

Supporting Information belonging to the manuscript:

Effect of the metal fragment on the aromaticity and synchronicity of the gold(I)-catalysed divinylcyclopropane-cycloheptadiene rearrangement

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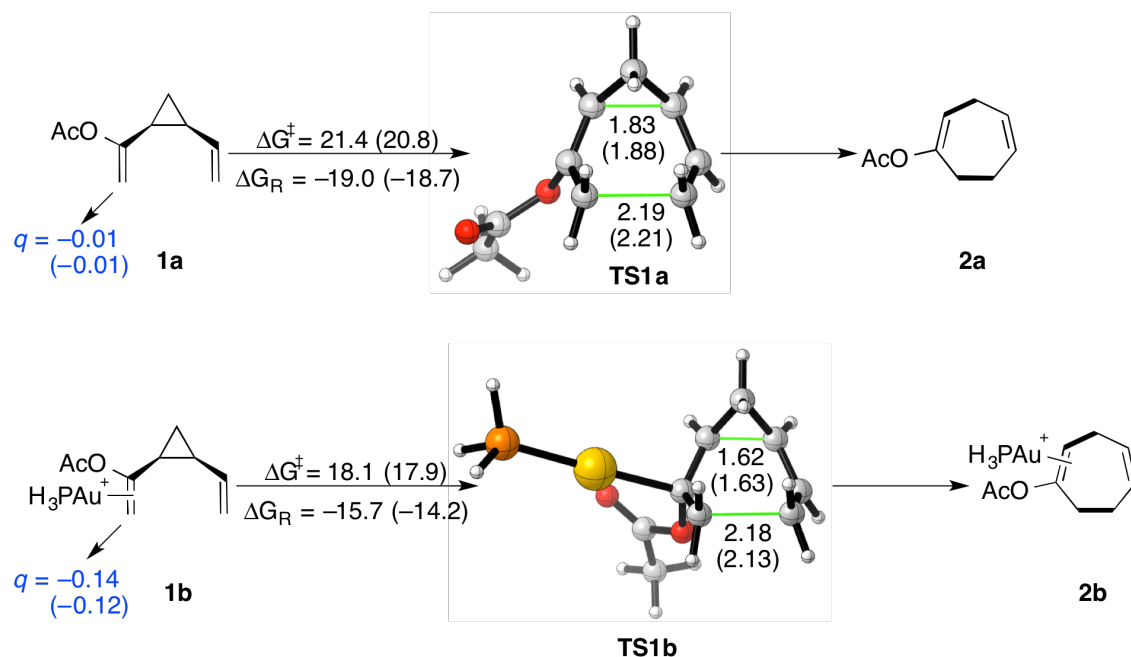


Figure S1. Comparison of the data computed at the PCM(CH₂Cl₂)-M06/def2-TZVP//M06/def2-SVP level (plain values) and PCM(CH₂Cl₂)-M06/def2-TZVP level (values within parantheses).

Cartesian coordinates (in Å) and free energies (in a. u.) of all the stationary points discussed in the text. All calculations have been performed at the M06/def2-SVP level.

1a: E= -499.669952

C	1.722958000	-1.528103000	0.219093000
C	-0.005304000	0.916862000	-0.123265000
C	2.045179000	-0.519559000	-0.813563000
C	1.168653000	0.714411000	-1.000949000
C	2.560870000	0.847541000	-0.490215000
H	1.307280000	-2.466476000	-0.172663000
H	2.395890000	-0.949162000	-1.759611000
H	0.983839000	0.985356000	-2.049201000
H	2.694806000	1.101692000	0.566138000
H	3.316099000	1.281487000	-1.151229000
C	1.854290000	-1.394305000	1.539372000
H	1.550294000	-2.192149000	2.222671000
H	2.267703000	-0.489390000	1.998352000
C	-0.056945000	1.736589000	0.928540000
H	-0.940164000	1.842229000	1.554514000
H	0.834816000	2.324894000	1.156611000
O	-1.033853000	0.115610000	-0.591553000
C	-2.225151000	-0.078743000	0.022060000
O	-2.561263000	0.429420000	1.053381000
C	-3.050156000	-1.027738000	-0.790220000
H	-2.529003000	-1.992544000	-0.882632000
H	-3.180455000	-0.635517000	-1.809924000
H	-4.026543000	-1.172392000	-0.312772000

TS1a: E= -499.636707

C	-2.257608000	0.363110000	-1.215350000
C	0.041111000	-0.089869000	0.470659000
C	-2.337492000	-0.852714000	-0.518914000
C	-0.878917000	-1.141620000	0.552835000
C	-2.297781000	-0.981513000	0.960763000
H	-2.074031000	0.298676000	-2.294739000
H	-2.505599000	-1.772912000	-1.087818000
H	-0.508867000	-2.149662000	0.343484000
H	-2.545534000	-0.084680000	1.541671000
H	-2.772228000	-1.875084000	1.380890000
C	-2.047824000	1.567676000	-0.561744000
H	-1.843478000	2.467363000	-1.152301000
H	-2.582010000	1.763436000	0.371908000
C	-0.296964000	1.231643000	0.707351000
H	0.426471000	2.014089000	0.463362000
H	-0.914895000	1.438861000	1.582331000
O	1.147078000	-0.400813000	-0.320423000
C	2.389117000	0.004676000	0.044179000
O	2.631874000	0.643302000	1.027167000
C	3.387942000	-0.474127000	-0.962625000
H	3.127131000	-0.091911000	-1.960892000
H	3.359083000	-1.572227000	-1.025322000
H	4.392834000	-0.139425000	-0.679443000

2a: E= -499.704538

C	2.533662000	1.063144000	-0.290493000
C	-0.084857000	-0.526245000	0.404972000
C	2.927836000	-0.212121000	-0.380086000

C	0.682863000	-1.480388000	-0.120493000
C	2.179207000	-1.491475000	-0.143611000
H	3.284384000	1.816851000	-0.562280000
H	3.970003000	-0.375527000	-0.685965000
H	0.165017000	-2.352571000	-0.535404000
H	2.501637000	-2.204257000	-0.923352000
H	2.556974000	-1.956642000	0.793631000
C	1.215564000	1.623128000	0.142819000
H	1.403244000	2.583317000	0.655678000
H	0.592102000	1.875586000	-0.734840000
C	0.401734000	0.726017000	1.064776000
H	1.020713000	0.449948000	1.940566000
H	-0.459670000	1.285779000	1.460212000
O	-1.461968000	-0.750051000	0.418862000
C	-2.253860000	0.125617000	-0.236364000
O	-1.833255000	1.067163000	-0.850413000
C	-3.691238000	-0.255743000	-0.082935000
H	-3.962992000	-0.267634000	0.983244000
H	-3.849132000	-1.276089000	-0.463021000
H	-4.325975000	0.452740000	-0.627565000

1b: E= -978.256573

C	4.015977000	-1.008150000	-0.203284000
C	1.341914000	0.487601000	-0.269319000
C	3.351582000	-0.530390000	1.028222000
C	1.993650000	0.232104000	1.006107000
C	2.134401000	-1.144764000	1.592198000
H	4.660170000	-0.276667000	-0.707805000
H	4.034970000	-0.058298000	1.746180000
H	1.939061000	1.071279000	1.706134000
H	1.673912000	-1.974009000	1.043263000
H	2.032249000	-1.217996000	2.678218000
C	3.926844000	-2.247081000	-0.688302000
H	3.332863000	-3.022497000	-0.190214000
C	0.912137000	-0.451224000	-1.196646000
H	0.731300000	-0.091717000	-2.217406000
O	1.249791000	1.789617000	-0.631955000
C	0.451787000	2.668101000	0.084244000
O	-0.345759000	2.261316000	0.876077000
C	0.726430000	4.067068000	-0.319894000
H	1.760272000	4.331607000	-0.049536000
H	0.650872000	4.163695000	-1.412957000
H	0.023346000	4.744760000	0.176721000
H	4.473663000	-2.547409000	-1.586131000
H	1.244198000	-1.490051000	-1.091925000
Au	-1.088532000	-0.463665000	-0.243977000
P	-3.285137000	-0.651020000	0.575414000
H	-4.318557000	-0.777938000	-0.382397000
H	-3.573466000	-1.742811000	1.427768000
H	-3.754394000	0.435821000	1.350141000

