.200900	3.093800
				H	-1.483400	-2.536900	4.474300
				H	-0.848900	-3.973300	3.634400
				H	0.885500	-2.895900	5.183100
				H	0.761000	-1.424100	4.164600
				Si	-2.819300	2.939100	-0.188000
				H	-2.285300	1.200400	-0.445600
				C	-4.056500	2.465400	1.193100
				H	-5.016300	2.936200	0.922000
				H	-3.702900	2.996400	2.093200
				C	-4.269700	0.983600	1.510300
				H	-3.310100	0.496900	1.737200

TS₁₂
SCF done: -1678.45444

C	6.733900	2.062600	-0.997600
C	5.508800	2.588300	-1.326600
C	4.356200	2.268800	-0.567300
C	4.489100	1.389900	0.551900
C	5.769700	0.868600	0.869400
C	6.866500	1.196100	0.112000
H	2.988100	3.495700	-1.710600
H	7.611000	2.311000	-1.588800

H	-4.937600	0.855100	2.373300
H	-4.711200	0.456200	0.653900
C	-3.352700	2.818500	-2.032100
H	-2.473900	3.106200	-2.634000
H	-4.107300	3.604400	-2.197400
C	-3.885600	1.460700	-2.500400
H	-4.737000	1.136600	-1.882900
H	-4.218300	1.498800	-3.546900
H	-3.100600	0.695600	-2.414400
C	-2.731000	4.858500	0.014400
H	-2.261700	5.093000	0.981500
H	-2.060700	5.267000	-0.759500
C	-4.101900	5.554700	-0.072800
H	-4.754800	5.245400	0.755300
H	-4.000600	6.647900	-0.022300
H	-4.617200	5.315300	-1.014600

TS₁₃

SCF done: -1337.411345

C	-6.346800	1.181200	-0.153800
C	-5.613800	0.794000	-1.248400
C	-4.501800	-0.069700	-1.105600
C	-4.157200	-0.539000	0.196700
C	-4.934500	-0.124500	1.306000
C	-6.004100	0.718000	1.136200
H	-3.994400	-0.132100	-3.207000
H	-7.197100	1.848100	-0.276200
H	-5.874300	1.148400	-2.244700
C	-3.711700	-0.473600	-2.212300
C	-3.030400	-1.379100	0.344300
H	-4.663400	-0.487100	2.296500
H	-6.593700	1.031400	1.994500
C	-2.247200	-1.705800	-0.742000
C	-2.601100	-1.255300	-2.036400
H	-2.746500	-1.736500	1.334100
H	-1.963800	-1.536800	-2.873100
C	-0.950600	-2.387700	-0.465800
O	-0.751100	-3.131500	0.458700
Pd	0.544800	-1.532400	-1.454700
P	1.397700	0.343700	-0.129800
C	3.059100	1.000200	-0.762600
C	4.078900	1.434200	0.292600
C	3.679900	-0.009000	-1.735700
H	2.777200	1.894600	-1.347600
C	5.345200	1.982100	-0.362000
H	4.350700	0.570300	0.921200
H	3.648300	2.184700	0.969100
C	4.953400	0.535300	-2.373700
H	3.909500	-0.942200	-1.195100
H	2.947000	-0.279200	-2.512200
C	5.960300	0.962600	-1.312500
H	6.067400	2.278400	0.409600
H	5.094700	2.896500	-0.923900
H	5.389400	-0.215100	-3.045300
H	4.697500	1.405100	-3.000500
H	6.865400	1.369700	-1.780600
H	6.276500	0.077400	-0.736800
C	0.336400	1.902500	-0.078700
C	-1.157800	1.574000	-0.008600
C	0.738500	2.952300	0.957700
H	0.520300	2.331000	-1.081900
C	-2.014000	2.831100	-0.102800
H	-1.389300	1.061100	0.938000
H	-1.420100	0.867900	-0.807700
C	-0.142000	4.196500	0.855800
H	0.642700	2.528600	1.970400
H	1.794900	3.228800	0.833200
C	-1.620800	3.842600	0.967000
H	-3.076200	2.558400	-0.021900
H	-1.883000	3.287300	-1.098000
H	0.145100	4.921900	1.628000