TS1b: E= -978.230981

C	3.774090000	-0.847593000	-0.189249000
C	1.111959000	-0.025089000	-0.177033000
C	3.159162000	-0.948028000	1.101264000
C	1.605192000	-0.485879000	1.124481000
C	2.025900000	-1.876551000	1.407532000
H	4.515843000	-0.048611000	-0.309485000
H	3.708875000	-0.520279000	1.945111000

H	1.384615000	0.167517000	1.976016000
H	1.802096000	-2.661082000	0.677402000
H	1.940083000	-2.217291000	2.442699000
C	3.327023000	-1.521528000	-1.298175000
H	2.911621000	-2.526846000	-1.183167000
C	1.251563000	-0.857742000	-1.309908000
H	1.221124000	-0.384242000	-2.297047000
O	1.525185000	1.293539000	-0.460203000
C	0.888161000	2.336563000	0.125221000
O	-0.093173000	2.188740000	0.807496000
C	1.551225000	3.627474000	-0.200232000
H	2.584503000	3.621873000	0.177810000
H	1.611960000	3.753794000	-1.291287000
H	0.992825000	4.456490000	0.248599000
H	3.770662000	-1.310678000	-2.275786000
H	0.906892000	-1.891735000	-1.256449000
Au	-1.102907000	-0.210223000	-0.081115000
P	-3.439749000	-0.440735000	0.063144000
H	-3.943730000	-1.382496000	0.991873000
H	-4.162508000	0.716722000	0.438558000
H	-4.140753000	-0.822518000	-1.105664000

2b: E= -978.284241

C	-3.780102000	-1.581524000	-0.054950000
C	-1.431256000	0.289247000	0.310069000
C	-2.898996000	-2.092689000	-0.922930000
C	-1.017214000	-0.402119000	-0.817243000
C	-1.407033000	-1.863536000	-0.961712000
H	-4.832356000	-1.853692000	-0.201125000
H	-3.290725000	-2.764355000	-1.695039000
H	-0.883260000	0.173234000	-1.743318000
H	-0.910770000	-2.488792000	-0.194016000
H	-1.004688000	-2.230112000	-1.917743000
C	-3.538502000	-0.682642000	1.119086000
H	-4.020390000	-1.125545000	2.008484000
C	-2.071735000	-0.405173000	1.462053000
H	-2.001725000	0.231125000	2.356833000
O	-1.541671000	1.627622000	0.414828000
C	-0.815487000	2.560232000	-0.316397000
O	0.128726000	2.243931000	-0.975806000
C	-1.372996000	3.915836000	-0.099130000
H	-2.412382000	3.948833000	-0.460765000
H	-1.403931000	4.142715000	0.976888000
H	-0.766376000	4.656982000	-0.631141000
H	-4.067326000	0.277884000	0.966124000
H	-1.553106000	-1.352967000	1.676600000
Au	1.087663000	-0.287242000	-0.051231000
P	3.370041000	-0.453892000	0.482105000
H	3.713309000	-0.683768000	1.835275000
H	4.081705000	-1.494262000	-0.160847000
H	4.179528000	0.664993000	0.174176000

1c: E= -1095.964217

C	4.494665000	-1.088129000	-0.016180000
C	1.832042000	0.376672000	-0.241900000
C	3.722591000	-0.688903000	1.180393000
C	2.367343000	0.056750000	1.079212000
C	2.465765000	-1.347651000	1.597870000

H	5.183187000	-0.327814000	-0.407348000
H	4.338048000	-0.264541000	1.984233000
H	2.232278000	0.853773000	1.816929000
H	2.070019000	-2.149993000	0.965898000
H	2.273483000	-1.487939000	2.664821000
C	4.442866000	-2.284229000	-0.602816000
H	3.803625000	-3.089919000	-0.222852000
C	1.460815000	-0.510114000	-1.230135000
H	1.360849000	-0.124335000	-2.251326000
O	1.856350000	1.697696000	-0.576539000
C	1.084241000	2.618761000	0.097736000
O	0.207809000	2.275456000	0.837493000
C	1.490466000	3.999814000	-0.261458000
H	2.507353000	4.189352000	0.115773000
H	1.531926000	4.111274000	-1.354546000
H	0.791693000	4.721491000	0.175987000
H	5.063715000	-2.519554000	-1.471426000
H	1.687892000	-1.574521000	-1.114982000
Au	-0.624146000	-0.376128000	-0.384975000
P	-2.871690000	-0.304915000	0.277983000
C	-3.358351000	1.404204000	0.660294000
H	-2.674368000	1.822118000	1.414634000
H	-3.282493000	2.020981000	-0.248240000
H	-4.394144000	1.435852000	1.035920000
C	-4.060655000	-0.890067000	-0.966143000
H	-5.089491000	-0.777062000	-0.586997000
H	-3.952114000	-0.308335000	-1.893727000
H	-3.875131000	-1.950126000	-1.195363000
C	-3.237336000	-1.262930000	1.779427000
H	-3.025323000	-2.328863000	1.607926000
H	-2.609211000	-0.909364000	2.610603000
H	-4.298881000	-1.144897000	2.051963000

TS2c: E= -1095.936990

C	4.283577000	-0.872587000	-0.132095000
C	1.621566000	-0.041006000	-0.178446000
C	3.644593000	-0.971000000	1.143261000
C	2.081527000	-0.498376000	1.130804000
C	2.495442000	-1.887681000	1.426357000
H	5.035894000	-0.081555000	-0.237119000
H	4.174046000	-0.541623000	1.999129000
H	1.853897000	0.159880000	1.976388000
H	2.283135000	-2.673015000	0.693599000
H	2.385643000	-2.226249000	2.460057000
C	3.836318000	-1.532150000	-1.252603000
H	3.427173000	-2.541115000	-1.146730000
C	1.788693000	-0.874549000	-1.305137000
H	1.767597000	-0.401334000	-2.292727000
O	2.034730000	1.280564000	-0.456976000
C	1.418055000	2.326875000	0.141804000
O	0.453396000	2.194023000	0.849745000
C	2.084677000	3.611695000	-0.207704000
H	3.133532000	3.591620000	0.123780000
H	2.099186000	3.742027000	-1.299944000
H	1.557277000	4.446564000	0.267310000
H	4.298602000	-1.321509000	-2.221745000
H	1.426514000	-1.903119000	-1.257205000
Au	-0.611841000	-0.219741000	-0.138282000
P	-2.949884000	-0.186676000	0.046599000
C	-3.516906000	1.521199000	0.314551000

H	-3.014011000	1.943359000	1.198323000
H	-3.250273000	2.138985000	-0.556459000
H	-4.608874000	1.551029000	0.460554000
C	-3.876713000	-0.781021000	-1.401411000
H	-4.960409000	-0.680316000	-1.226560000
H	-3.598990000	-0.194755000	-2.290189000
H	-3.639091000	-1.838111000	-1.592850000
C	-3.606314000	-1.136264000	1.452522000
H	-3.362363000	-2.202669000	1.335010000
H	-3.155941000	-0.775517000	2.389488000
H	-4.700928000	-1.020435000	1.509589000

2c: E= -1095.991714

C	-4.168969000	-1.764610000	0.111926000
C	-1.891693000	0.227422000	0.311856000
C	-3.343124000	-2.206865000	-0.844071000
C	-1.561387000	-0.406309000	-0.866522000
C	-1.880319000	-1.880852000	-1.029222000
H	-5.209881000	-2.106206000	0.059793000
H	-3.764234000	-2.896094000	-1.584960000
H	-1.490582000	0.200422000	-1.777788000
H	-1.268546000	-2.503965000	-0.347482000
H	-1.563645000	-2.187838000	-2.037122000
C	-3.875533000	-0.865563000	1.274028000
H	-4.265019000	-1.338418000	2.192816000
C	-2.399587000	-0.529722000	1.493001000
H	-2.271582000	0.079942000	2.400079000
O	-2.063396000	1.562405000	0.471559000
C	-1.458346000	2.545639000	-0.288798000
O	-0.560730000	2.306738000	-1.041471000
C	-2.069081000	3.864492000	0.010795000
H	-3.124753000	3.858252000	-0.302211000
H	-2.060359000	4.051121000	1.094518000
H	-1.528310000	4.654482000	-0.522188000
H	-4.456326000	0.072097000	1.176189000
H	-1.824106000	-1.460188000	1.624571000
Au	0.596566000	-0.205854000	-0.150483000
P	2.906938000	-0.219733000	0.244859000
C	3.795284000	-1.486470000	-0.709804000
H	3.435022000	-2.488585000	-0.432942000
H	3.621764000	-1.337928000	-1.786103000
H	4.876637000	-1.421820000	-0.506170000
C	3.684853000	1.360435000	-0.205660000
H	4.770622000	1.318639000	-0.020668000
H	3.505362000	1.574774000	-1.269997000
H	3.245692000	2.175336000	0.389104000
C	3.372754000	-0.511441000	1.977997000
H	2.933307000	0.264661000	2.622283000
H	3.000117000	-1.492392000	2.308971000
H	4.469938000	-0.487894000	2.080717000

1d: E= -1670.152020

C	5.592966000	-1.647731000	-0.113091000
C	3.240435000	0.281399000	-0.394407000
C	4.836621000	-1.166236000	1.063256000
C	3.646747000	-0.186836000	0.931853000
C	3.458500000	-1.605177000	1.381339000
H	6.429222000	-1.010079000	-0.428308000

H	5.470022000	-0.899753000	1.919379000
H	3.603626000	0.586598000	1.704029000
H	2.964360000	-2.295576000	0.688234000
H	3.179733000	-1.751694000	2.428381000
C	5.357604000	-2.784409000	-0.768942000
H	4.561009000	-3.474073000	-0.465693000
C	2.794313000	-0.481021000	-1.449865000
H	2.786411000	-0.021527000	-2.444371000
O	3.496335000	1.595821000	-0.658200000
C	2.866381000	2.594304000	0.047718000
O	1.948017000	2.358273000	0.778090000
C	3.468213000	3.913927000	-0.267891000
H	2.917479000	4.708765000	0.247165000
H	4.523842000	3.922651000	0.043251000
H	3.456735000	4.080265000	-1.355079000
H	5.973429000	-3.089131000	-1.619430000
H	2.854048000	-1.572320000	-1.398994000
Au	0.724874000	-0.140051000	-0.601473000
P	-1.545972000	-0.103344000	0.013634000
C	-1.787543000	-0.793888000	1.678473000
C	-2.670209000	-0.201518000	2.587361000
C	-1.105932000	-1.966792000	2.028397000
C	-2.867931000	-0.783096000	3.838110000
H	-3.204652000	0.716785000	2.321463000
C	-1.311808000	-2.544372000	3.276571000
H	-0.415533000	-2.433930000	1.314979000
C	-2.191818000	-1.950973000	4.182133000
H	-3.556812000	-0.318684000	4.548570000
H	-0.781443000	-3.461431000	3.547003000
H	-2.348673000	-2.403400000	5.165158000
C	-2.580732000	-1.081424000	-1.115772000
C	-3.581421000	-1.934814000	-0.639938000
C	-2.397301000	-0.917114000	-2.494835000
C	-4.393320000	-2.617240000	-1.544246000
H	-3.729634000	-2.069120000	0.436728000
C	-3.215751000	-1.595715000	-3.390884000
H	-1.614645000	-0.246416000	-2.870067000
C	-4.212855000	-2.447373000	-2.914617000
H	-5.173552000	-3.286716000	-1.172600000
H	-3.073895000	-1.464010000	-4.466736000
H	-4.852560000	-2.985180000	-3.619441000
C	-2.249549000	1.571578000	0.043659000
C	-1.498528000	2.599568000	0.629139000
C	-3.537123000	1.828040000	-0.440220000
C	-2.043911000	3.874647000	0.738225000
H	-0.484510000	2.407932000	1.000036000
C	-4.070960000	3.110380000	-0.332499000
H	-4.126837000	1.028850000	-0.901692000
C	-3.328135000	4.130282000	0.257847000
H	-1.460210000	4.676002000	1.198963000
H	-5.076443000	3.311727000	-0.711484000
H	-3.752480000	5.134532000	0.342053000

TS1d: E= -1670.124701

C	5.584498000	-1.212963000	-0.202773000
C	3.023992000	-0.098213000	-0.226510000
C	4.935596000	-1.277371000	1.068598000
C	3.433120000	-0.627582000	1.070131000
C	3.689243000	-2.061946000	1.330446000
H	6.418089000	-0.505032000	-0.284148000

H	5.506950000	-0.932507000	1.935686000
H	3.282288000	0.033470000	1.930555000
H	3.385645000	-2.797231000	0.577844000
H	3.539627000	-2.411725000	2.355408000
C	5.069005000	-1.783937000	-1.343164000
H	4.560006000	-2.749469000	-1.270010000
C	3.104905000	-0.917849000	-1.372577000
H	3.128511000	-0.421147000	-2.348438000
O	3.562730000	1.183422000	-0.476938000
C	3.035577000	2.271306000	0.128520000
O	2.068072000	2.212240000	0.843106000
C	3.799159000	3.501810000	-0.218979000
H	3.344676000	4.372867000	0.266598000
H	4.846279000	3.397116000	0.101305000
H	3.809303000	3.639183000	-1.310389000
H	5.553739000	-1.592911000	-2.305508000
H	2.637585000	-1.903993000	-1.345904000
Au	0.776501000	-0.089186000	-0.180243000
P	-1.572252000	-0.067071000	-0.017718000
C	-2.149596000	-0.821041000	1.534773000
C	-3.080555000	-0.186803000	2.362742000
C	-1.659756000	-2.088578000	1.878291000
C	-3.520498000	-0.822607000	3.522759000
H	-3.464459000	0.805915000	2.106348000
C	-2.108626000	-2.720018000	3.032279000
H	-0.929699000	-2.588865000	1.230076000
C	-3.039262000	-2.085705000	3.856193000
H	-4.247069000	-0.324146000	4.169813000
H	-1.730183000	-3.711782000	3.294115000
H	-3.388726000	-2.580552000	4.766363000
C	-2.419058000	-0.958234000	-1.359593000
C	-3.511641000	-1.795917000	-1.113118000
C	-1.986361000	-0.743165000	-2.674371000
C	-4.163158000	-2.414065000	-2.178954000
H	-3.857827000	-1.967616000	-0.088380000
C	-2.645446000	-1.357308000	-3.733563000
H	-1.130289000	-0.085794000	-2.869230000
C	-3.732997000	-2.194897000	-3.485152000
H	-5.015215000	-3.070902000	-1.984882000
H	-2.308171000	-1.185659000	-4.759236000
H	-4.247608000	-2.682274000	-4.317709000
C	-2.216699000	1.632459000	-0.044151000
C	-1.450024000	2.656947000	0.525983000
C	-3.485810000	1.911861000	-0.565690000
C	-1.960946000	3.950748000	0.582784000
H	-0.446382000	2.450847000	0.918048000
C	-3.986042000	3.209707000	-0.508201000
H	-4.086230000	1.115132000	-1.018376000
C	-3.226296000	4.226768000	0.067532000
H	-1.362515000	4.750036000	1.027805000
H	-4.976199000	3.427936000	-0.917128000
H	-3.622309000	5.245128000	0.109611000

2d: E= -1670.179401

C	-5.455215000	-1.932423000	0.102202000
C	-3.232135000	0.129900000	0.261647000
C	-4.657120000	-2.322130000	-0.899220000
C	-2.941857000	-0.462085000	-0.947887000
C	-3.215536000	-1.941615000	-1.137962000
H	-6.485696000	-2.307736000	0.084251000