H	0.038400	4.685700	-0.115400
H	-2.238400	4.746900	0.895300
H	-1.814200	3.408500	1.962100
C	1.714100	-0.215300	1.639100
C	0.413000	-0.408800	2.425300
C	2.499900	-1.532200	1.596300
H	2.318800	0.550800	2.152700
C	0.690100	-0.951800	3.825000
H	-0.234600	-1.116100	1.882300
H	-0.137800	0.538000	2.501700
C	2.776200	-2.063400	2.999000
H	1.905100	-2.271100	1.033700
H	3.442800	-1.405400	1.044900
C	1.476500	-2.254400	3.770500
H	-0.257000	-1.092200	4.362000
H	1.265000	-0.202900	4.394600
H	3.332800	-3.007100	2.936800
H	3.422400	-1.351400	3.539400
H	1.678700	-2.624900	4.783700
H	0.869100	-3.021600	3.265700
H	-0.059800	-2.833000	-2.250400

TS₁₄

SCF done: -1337.387027

C	6.144100	0.661300	0.601200
C	5.330600	-0.285100	1.172600
C	4.176000	-0.749900	0.498800
C	3.872500	-0.226000	-0.793100
C	4.733000	0.747300	-1.357200
C	5.841700	1.183500	-0.676400
H	3.554800	-2.119400	2.052400
H	7.027000	1.012600	1.130300
H	5.557900	-0.691600	2.157400
C	3.308600	-1.715500	1.070200
C	2.699200	-0.671500	-1.452400
H	4.494500	1.144000	-2.343300
H	6.494300	1.932600	-1.118800
C	1.854300	-1.583800	-0.863600
C	2.183000	-2.128900	0.403500
H	2.461400	-0.253900	-2.433200
H	1.526000	-2.876800	0.849100
C	0.818900	-2.686000	-2.074400
O	1.384600	-3.537700	-2.631700
Pd	-0.341200	-1.398800	-1.251500
P	-1.317300	0.276500	0.178300
C	-2.597400	-0.545600	1.297300
C	-3.955100	-0.806700	0.645900
C	-2.010500	-1.854800	1.839700
H	-2.760100	0.143000	2.144800
C	-4.908200	-1.499000	1.617900
H	-3.810700	-1.440400	-0.244500
H	-4.404000	0.134900	0.303200
C	-2.967500	-2.538600	2.811000
H	-1.811300	-2.523300	0.985000
H	-1.040500	-1.678400	2.326600
C	-4.317000	-2.796100	2.153400
H	-5.870200	-1.685700	1.123500
H	-5.117800	-0.821400	2.461800
H	-2.526600	-3.475600	3.174600
H	-3.110800	-1.895700	3.694700
H	-5.008400	-3.271300	2.861000
H	-4.182400	-3.503900	1.320200
C	-0.214200	1.058700	1.499800
C	1.168100	1.474500	0.990600
C	-0.847400	2.174300	2.336000
H	-0.047400	0.194800	2.170700
C	2.077800	1.868400	2.149200
H	1.081500	2.328900	0.302500
H	1.616600	0.657800	0.416800
C	0.072900	2.568700	3.490300
H	-1.024900	3.058500	1.703900

H	-1.829300	1.874100	2.726800
C	1.453900	2.977000	2.988500
H	3.060500	2.171600	1.762200
H	2.254600	0.982600	2.782200
H	-0.383700	3.379400	4.073100
H	0.175300	1.710900	4.174300
H	2.104400	3.241600	3.831900
H	1.357100	3.885600	2.371500
C	-2.204300	1.683500	-0.707300
C	-1.229500	2.772900	-1.169000
C	-2.978500	1.165400	-1.927000
H	-2.911400	2.126200	0.018400
C	-1.956000	3.901900	-1.896200
H	-0.482800	2.315700	-1.842100
H	-0.672800	3.190800	-0.323000
C	-3.723100	2.293400	-2.633400
H	-2.257200	0.703600	-2.619900
H	-3.672700	0.364300	-1.653800
C	-2.762800	3.386800	-3.079800
H	-1.231800	4.661100	-2.218800
H	-2.634800	4.400700	-1.185200
H	-4.279300	1.891400	-3.489600
H	-4.471900	2.721900	-1.946600
H	-3.303600	4.209400	-3.565000
H	-2.074600	2.974100	-3.834700
H	-1.846300	-1.656300	-1.771200