H	-5.087513000	-3.005901000	-1.639942000
H	-2.914382000	0.169134000	-1.843688000
H	-2.553270000	-2.560189000	-0.500820000
H	-2.933209000	-2.209763000	-2.166884000
C	-5.142077000	-1.054137000	1.275154000
H	-5.476400000	-1.565082000	2.195442000
C	-3.670792000	-0.674040000	1.441626000
H	-3.524542000	-0.082620000	2.358086000
O	-3.440298000	1.456742000	0.471192000
C	-2.933533000	2.480538000	-0.300986000
O	-2.110387000	2.297881000	-1.149310000
C	-3.538779000	3.771957000	0.112884000
H	-3.073799000	4.594376000	-0.442105000
H	-4.621439000	3.751348000	-0.085603000
H	-3.416208000	3.918550000	1.195879000
H	-5.758356000	-0.135367000	1.227524000
H	-3.060291000	-1.587117000	1.529036000
Au	-0.776804000	-0.195344000	-0.260612000
P	1.549699000	-0.085797000	0.063115000
C	2.437412000	-0.927181000	-1.281148000
C	3.482439000	-0.306945000	-1.972490000
C	2.062205000	-2.238159000	-1.606095000
C	4.148579000	-1.000427000	-2.981795000
H	3.777093000	0.718824000	-1.728083000
C	2.737020000	-2.926049000	-2.607934000
H	1.241953000	-2.726941000	-1.065572000
C	3.779403000	-2.305102000	-3.297399000
H	4.963358000	-0.513985000	-3.524580000
H	2.447413000	-3.950416000	-2.856744000
H	4.305639000	-2.843876000	-4.089996000
C	2.108420000	-0.838545000	1.620374000
C	3.235391000	-1.664354000	1.676500000
C	1.411141000	-0.523791000	2.793865000
C	3.658013000	-2.172158000	2.904067000
H	3.787161000	-1.912474000	0.763627000
C	1.841935000	-1.029008000	4.015290000
H	0.530084000	0.128282000	2.751473000
C	2.964224000	-1.855767000	4.069315000
H	4.537705000	-2.819692000	2.947458000
H	1.298236000	-0.780765000	4.930672000
H	3.299877000	-2.257200000	5.029369000
C	2.119724000	1.638986000	0.078656000
C	1.476052000	2.570793000	-0.745590000
C	3.226583000	2.025584000	0.843919000
C	1.945893000	3.879238000	-0.809287000
H	0.601826000	2.278234000	-1.339713000
C	3.686746000	3.338157000	0.777319000
H	3.732330000	1.303095000	1.493509000
C	3.049495000	4.262450000	-0.048520000
H	1.444038000	4.604783000	-1.454751000
H	4.549964000	3.640405000	1.376285000
H	3.414136000	5.292134000	-0.096563000

1e: E= -1321.364661

C	4.703433000	-1.536592000	0.067930000
C	2.293624000	0.317782000	-0.232645000
C	3.967265000	-1.017781000	1.240845000
C	2.744117000	-0.071284000	1.099342000
C	2.614593000	-1.472781000	1.623134000
H	5.504338000	-0.888670000	-0.311162000

H	4.616821000	-0.683566000	2.060371000
H	2.711942000	0.741405000	1.831132000
H	2.114563000	-2.206699000	0.981119000
H	2.370880000	-1.572614000	2.684077000
C	4.491932000	-2.720146000	-0.508463000
H	3.733506000	-3.418896000	-0.135798000
C	1.850069000	-0.510393000	-1.243897000
H	1.816656000	-0.092562000	-2.257016000
O	2.463166000	1.630168000	-0.550013000
C	1.761577000	2.615272000	0.109052000
O	0.839923000	2.343613000	0.823039000
C	2.295571000	3.956368000	-0.230982000
H	3.321085000	4.051278000	0.158117000
H	2.358509000	4.072568000	-1.322667000
H	1.658374000	4.733966000	0.204469000
H	5.093472000	-3.054885000	-1.357856000
H	1.988948000	-1.593066000	-1.154903000
Au	-0.233321000	-0.268116000	-0.442900000
P	-2.481963000	-0.282072000	0.135808000
O	-2.727729000	-1.249515000	1.372173000
O	-3.124492000	1.146687000	0.490092000
O	-3.510472000	-0.812834000	-0.962930000
C	-4.042876000	-1.552130000	1.856583000
H	-4.519963000	-2.299350000	1.206585000
H	-3.925832000	-1.959689000	2.867708000
H	-4.665530000	-0.644348000	1.892214000
C	-2.566386000	1.977982000	1.507596000
H	-1.494782000	2.170136000	1.330020000
H	-3.112905000	2.928404000	1.482114000
H	-2.697626000	1.513153000	2.498597000
C	-3.694431000	-0.139196000	-2.203787000
H	-2.728018000	0.013141000	-2.716133000
H	-4.329951000	-0.777698000	-2.828986000
H	-4.186763000	0.832671000	-2.047143000

TS1e: E= -1321.339227

C	-4.650173000	-1.019312000	0.050271000
C	-2.022277000	-0.088461000	0.170983000
C	-3.984450000	-1.050665000	-1.216175000
C	-2.445100000	-0.520538000	-1.160933000
C	-2.797886000	-1.915037000	-1.508844000
H	-5.432064000	-0.258953000	0.166171000
H	-4.516695000	-0.613811000	-2.066592000
H	-2.224942000	0.171051000	-1.981565000
H	-2.567284000	-2.716095000	-0.799101000
H	-2.656153000	-2.212900000	-2.551058000
C	-4.206601000	-1.702554000	1.156310000
H	-3.751466000	-2.689008000	1.028745000
C	-2.174514000	-0.961658000	1.268674000
H	-2.195300000	-0.520134000	2.270735000
O	-2.488958000	1.208712000	0.483698000
C	-1.895599000	2.292646000	-0.063475000
O	-0.908966000	2.211774000	-0.750998000
C	-2.617279000	3.543874000	0.295404000
H	-3.590434000	3.563649000	-0.218928000
H	-2.822841000	3.573948000	1.374783000
H	-2.027773000	4.415500000	-0.011076000
H	-4.694115000	-1.540232000	2.122342000
H	-1.777842000	-1.975933000	1.195907000
Au	0.210704000	-0.200636000	0.143463000

P	2.526609000	-0.229588000	-0.009185000
O	2.992465000	-1.094685000	-1.259595000
O	3.176776000	1.235434000	-0.154452000
O	3.400594000	-0.826343000	1.188002000
C	4.375336000	-1.323648000	-1.555599000
H	4.784816000	-2.088175000	-0.879933000
H	4.426586000	-1.677444000	-2.592092000
H	4.956024000	-0.393324000	-1.453652000
C	2.666510000	2.166849000	-1.107252000
H	1.575869000	2.301213000	-0.997455000
H	3.167521000	3.125197000	-0.924039000
H	2.892901000	1.832148000	-2.133008000
C	3.443645000	-0.206210000	2.467937000
H	2.427919000	-0.085285000	2.883981000
H	4.020854000	-0.864843000	3.128005000
H	3.934738000	0.776671000	2.404958000

2e: E= -1321.391655

C	-4.560890000	-1.801331000	0.038625000
C	-2.292095000	0.192174000	0.298175000
C	-3.736108000	-2.208451000	-0.933692000
C	-1.958978000	-0.401918000	-0.900169000
C	-2.275746000	-1.870935000	-1.115279000
H	-5.599998000	-2.147015000	-0.020812000
H	-4.156275000	-2.876652000	-1.694010000
H	-1.894886000	0.237028000	-1.790401000
H	-1.656546000	-2.517995000	-0.463191000
H	-1.963998000	-2.138064000	-2.135863000
C	-4.268902000	-0.939244000	1.228805000
H	-4.651866000	-1.444929000	2.132670000
C	-2.793839000	-0.602808000	1.455867000
H	-2.667399000	-0.021001000	2.381311000
O	-2.464074000	1.521730000	0.496788000
C	-1.831091000	2.530388000	-0.202700000
O	-0.909633000	2.315388000	-0.935118000
C	-2.442060000	3.840123000	0.131250000
H	-3.495960000	3.844831000	-0.187375000
H	-2.439454000	3.992924000	1.220448000
H	-1.896078000	4.645577000	-0.372374000
H	-4.855310000	-0.002250000	1.164568000
H	-2.213790000	-1.534277000	1.556850000
Au	0.197716000	-0.230585000	-0.207517000
P	2.484998000	-0.255836000	0.170710000
O	3.202946000	-1.098047000	-0.966620000
O	3.160812000	1.202925000	0.214791000
O	3.047209000	-0.893757000	1.520104000
C	4.613420000	-1.359139000	-0.956308000
H	4.838765000	-2.173576000	-0.253367000
H	4.889779000	-1.658345000	-1.974168000
H	5.175332000	-0.456614000	-0.669283000
C	2.903836000	2.154653000	-0.816246000
H	1.821689000	2.347008000	-0.922553000
H	3.408784000	3.085599000	-0.531566000
H	3.309515000	1.803680000	-1.779357000
C	2.768158000	-0.324559000	2.794913000
H	1.679458000	-0.228848000	2.952568000
H	3.177400000	-1.006237000	3.550034000
H	3.243971000	0.663255000	2.890045000

1f: E= -1895.582332

C	5.354298000	-2.310810000	-0.186113000
C	3.146873000	-0.299088000	-0.898074000
C	4.742181000	-1.426081000	0.828609000
C	3.630536000	-0.401740000	0.474613000
C	3.367722000	-1.599530000	1.341908000
H	6.205041000	-1.883275000	-0.732478000
H	5.467715000	-0.978409000	1.520438000
H	3.726737000	0.561566000	0.985028000
H	2.757600000	-2.407113000	0.920721000
H	3.156903000	-1.388090000	2.394679000
C	4.982164000	-3.565963000	-0.438222000
H	4.166398000	-4.051468000	0.110559000
C	2.572294000	-1.297951000	-1.661961000
H	2.517673000	-1.131065000	-2.744017000
O	3.410359000	0.870511000	-1.536999000
C	2.884828000	2.068415000	-1.091995000
O	2.005398000	2.097725000	-0.283342000
C	3.537648000	3.205792000	-1.786352000
H	3.070097000	4.148714000	-1.481484000
H	4.610674000	3.221501000	-1.541680000
H	3.465021000	3.072903000	-2.875942000
H	5.499381000	-4.173051000	-1.186034000
H	2.629224000	-2.337278000	-1.321117000
Au	0.588859000	-0.688337000	-0.841543000
P	-1.589944000	-0.352164000	-0.093105000
O	-2.531642000	-1.596060000	-0.388496000
O	-1.669377000	-0.081214000	1.502134000
O	-2.442448000	0.858503000	-0.725169000
C	-3.933403000	-1.637151000	-0.343825000
C	-4.635846000	-1.111736000	0.734311000
C	-4.570518000	-2.259480000	-1.408210000
C	-6.025413000	-1.213240000	0.732034000
C	-5.959152000	-2.357464000	-1.391297000
C	-6.687591000	-1.833319000	-0.325219000
H	-4.105043000	-0.641732000	1.566508000
H	-3.973485000	-2.660318000	-2.230757000
H	-6.594144000	-0.805811000	1.572053000
H	-6.474913000	-2.847592000	-2.221225000
H	-7.777555000	-1.910536000	-0.317009000
C	-0.550177000	0.072536000	2.315041000
C	-0.281646000	-0.915458000	3.257940000
C	0.245176000	1.207913000	2.194618000
C	0.803534000	-0.748799000	4.114260000
C	1.336941000	1.352911000	3.049367000
C	1.613775000	0.383235000	4.011545000
H	-0.938597000	-1.786693000	3.323614000
H	0.005614000	1.975440000	1.451341000
H	1.010774000	-1.506954000	4.874501000
H	1.963331000	2.245785000	2.966776000
H	2.455751000	0.515164000	4.696816000
C	-2.067272000	2.182185000	-0.505975000
C	-1.148696000	2.776206000	-1.364143000
C	-2.629513000	2.871665000	0.562497000
C	-0.779565000	4.100424000	-1.137165000
C	-2.254231000	4.195548000	0.774776000
C	-1.328200000	4.807995000	-0.069798000
H	-0.746406000	2.201291000	-2.204485000
H	-3.350794000	2.362554000	1.207297000
H	-0.063611000	4.584778000	-1.806679000
H	-2.691820000	4.754216000	1.606187000

H	-1.041112000	5.848737000	0.100846000
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TS1f: E= -1895.557106

C	5.401991000	-1.802836000	-0.073992000
C	2.911332000	-0.693966000	-0.684525000
C	4.781451000	-1.170391000	1.049517000
C	3.322915000	-0.526368000	0.709467000
C	3.499859000	-1.646346000	1.659192000
H	6.269702000	-1.286962000	-0.502814000
H	5.392396000	-0.470548000	1.627536000
H	3.209511000	0.481253000	1.127504000
H	3.144680000	-2.642539000	1.374549000
H	3.339868000	-1.418608000	2.716834000
C	4.831557000	-2.848035000	-0.760072000
H	4.256307000	-3.596077000	-0.206787000
C	2.914441000	-1.981701000	-1.262992000
H	2.951797000	-2.047146000	-2.355562000
O	3.516590000	0.253476000	-1.538141000
C	3.050721000	1.521288000	-1.581458000
O	2.067862000	1.873900000	-0.980229000
C	3.904136000	2.376272000	-2.451957000
H	4.033600000	1.906124000	-3.437674000
H	3.455102000	3.370429000	-2.557127000
H	4.907274000	2.468737000	-2.008476000
H	5.300626000	-3.211103000	-1.679487000
H	2.395550000	-2.792953000	-0.749172000
Au	0.693690000	-0.516715000	-0.542811000
P	-1.588830000	-0.347961000	-0.111102000
O	-2.438731000	-1.668368000	-0.359399000
O	-1.802184000	0.054669000	1.452315000
O	-2.465977000	0.752386000	-0.896826000
C	-3.834748000	-1.791660000	-0.388581000
C	-4.630898000	-1.223002000	0.599181000
C	-4.371367000	-2.539124000	-1.427886000
C	-6.010002000	-1.410098000	0.528869000
C	-5.750769000	-2.721171000	-1.479242000
C	-6.571447000	-2.155739000	-0.505157000
H	-4.180033000	-0.655368000	1.417680000
H	-3.703939000	-2.969098000	-2.178599000
H	-6.650494000	-0.970447000	1.298026000
H	-6.186531000	-3.309387000	-2.291096000
H	-7.653812000	-2.298982000	-0.550768000
C	-0.720405000	0.317586000	2.282971000
C	-0.401066000	-0.615320000	3.265331000
C	0.015014000	1.490007000	2.121788000
C	0.671867000	-0.359079000	4.115528000
C	1.093257000	1.727496000	2.973451000
C	1.421479000	0.809119000	3.969925000
H	-1.008882000	-1.518987000	3.360210000
H	-0.263846000	2.213157000	1.347686000
H	0.917159000	-1.075462000	4.904625000
H	1.668794000	2.650789000	2.862637000
H	2.253674000	1.012655000	4.649675000
C	-2.200250000	2.108246000	-0.713490000
C	-1.168005000	2.703846000	-1.429079000
C	-2.976811000	2.823327000	0.191388000
C	-0.903893000	4.056656000	-1.224040000
C	-2.709047000	4.176630000	0.378150000
C	-1.672187000	4.792253000	-0.324091000
H	-0.582528000	2.108159000	-2.136043000

H	-3.776470000	2.308969000	0.731629000
H	-0.091837000	4.537184000	-1.776017000
H	-3.315346000	4.755420000	1.079872000
H	-1.466611000	5.854846000	-0.171169000

2f: E= -1895.610968

Au	-0.805063000	-0.259572000	0.003561000
P	1.506321000	-0.212238000	-0.250056000
O	2.130905000	-1.435711000	-1.044678000
O	1.944026000	1.142251000	-1.030529000
O	2.405487000	-0.178621000	1.083972000
C	3.480609000	-1.809035000	-1.133413000
C	4.481998000	-0.865062000	-1.328198000
C	3.751510000	-3.167737000	-1.050112000
C	5.798364000	-1.309570000	-1.432731000
C	5.071718000	-3.594532000	-1.162998000
C	6.095631000	-2.668133000	-1.350413000
H	4.237577000	0.197911000	-1.407796000
H	2.928955000	-3.871303000	-0.901437000
H	6.598669000	-0.580619000	-1.585012000
H	5.299816000	-4.661775000	-1.101532000
H	7.131177000	-3.006690000	-1.435485000
C	0.984700000	2.059046000	-1.449625000
C	0.614022000	2.072050000	-2.790123000
C	0.418856000	2.931733000	-0.522872000
C	-0.339978000	2.994764000	-3.214814000
C	-0.539384000	3.845367000	-0.962393000
C	-0.917013000	3.879177000	-2.303782000
H	1.087716000	1.372718000	-3.484513000
H	0.750484000	2.906502000	0.521229000
H	-0.628861000	3.025210000	-4.268778000
H	-0.980092000	4.547310000	-0.249073000
H	-1.658141000	4.606809000	-2.644912000
C	2.264144000	0.888993000	1.972292000
C	1.245528000	0.861851000	2.919744000
C	3.154092000	1.952768000	1.875387000
C	1.119125000	1.942968000	3.791669000
C	3.019210000	3.021025000	2.758449000
C	2.000896000	3.019327000	3.711776000
H	0.571807000	0.001043000	2.981766000
H	3.937494000	1.925191000	1.113167000
H	0.328701000	1.935383000	4.546684000
H	3.716437000	3.860930000	2.700971000
H	1.900299000	3.859379000	4.403696000
C	-5.536566000	-0.208382000	-1.595115000
C	-3.183880000	-1.213280000	0.044348000
C	-4.839013000	0.919361000	-1.412641000
C	-3.020929000	0.150497000	0.173000000
C	-3.399262000	1.058686000	-0.982633000
H	-6.586406000	-0.095568000	-1.891880000
H	-5.363156000	1.863331000	-1.601503000
H	-3.035284000	0.581335000	1.182313000
H	-2.728306000	0.903157000	-1.851607000
H	-3.201071000	2.097897000	-0.678141000
C	-5.086140000	-1.631461000	-1.463614000
H	-5.385245000	-2.181848000	-2.373054000
C	-3.585388000	-1.836243000	-1.251062000
H	-3.339538000	-2.908502000	-1.229989000
O	-3.273061000	-2.096575000	1.069460000
C	-2.678566000	-1.952265000	2.306458000