TS₁₅

SCF done: -1224.095211

C	-6.858100	0.129900	-3.836900
C	-6.055100	-0.953600	-3.581000
C	-4.718800	-0.781400	-3.147000
C	-4.210200	0.539200	-2.976500
C	-5.065500	1.636500	-3.245500
C	-6.357300	1.440000	-3.665700
H	-4.248400	-2.885300	-3.003600
H	-7.882600	-0.015800	-4.172700
H	-6.434100	-1.967200	-3.710700
C	-3.860400	-1.874100	-2.873100
C	-2.870900	0.707300	-2.537600
H	-4.671900	2.644400	-3.113700
H	-7.001300	2.292800	-3.870400
C	-2.021200	-0.356200	-2.276900
C	-2.568900	-1.664000	-2.454700
H	-2.521100	1.735700	-2.400800
H	-1.938700	-2.533100	-2.249300
Pd	-0.004000	-0.103600	-1.822300
P	1.493000	0.056600	-0.171600
C	2.727300	-1.357700	-0.279600
C	3.563500	-1.606700	0.977600
C	2.071400	-2.649700	-0.778200
H	3.399700	-1.005700	-1.081800
C	4.595100	-2.706600	0.732600
H	2.908400	-1.911000	1.808500
H	4.070600	-0.687400	1.297500
C	3.114300	-3.738300	-1.006700
H	1.331800	-3.002100	-0.042300
H	1.514700	-2.440500	-1.702500
C	3.933000	-3.991900	0.253400
H	5.173500	-2.883500	1.648400
H	5.312500	-2.362300	-0.029600
H	2.623900	-4.659800	-1.344500
H	3.788500	-3.426500	-1.820700
H	4.687200	-4.769200	0.076800
H	3.268500	-4.373400	1.045800
C	2.529400	1.624600	-0.285300
C	1.762900	2.770600	-0.954600
C	3.171900	2.094300	1.023900
H	3.332500	1.318900	-0.980200
C	2.671700	3.973900	-1.183000
H	0.911000	3.068000	-0.321400

H	1.337500	2.416000	-1.902600
C	4.079100	3.298700	0.778900
H	2.386400	2.384900	1.738800
H	3.743800	1.288700	1.502300
C	3.316100	4.438600	0.117100
H	2.102800	4.788600	-1.648200
H	3.461400	3.695900	-1.899500
H	4.523300	3.626800	1.727400
H	4.916000	2.994800	0.129700
H	3.981300	5.292300	-0.063600
H	2.530500	4.793000	0.804300
C	0.744900	0.041700	1.555900
C	-0.228200	1.215000	1.719800
C	0.055100	-1.293500	1.851300
H	1.591000	0.172100	2.254700
C	-0.937300	1.188100	3.070400
H	-0.980200	1.154700	0.918800
H	0.295700	2.172500	1.594200
C	-0.652100	-1.282900	3.202900
H	-0.688300	-1.488200	1.063600
H	0.780700	-2.117500	1.820400
C	-1.652400	-0.138800	3.282700
H	-1.642800	2.026600	3.127800
H	-0.201800	1.338300	3.878400
H	-1.147600	-2.249100	3.361900
H	0.092300	-1.173800	4.009400
H	-2.177400	-0.147400	4.246200
H	-2.416200	-0.271300	2.498400
H	-0.619700	-0.162200	-3.365200