O	-1.886342000	-1.085278000	2.535774000
C	-3.147539000	-3.020928000	3.222500000
H	-4.235270000	-2.931584000	3.366155000
H	-2.966462000	-4.008981000	2.774020000
H	-5.644873000	-2.124613000	-0.644600000
H	-3.026663000	-1.379756000	-2.084004000
H	-2.633231000	-2.937493000	4.186352000

1g: E= -861.106355

C	4.513562000	-0.468056000	0.386249000
C	1.656802000	0.340236000	-0.213638000
C	3.534713000	-0.240039000	1.471834000
C	2.073934000	0.173923000	1.180214000
C	2.413297000	-1.163307000	1.764462000
H	5.066441000	0.422079000	0.058356000
H	3.938531000	0.319684000	2.325308000
H	1.666131000	0.930531000	1.858279000
H	2.294696000	-2.044035000	1.124681000
H	2.125854000	-1.330973000	2.805598000
C	4.786910000	-1.646380000	-0.174140000
H	4.294778000	-2.571785000	0.147438000
C	1.551178000	-0.639899000	-1.180385000
H	1.530734000	-0.330025000	-2.231048000
O	1.577661000	1.640103000	-0.644547000
C	0.681962000	2.537982000	-0.131980000
O	-0.228391000	2.199061000	0.575981000
C	0.991606000	3.910126000	-0.604404000
H	0.233873000	4.613477000	-0.241896000
H	1.987414000	4.208336000	-0.242478000
H	1.037706000	3.926271000	-1.703285000
H	5.541027000	-1.740965000	-0.959992000
H	1.892109000	-1.655815000	-0.960995000
Au	-0.568419000	-0.614097000	-0.468887000
C	-2.513426000	-0.390822000	0.154627000
C	-4.700565000	-0.496033000	0.684294000
C	-4.238773000	0.716110000	1.088264000
H	-5.689938000	-0.940494000	0.752347000
H	-4.747384000	1.540269000	1.581363000
N	-3.622751000	-1.149735000	0.118344000
H	-3.649136000	-2.083679000	-0.279709000
N	-2.902142000	0.751982000	0.751933000
H	-2.244818000	1.518689000	0.912344000

TS1g: E= -861.076637

C	4.269515000	-0.755031000	-0.017448000
C	1.578268000	-0.040709000	-0.150824000
C	3.617158000	-0.800183000	1.253984000
C	2.037325000	-0.397106000	1.190566000
C	2.502105000	-1.745287000	1.581178000
H	4.991917000	0.057449000	-0.161769000
H	4.116831000	-0.296200000	2.086815000
H	1.768393000	0.303455000	1.988945000
H	2.334906000	-2.584418000	0.898261000
H	2.389806000	-2.020185000	2.633274000
C	3.866409000	-1.500386000	-1.100720000
H	3.500487000	-2.518363000	-0.937956000
C	1.802743000	-0.933121000	-1.222843000
H	1.781259000	-0.520692000	-2.237329000

O	1.954766000	1.277689000	-0.502773000
C	1.295150000	2.340827000	0.010302000
O	0.323514000	2.231484000	0.713954000
C	1.931554000	3.618583000	-0.416071000
H	1.322316000	4.467479000	-0.085713000
H	2.938262000	3.694410000	0.022391000
H	2.057138000	3.635963000	-1.508278000
H	4.336342000	-1.330929000	-2.074320000
H	1.478551000	-1.970274000	-1.120196000
Au	-0.618137000	-0.295790000	-0.163478000
C	-2.665556000	-0.247434000	0.001039000
C	-4.887201000	-0.651257000	-0.008278000
C	-4.702638000	0.599132000	0.487410000
H	-5.795348000	-1.223285000	-0.178278000
H	-5.417681000	1.338188000	0.838611000
N	-3.627259000	-1.141099000	-0.295111000
H	-3.430914000	-2.058037000	-0.684534000
N	-3.339316000	0.816662000	0.480853000
H	-2.868603000	1.662372000	0.795392000

2g: E= -861.131316

N	3.514271000	0.639963000	-0.337390000
C	2.624225000	-0.249049000	0.143683000
N	3.378087000	-1.140536000	0.814897000
C	4.719830000	-0.820276000	0.759906000
C	4.806320000	0.317235000	0.023025000
Au	0.593334000	-0.215422000	-0.151458000
C	-1.532225000	-0.361000000	-0.891850000
C	-1.880462000	-1.817229000	-1.136738000
C	-3.344307000	-2.123985000	-0.928463000
C	-4.130590000	-1.725924000	0.079049000
C	-3.783437000	-0.909901000	1.287300000
C	-2.295867000	-0.616996000	1.485460000
C	-1.801280000	0.203153000	0.338144000
O	-1.971204000	1.529861000	0.583622000
C	-1.408875000	2.558422000	-0.143530000
C	-1.988903000	3.856122000	0.285947000
O	-0.562819000	2.371845000	-0.968001000
H	-5.180634000	-2.040061000	0.036828000
H	-3.803991000	-2.752936000	-1.699363000
H	-1.481780000	0.299721000	-1.765233000
H	-1.262502000	-2.490416000	-0.511484000
H	-1.597095000	-2.066522000	-2.170014000
H	-4.157304000	-1.434050000	2.184589000
H	-2.130766000	-0.065063000	2.423185000
H	-1.490672000	4.678224000	-0.239994000
H	-3.067314000	3.868806000	0.065139000
H	-1.886152000	3.975382000	1.374486000
H	-4.347812000	0.042513000	1.266622000
H	-1.737042000	-1.563972000	1.550882000
H	5.489430000	-1.417463000	1.241610000
H	5.667123000	0.913388000	-0.268086000
H	2.987711000	-1.944945000	1.296894000
H	3.244498000	1.442639000	-0.899974000