TS₁₆

SCF done: -1436.629709

C	-7.660000	0.277000	-0.597300
C	-6.818300	-0.805900	-0.638800
C	-5.453600	-0.675400	-0.288400
C	-4.965000	0.603500	0.112000
C	-5.858400	1.702200	0.144700
C	-7.175900	1.543700	-0.201600
H	-4.946100	-2.750700	-0.620700
H	-8.706600	0.164000	-0.870300
H	-7.187300	-1.784000	-0.944200
C	-4.562700	-1.777800	-0.315000
C	-3.600100	0.733600	0.466300
H	-5.476500	2.675200	0.450800
H	-7.853500	2.393800	-0.173800
C	-2.756900	-0.351900	0.417000
C	-3.247400	-1.625800	0.036900
H	-3.228900	1.710600	0.778000
H	-2.569700	-2.478500	0.018700
C	-1.357600	-0.381300	1.766800
O	-1.584300	-0.593300	2.887500
F	-0.421600	0.288100	-1.898900
Pd	-0.654100	-0.037200	0.084800
P	1.699800	0.072600	-0.158000
C	2.116100	-1.326500	-1.328600
C	3.608500	-1.551900	-1.564800
C	1.391300	-2.634800	-0.998400
H	1.645700	-0.935400	-2.246000
C	3.839000	-2.612300	-2.639700
H	4.086900	-1.880200	-0.626200
H	4.101000	-0.613400	-1.856200
C	1.632600	-3.671700	-2.090700
H	1.744600	-3.040700	-0.038100
H	0.315700	-2.437400	-0.882100
C	3.123400	-3.913200	-2.297200
H	4.915000	-2.782500	-2.775200
H	3.456600	-2.232800	-3.600600
H	1.119400	-4.608700	-1.839000
H	1.187400	-3.312400	-3.031800
H	3.289500	-4.661400	-3.082600
H	3.553600	-4.329600	-1.371100

C	2.286400	1.595400	-1.100500	H	-4.427000	0.396900	-0.838300
C	1.248600	2.720600	-1.035400	H	-6.071900	-1.386000	-1.502500
C	3.690400	2.087800	-0.741600	H	-5.271000	-2.532000	-0.406200
H	2.301700	1.240900	-2.145000	C	-0.249600	-2.432900	1.382600
C	1.677900	3.911000	-1.885700	C	-0.678700	-1.692100	2.661400
H	1.113600	3.043700	0.011200	C	-0.954800	-3.791600	1.255700
H	0.295300	2.309600	-1.388100	H	0.838100	-2.603400	1.458100
C	4.086900	3.275100	-1.615500	C	-0.377700	-2.567200	3.889600
H	3.719100	2.404600	0.313300	H	-1.756700	-1.475200	2.626900
H	4.430600	1.281500	-0.844600	H	-0.137300	-0.735900	2.729300
C	3.068500	4.403200	-1.505000	C	-0.649000	-4.652200	2.494100
H	0.940300	4.718700	-1.796600	H	-2.042500	-3.632500	1.191900
H	1.680200	3.608800	-2.945300	H	-0.633200	-4.312500	0.341400
H	5.089700	3.624600	-1.337200	C	-1.086700	-3.924500	3.773200
H	4.149300	2.945500	-2.665200	H	-0.693900	-2.046100	4.803600
H	3.366700	5.252500	-2.133200	H	0.709600	-2.729900	3.955200
H	3.052200	4.772400	-0.466200	H	-1.159300	-5.621700	2.409500
C	2.725600	-0.050500	1.407400	H	0.434800	-4.844200	2.538200
C	2.278000	1.054600	2.373500	H	-0.870100	-4.543500	4.654400
C	2.581700	-1.425800	2.063800	H	-2.176200	-3.761200	3.738700
H	3.786700	0.105300	1.149600	Si	3.786800	1.763100	0.685000
C	3.012200	0.974400	3.707800	H	2.238200	2.037000	0.567200
H	1.195300	0.945000	2.550400	C	3.866300	3.708100	0.950600
H	2.414300	2.046100	1.919800	H	4.931800	3.987100	1.027900
C	3.302500	-1.490700	3.407400	H	3.393000	3.949900	1.916600
H	1.510400	-1.643100	2.216100	C	3.187600	4.490900	-0.178400
H	2.970200	-2.208400	1.399100	H	2.145700	4.152700	-0.306300
C	2.821200	-0.394000	4.347400	H	3.163600	5.572800	0.016900
H	2.657800	1.769900	4.375600	H	3.711500	4.336200	-1.133600
H	4.087400	1.156000	3.546100	C	4.769100	1.562600	-0.948700
H	3.159400	-2.481400	3.857300	H	5.464900	0.716800	-0.836400
H	4.386100	-1.375300	3.241900	H	5.369800	2.465500	-1.129600
H	3.346700	-0.450300	5.309000	C	3.850200	1.285200	-2.156400
H	1.750300	-0.544800	4.561800	H	3.141200	2.111500	-2.316200
TS₁₇				H	4.422500	1.134900	-3.082800
SCF done: -1436.626543				H	3.268700	0.378600	-1.946900
C	-5.392200	3.849200	0.067900	C	4.598900	1.178300	2.323500
C	-4.510300	3.578900	-0.948800	H	5.177400	2.017900	2.736500
C	-3.250800	2.986700	-0.678900	H	3.791800	0.970300	3.045300
C	-2.903500	2.682200	0.672800	C	5.490500	-0.068700	2.187400
C	-3.833700	2.981100	1.701400	H	6.329800	0.123100	1.504100
C	-5.049400	3.546500	1.405800	H	5.909400	-0.371500	3.157400
H	-2.588300	2.918500	-2.739100	H	4.906000	-0.900100	1.779600
H	-6.357100	4.298900	-0.149500	C	0.545300	-2.254100	-1.538800
H	-4.765900	3.810800	-1.980900	C	0.620800	-1.337400	-2.775000
C	-2.334500	2.657400	-1.712800	C	1.959500	-2.641800	-1.064000
C	-1.668900	2.026000	0.941700	H	-0.013600	-3.169000	-1.797200
H	-3.564000	2.750700	2.730500	C	1.382700	-2.035700	-3.911500
H	-5.755900	3.768200	2.201300	H	1.160700	-0.418300	-2.490300
C	-0.832600	1.673500	-0.089100	H	-0.387100	-1.046000	-3.110100
C	-1.156100	2.010400	-1.431400	C	2.728800	-3.318400	-2.212300
H	-1.430900	1.768300	1.974600	H	2.500700	-1.748700	-0.711100
H	-0.466300	1.750000	-2.233500	H	1.891500	-3.345700	-0.221100
F	3.141100	0.034300	0.430200	C	2.796700	-2.408100	-3.445400
P	-0.401200	-1.333300	-0.163700	H	1.428500	-1.374400	-4.787700
Pd	0.843000	0.649600	0.218400	H	0.840600	-2.949600	-4.204900
C	-2.211600	-1.207900	-0.762800	H	3.741400	-3.572400	-1.869900
C	-2.733400	-2.407100	-1.571300	H	2.219800	-4.257700	-2.484900
C	-3.189600	-0.880500	0.380800	H	3.347500	-2.905400	-4.255600
H	-2.184500	-0.329300	-1.429300	H	3.340900	-1.487700	-3.183200
C	-4.109900	-2.046500	-2.164300	TS₁₈			
H	-2.838800	-3.285100	-0.915500	SCF done: -1436.630179			
H	-2.041300	-2.668400	-2.383800	C	-7.668200	0.444100	-0.320000
C	-4.555000	-0.501800	-0.214200	C	-6.850400	-0.252900	-1.174000
H	-3.306200	-1.764600	1.026800	C	-5.456600	-0.333400	-0.940500
H	-2.807100	-0.047500	0.981600	C	-4.910200	0.323100	0.201600
C	-5.104800	-1.659800	-1.059300	C	-5.780400	1.030800	1.066900
H	-4.495500	-2.893700	-2.748100	C	-7.127400	1.092100	0.813100
H	-3.984700	-1.194000	-2.850700	H	-5.015400	-1.580500	-2.650400
H	-5.254500	-0.243100	0.592900	H	-8.737600	0.498600	-0.511200