1h: E= -1322.351842

C	-4.040323000	-3.231738000	-0.953917000
C	-2.068492000	-1.378726000	0.390286000

C	-3.902649000	-1.821915000	-1.381487000
C	-2.899416000	-0.865873000	-0.707284000
C	-2.724323000	-1.311003000	-2.125565000
H	-4.771447000	-3.407415000	-0.153786000
H	-4.859164000	-1.322594000	-1.582777000
H	-3.261952000	0.154501000	-0.544642000
H	-1.915352000	-2.013769000	-2.349715000
H	-2.878504000	-0.555998000	-2.901738000
C	-3.382088000	-4.269125000	-1.471026000
H	-2.671336000	-4.153531000	-2.297565000
C	-1.053092000	-2.305113000	0.301239000
H	-0.725195000	-2.798359000	1.222388000
O	-2.496210000	-1.069026000	1.649073000
C	-2.609351000	0.241251000	2.063048000
O	-2.145980000	1.141316000	1.427848000
C	-3.326308000	0.310213000	3.361913000
H	-3.367650000	1.348451000	3.709417000
H	-4.344026000	-0.092196000	3.245828000
H	-2.818334000	-0.322264000	4.104794000
H	-3.548313000	-5.286637000	-1.107186000
H	-0.861104000	-2.822391000	-0.643285000
C	2.500615000	3.042568000	-0.599947000
N	1.331761000	2.313950000	-0.456223000
C	1.608976000	1.012686000	-0.213492000
N	2.957820000	0.925583000	-0.209064000
C	3.525514000	2.166992000	-0.448885000
Au	0.210302000	-0.474897000	0.068946000
H	4.604082000	2.307686000	-0.472433000
H	2.489029000	4.110737000	-0.806477000
C	3.710149000	-0.271255000	0.016861000
C	0.012053000	2.865701000	-0.532785000
C	-0.358664000	3.858627000	0.370166000
C	-1.647696000	4.378888000	0.315186000
C	-2.554067000	3.903287000	-0.629549000
C	-2.168814000	2.914882000	-1.533292000
C	-0.878798000	2.393981000	-1.494081000
H	0.357887000	4.206481000	1.120376000
H	-1.947859000	5.157029000	1.021395000
H	-3.565950000	4.314971000	-0.669683000
H	-2.873559000	2.558788000	-2.290676000
H	-0.551450000	1.637211000	-2.214275000
C	4.641588000	-0.675384000	-0.937578000
C	5.385745000	-1.830530000	-0.714372000
C	5.191906000	-2.574751000	0.447574000
C	4.258137000	-2.160675000	1.395782000
C	3.515957000	-1.001122000	1.188518000
H	4.770942000	-0.091755000	-1.854021000
H	6.117027000	-2.155258000	-1.458844000
H	5.777613000	-3.481506000	0.618922000
H	4.116641000	-2.735801000	2.314436000
H	2.805187000	-0.645756000	1.940585000

TS1h: E= -1322.321644

C	2.172567000	4.548727000	0.288582000
C	1.417881000	1.868385000	0.009882000
C	1.435298000	4.302317000	-0.908567000
C	0.989198000	2.731826000	-1.082130000
C	0.014064000	3.832483000	-0.934534000
H	3.241476000	4.758498000	0.161225000
H	1.856869000	4.687919000	-1.841685000

H	1.224994000	2.371580000	-2.089411000
H	-0.560378000	3.901871000	-0.004430000
H	-0.570730000	4.099329000	-1.819216000
C	1.680371000	4.290477000	1.547170000
H	0.623522000	4.480330000	1.755845000
C	1.096561000	2.223756000	1.340100000
H	1.661376000	1.764937000	2.157963000
O	2.750696000	1.480903000	-0.230831000
C	3.269391000	0.338852000	0.294250000
O	2.634681000	-0.429603000	0.963258000
C	4.699564000	0.190393000	-0.099451000
H	4.770955000	0.080795000	-1.192522000
H	5.266448000	1.094603000	0.166229000
H	5.131876000	-0.688111000	0.393673000
H	2.343025000	4.384902000	2.412921000
H	0.057170000	2.467035000	1.572453000
Au	-0.010687000	0.166360000	0.013265000
C	-1.256945000	-1.465670000	-0.116007000
C	-3.029223000	-2.852125000	-0.045900000
C	-1.911702000	-3.620125000	-0.079184000
H	-4.084297000	-3.117490000	-0.035750000
H	-1.781341000	-4.699990000	-0.101642000
N	-2.608011000	-1.531717000	-0.078019000
N	-0.834823000	-2.751177000	-0.131661000
C	0.539782000	-3.149830000	-0.165508000
C	1.044518000	-3.949314000	0.856674000
C	1.351935000	-2.724977000	-1.216007000
C	2.384133000	-4.326299000	0.825753000
H	0.391993000	-4.259534000	1.678290000
C	2.691172000	-3.102638000	-1.233080000
H	0.924335000	-2.123007000	-2.023739000
C	3.207545000	-3.901572000	-0.214817000
H	2.787897000	-4.951754000	1.625812000
H	3.331177000	-2.788116000	-2.062274000
H	4.258312000	-4.202593000	-0.235700000
C	-3.487104000	-0.404596000	-0.044098000
C	-3.370989000	0.594751000	-1.009848000
C	-4.459157000	-0.330498000	0.951852000
C	-4.233208000	1.686673000	-0.964212000
H	-2.623435000	0.500336000	-1.802948000
C	-5.324123000	0.760176000	0.980246000
H	-4.527162000	-1.118234000	1.708203000
C	-5.209866000	1.769916000	0.027056000
H	-4.153302000	2.469510000	-1.723368000
H	-6.088483000	0.823846000	1.758825000
H	-5.891224000	2.624211000	0.052344000

2h: E= -1322.379497

C	0.600021000	-4.014778000	0.298298000
N	0.994653000	-2.695971000	0.145617000
C	-0.086188000	-1.885914000	0.063944000
N	-1.159677000	-2.702608000	0.168167000
C	-0.756488000	-4.019632000	0.308477000
Au	-0.132573000	0.152556000	-0.217051000
C	0.177131000	2.492202000	0.317588000
O	1.510345000	2.695889000	0.524006000
C	2.514241000	2.350827000	-0.352703000
O	2.310976000	1.754574000	-1.369688000
C	-0.441182000	2.287173000	-0.899637000
C	-1.926975000	2.556077000	-1.037159000

C	-2.311640000	3.976928000	-0.701515000
C	-1.899390000	4.720645000	0.332258000
C	-0.984919000	4.348794000	1.459759000
C	-0.604394000	2.871696000	1.537076000
C	3.828353000	2.781611000	0.192232000
H	-2.282843000	5.747085000	0.383156000
H	-3.018352000	4.444000000	-1.397236000
H	0.171620000	2.306775000	-1.806696000
H	-2.525464000	1.848810000	-0.429306000
H	-2.217161000	2.335407000	-2.074991000
H	-1.465201000	4.637352000	2.411551000
H	0.005662000	2.670574000	2.430841000
H	4.610025000	2.629238000	-0.561233000
H	3.793270000	3.835201000	0.504509000
H	4.059182000	2.185864000	1.089650000
H	-0.066592000	4.966057000	1.414227000
H	-1.517582000	2.258477000	1.611218000
H	-1.473346000	-4.831062000	0.415429000
H	1.321031000	-4.826444000	0.368041000
C	-2.525713000	-2.273685000	0.148266000
C	2.359196000	-2.263100000	0.102462000
C	3.236897000	-2.690359000	1.098471000
C	4.563519000	-2.271399000	1.061028000
C	5.002368000	-1.423074000	0.045315000
C	4.115659000	-0.999250000	-0.942413000
C	2.790672000	-1.427438000	-0.925625000
H	2.878317000	-3.334315000	1.907129000
H	5.256905000	-2.604748000	1.837354000
H	6.045685000	-1.097204000	0.021035000
H	4.450952000	-0.337046000	-1.745273000
H	2.098039000	-1.119175000	-1.714049000
C	-3.394687000	-2.816642000	-0.795270000
C	-4.725402000	-2.406659000	-0.809227000
C	-5.176401000	-1.458784000	0.106960000
C	-4.298558000	-0.923070000	1.048362000
C	-2.968481000	-1.333087000	1.078731000
H	-3.023884000	-3.546584000	-1.521346000
H	-5.412834000	-2.827323000	-1.547456000
H	-6.221937000	-1.140600000	0.092388000
H	-4.657508000	-0.193907000	1.779715000
H	-2.275928000	-0.946481000	1.833261000

1i: E= -1793.069461

C	-4.896119000	-2.751618000	-1.459112000
C	-2.326357000	-1.908063000	-0.175910000
C	-4.659925000	-1.331270000	-1.113633000
C	-3.346537000	-0.882309000	-0.453879000
C	-3.694627000	-0.469934000	-1.847745000
H	-5.405667000	-3.339569000	-0.684106000
H	-5.530917000	-0.825669000	-0.678241000
H	-3.448273000	-0.125482000	0.331439000
H	-3.141721000	-0.917585000	-2.680128000
H	-3.939154000	0.586041000	-1.994024000
C	-4.558698000	-3.346543000	-2.603297000
H	-4.081907000	-2.800821000	-3.425625000
C	-1.434015000	-2.444460000	-1.077164000
H	-0.918921000	-3.373480000	-0.812183000
O	-2.421739000	-2.556836000	1.024343000
C	-2.460864000	-1.884051000	2.223035000
O	-2.238113000	-0.711511000	2.303665000