H	-7.262300	-0.757200	-2.047700	C	0.907878	-0.568552	0.000068
C	-4.588200	-1.060300	-1.792800	C	1.933347	-1.546930	0.000240
C	-3.515100	0.236400	0.439500	C	3.252811	-1.174626	0.000176
H	-5.355900	1.525700	1.939800	H	0.516847	2.841997	-0.000522
H	-7.785000	1.639800	1.484900	H	4.654697	0.476550	-0.000117
C	-2.683300	-0.429800	-0.433000	H	2.904509	2.219002	-0.000423
C	-3.240500	-1.123200	-1.539700	C	0.235853	1.790192	-0.000342
H	-3.110200	0.706600	1.338000	C	-0.457959	-0.919032	0.000140
H	-2.590500	-1.705200	-2.192100	H	1.650450	-2.598246	0.000428
C	-1.105800	-1.648500	0.856900	H	4.034001	-1.930644	0.000310
O	-1.185500	-1.609800	2.045000	C	-1.435853	0.053027	-0.000048
F	-1.144800	-2.829900	0.200300	C	-1.083517	1.426138	-0.000297
Pd	-0.660500	-0.152300	-0.342600	H	-0.753622	-1.967034	0.000341
P	1.745700	0.175600	-0.234600	H	-1.867290	2.176901	-0.000438
C	2.774700	-1.088600	-1.164100	C	-2.837829	-0.390418	0.000040
C	4.285700	-1.028100	-0.941600	O	-3.247260	-1.510964	-0.000392
C	2.232300	-2.510700	-0.987000	F	-3.696036	0.646449	0.000729
H	2.574800	-0.804400	-2.214900				
C	5.011600	-2.026400	-1.841700				
H	4.512000	-1.261500	0.111000				
H	4.664800	-0.012700	-1.123900				
C	2.966100	-3.482800	-1.904500				
H	2.368400	-2.834500	0.056100				
H	1.149900	-2.528500	-1.172300				
C	4.469600	-3.439600	-1.657600				
H	6.090700	-1.994200	-1.643700				
H	4.877800	-1.723900	-2.892900				
H	2.577200	-4.498800	-1.762700				
H	2.763400	-3.214100	-2.954100				
H	4.991900	-4.138100	-2.323600				
H	4.675800	-3.774800	-0.627900				
C	2.281400	1.810900	-1.021600				
C	1.060100	2.713500	-1.236800				
C	3.405100	2.580600	-0.324600				
H	2.649100	1.510100	-2.019500				
C	1.427300	3.977300	-2.006300				
H	0.632800	2.988400	-0.257600				
H	0.270900	2.159100	-1.770400				
C	3.769500	3.841200	-1.105100				
H	3.082800	2.871100	0.688700				
H	4.293100	1.947300	-0.196200				
C	2.553400	4.735700	-1.313500				
H	0.543600	4.616800	-2.124200				
H	1.749000	3.697200	-3.022400				
H	4.565000	4.386600	-0.581200				
H	4.182800	3.553300	-2.085300				
H	2.827600	5.627500	-1.891000				
H	2.197500	5.094600	-0.334200				
C	2.307300	0.258200	1.556800				
C	1.326300	1.169000	2.308300				
C	2.367000	-1.113500	2.236200				
H	3.315000	0.705200	1.591400				
C	1.706000	1.310300	3.777500				
H	0.317200	0.728400	2.231100				
H	1.269600	2.159200	1.832500				
C	2.737700	-0.975200	3.711100				
H	1.386400	-1.608100	2.150600				
H	3.097500	-1.762900	1.736700				
C	1.775700	-0.054700	4.451000				
H	0.979200	1.955700	4.287000				
H	2.684300	1.813100	3.858200				
H	2.757800	-1.967600	4.179000				
H	3.760700	-0.571600	3.789500				
H	2.077100	0.048200	5.501400				
H	0.771900	-0.506900	4.449300				
substrate							
SCF done: -598.087800							
C	3.604586	0.194017	-0.000067				
C	2.634302	1.164216	-0.000237				
C	1.263517	0.813827	-0.000174				
				naphthene			
				SCF done: -385.582067			
C	2.424371	0.706250	0.000065				
C	1.239701	1.397977	-0.000054				
C	0.000065	0.713009	-0.000094				
C	-0.000002	-0.712564	-0.000014				
C	1.239522	-1.397879	-0.000137				
C	2.424368	-0.706462	0.000044				
H	-1.233323	2.487200	-0.000161				
H	3.369835	1.243891	0.000396				
H	1.233072	2.487214	-0.000002				
C	-1.239729	1.397942	-0.000009				
C	-1.239614	-1.398001	0.000182				
H	1.232363	-2.487115	-0.000303				
H	3.369779	-1.244170	0.000003				
C	-2.424297	-0.706535	-0.000021				
C	-2.424387	0.706290	0.000048				
H	-1.232019	-2.487214	0.000163				
H	-3.369756	1.244039	0.000095				
H	-3.369936	-1.244003	-0.000255				
				aldehyde			
				SCF done: -498.849564			
C	3.256192	0.042432	-0.000113				
C	2.349865	1.072532	-0.000079				
C	0.958742	0.811284	0.000033				
C	0.513072	-0.545581	0.000107				
C	1.475254	-1.586959	0.000120				
C	2.815796	-1.300691	0.000008				
H	0.347585	2.885164	0.000066				
H	4.322341	0.257000	-0.000210				
H	2.686579	2.108125	-0.000189				
C	-0.001907	1.853924	0.000057				
C	-0.871663	-0.808652	0.000027				
H	1.125498	-2.618011	0.000220				
H	3.546671	-2.105609	-0.000014				
C	-1.785179	0.224014	-0.000024				
C	-1.341352	1.567986	0.000017				
H	-1.239210	-1.834151	0.000014				
H	-2.081719	2.367656	0.000030				
C	-3.228862	-0.070450	-0.000035				
O	-3.708611	-1.182293	-0.000160				
H	-3.878607	0.839131	0.000648				
				Et3SiH			
				SCF done: -241.960539			
Si	0.145671	-0.004158	0.582084				
H	-0.400565	-0.134372	1.967173				
C	-0.387875	1.669746	-0.113893				
H	0.085760	1.807895	-1.098834				
H	0.021610	2.463629	0.529253				
C	-1.901747	1.818622	-0.243261				
H	-2.407084	1.648354	0.718372				

H	-2.193970	2.817157	-0.595000
H	-2.312436	1.090068	-0.956685
C	-0.561983	-1.414490	-0.467275
H	0.137513	-2.264297	-0.423759
H	-0.570687	-1.093460	-1.521648
C	-1.956469	-1.869838	-0.041746
H	-2.685993	-1.049355	-0.088938
H	-2.338026	-2.682210	-0.674866
H	-1.955045	-2.231470	0.995271
C	2.030437	-0.125678	0.626691
H	2.432924	0.667361	1.274469
H	2.301853	-1.075274	1.113022
C	2.667671	-0.048822	-0.759590
H	2.475678	0.920776	-1.239840
H	3.757376	-0.179427	-0.721744
H	2.271483	-0.824408	-1.430971

Et3SiF

SCF done: -341.242117

Si	0.184331	0.003520	0.337632
C	-0.311613	1.696919	-0.295842
H	0.214431	1.881183	-1.246153
H	0.065063	2.455374	0.407255
C	-1.818456	1.850848	-0.492063
H	-2.366614	1.615423	0.430552
H	-2.096248	2.869962	-0.790743
H	-2.187883	1.170134	-1.271854
C	-0.478517	-1.370764	-0.764086
H	0.215214	-2.224858	-0.717470
H	-0.438537	-1.014272	-1.806639
C	-1.893864	-1.830476	-0.416277
H	-2.614908	-1.003222	-0.464200
H	-2.247518	-2.613128	-1.100121
H	-1.941526	-2.231894	0.603237
C	2.043414	-0.139024	0.520998
H	2.410766	0.631920	1.213772
H	2.274514	-1.106667	0.991338
C	2.756099	-0.025567	-0.827004
H	2.598430	0.959559	-1.287861
H	3.840589	-0.165215	-0.732126
H	2.395984	-0.778688	-1.542830
F	-0.498307	-0.176279	1.803625

CO

SCF done: -113.248634

C	0.000000	0.000000	-0.649940
O	0.000000	0.000000	0.487455