C	-2.760104000	-2.829904000	3.329381000
H	-1.963565000	-3.587304000	3.389377000
H	-2.829604000	-2.284347000	4.277069000
H	-3.696599000	-3.369483000	3.125246000
H	-4.770580000	-4.404923000	-2.777066000
H	-1.500663000	-2.182427000	-2.137182000
Au	-0.203355000	-0.741436000	-0.294447000
C	1.080539000	0.789997000	0.178557000
C	2.903747000	2.058967000	0.477447000
C	1.815132000	2.855584000	0.650903000
H	3.970480000	2.270377000	0.524606000
H	1.728299000	3.916096000	0.880493000
N	2.427163000	0.791238000	0.191872000
N	0.704446000	2.052482000	0.474244000
C	3.237423000	-0.351054000	-0.142197000
C	3.540825000	-0.569164000	-1.496438000
C	3.659016000	-1.206275000	0.889642000
C	4.307305000	-1.695652000	-1.805863000
C	4.420489000	-2.318575000	0.522071000
C	4.743231000	-2.560058000	-0.808589000
H	4.564775000	-1.900816000	-2.850135000
H	4.763909000	-3.013764000	1.294127000
H	5.342210000	-3.436202000	-1.071923000
C	-0.673265000	2.471713000	0.476106000
C	-1.243004000	2.797146000	-0.770772000
C	-1.402372000	2.478012000	1.677861000
C	-2.600006000	3.125735000	-0.797538000
C	-2.760174000	2.807547000	1.583555000
C	-3.356167000	3.122267000	0.369019000
H	-3.069589000	3.397330000	-1.749021000
H	-3.358326000	2.820184000	2.501030000
H	-4.418243000	3.381374000	0.334403000
C	-0.440402000	2.831161000	-2.055982000
H	0.585778000	2.484304000	-1.838801000
C	-0.849970000	2.267359000	3.078021000
H	-1.721909000	1.921945000	3.663625000
C	0.234302000	1.219814000	3.290404000
H	0.342603000	1.037457000	4.372193000
H	-0.018607000	0.257600000	2.819817000
H	1.224472000	1.550549000	2.934600000
C	-0.415859000	3.612930000	3.660089000
H	-0.128311000	3.505179000	4.718472000
H	0.459086000	4.017353000	3.121244000
H	-1.218968000	4.364274000	3.600883000
C	-1.012317000	1.887845000	-3.107602000
H	-0.367616000	1.864386000	-4.001504000
H	-1.094965000	0.856908000	-2.717329000
H	-2.016143000	2.203576000	-3.439323000
C	-0.331584000	4.257820000	-2.585310000
H	0.293741000	4.292799000	-3.491984000
H	-1.322323000	4.664516000	-2.849754000
H	0.113991000	4.934489000	-1.837905000
C	3.268901000	-0.989803000	2.336398000
H	2.865687000	0.034494000	2.432172000
C	2.156436000	-1.958211000	2.735518000
H	1.844214000	-1.787614000	3.779354000
H	1.265170000	-1.846737000	2.090654000
H	2.498944000	-3.004247000	2.653617000
C	4.455285000	-1.102900000	3.286230000
H	4.845050000	-2.133230000	3.337646000
H	5.286248000	-0.445594000	2.984971000

H	4.155744000	-0.824162000	4.309058000
C	3.053658000	0.343175000	-2.602208000
H	2.501228000	1.182284000	-2.140726000
C	4.216942000	0.944231000	-3.383168000
H	4.911545000	1.485953000	-2.720801000
H	4.797037000	0.167109000	-3.908383000
H	3.852308000	1.652095000	-4.144796000
C	2.078891000	-0.387446000	-3.521062000
H	1.675468000	0.295273000	-4.287343000
H	2.571596000	-1.221450000	-4.048755000
H	1.227062000	-0.808931000	-2.955226000

TS1i: E= -1793.039345

C	2.124651000	-1.938465000	0.381451000
O	1.936973000	-3.221406000	-0.176393000
C	1.397307000	-3.353925000	-1.409313000
O	1.027603000	-2.414885000	-2.064144000
C	1.319073000	-4.789351000	-1.803283000
H	2.297259000	-5.275589000	-1.678206000
H	0.614621000	-5.313166000	-1.139215000
H	0.979560000	-4.873713000	-2.841822000
Au	0.416734000	-0.538036000	0.156242000
C	-0.981373000	0.939165000	-0.148488000
C	-2.854690000	2.174998000	-0.222255000
C	-1.820182000	2.979309000	-0.582200000
H	-3.922319000	2.365933000	-0.128777000
H	-1.787910000	4.029815000	-0.865567000
N	-2.314850000	0.925984000	0.037037000
N	-0.679798000	2.195331000	-0.550809000
C	-3.066969000	-0.239195000	0.414856000
C	-3.261160000	-0.500064000	1.781293000
C	-3.556705000	-1.068335000	-0.607945000
C	-3.990496000	-1.644762000	2.112686000
C	-4.278249000	-2.199913000	-0.218215000
C	-4.494261000	-2.484039000	1.125410000
H	-4.168166000	-1.885309000	3.165754000
H	-4.682618000	-2.871363000	-0.982233000
H	-5.065810000	-3.372624000	1.407657000
C	0.675635000	2.644778000	-0.733595000
C	1.365590000	3.070339000	0.416073000
C	1.275543000	2.575778000	-2.006357000
C	2.709788000	3.426296000	0.273437000
C	2.624385000	2.939290000	-2.083313000
C	3.336716000	3.355433000	-0.963511000
H	3.271926000	3.770484000	1.147825000
H	3.121226000	2.902391000	-3.058309000
H	4.387711000	3.642343000	-1.062397000
C	0.711444000	3.167626000	1.779664000
H	-0.332870000	2.818985000	1.692902000
C	0.588135000	2.132397000	-3.288211000
H	1.323082000	2.367303000	-4.080106000
C	0.347712000	0.627466000	-3.364332000
H	0.031830000	0.347142000	-4.382810000
H	1.249034000	0.041952000	-3.122119000
H	-0.449011000	0.293429000	-2.677850000
C	-0.675134000	2.911598000	-3.641262000
H	-0.930108000	2.745553000	-4.700158000
H	-1.549312000	2.587839000	-3.052828000
H	-0.545206000	3.997227000	-3.499451000
C	1.396886000	2.262214000	2.797086000

H	0.878424000	2.304498000	3.768979000
H	1.391750000	1.210476000	2.456239000
H	2.444836000	2.561554000	2.971048000
C	0.666335000	4.615003000	2.258963000
H	0.143137000	4.691695000	3.225573000
H	1.680175000	5.026299000	2.398185000
H	0.143088000	5.263068000	1.537229000
C	-3.357277000	-0.756755000	-2.076636000
H	-2.698190000	0.127567000	-2.155578000
C	-2.660583000	-1.894031000	-2.814207000
H	-2.501975000	-1.625288000	-3.871454000
H	-1.673741000	-2.123985000	-2.377737000
H	-3.263550000	-2.817775000	-2.802857000
C	-4.684840000	-0.390684000	-2.734520000
H	-5.384554000	-1.243418000	-2.729865000
H	-5.180959000	0.445814000	-2.214880000
H	-4.532317000	-0.096074000	-3.785320000
C	-2.688535000	0.382374000	2.870822000
H	-2.245358000	1.274491000	2.392100000
C	-3.764131000	0.873274000	3.832875000
H	-4.576160000	1.395687000	3.301900000
H	-4.217445000	0.042172000	4.398502000
H	-3.336374000	1.571625000	4.570099000
C	-1.565688000	-0.336653000	3.613448000
H	-1.114810000	0.322344000	4.373935000
H	-1.940278000	-1.234566000	4.134087000
H	-0.768263000	-0.659521000	2.919530000
C	2.058671000	-1.990732000	1.791291000
H	1.473021000	-2.801488000	2.238361000
H	2.087828000	-1.055964000	2.354808000
C	3.203918000	-1.188224000	-0.255999000
H	3.163989000	-1.114258000	-1.348087000
C	4.098239000	-0.256600000	0.464758000
H	3.846988000	0.025532000	1.493234000
H	4.519866000	0.568078000	-0.116926000
C	4.703118000	-1.611110000	0.257875000
H	5.381185000	-1.742381000	-0.590575000
C	4.688986000	-2.639455000	1.248087000
C	4.027552000	-2.517114000	2.449165000
H	4.034590000	-1.548485000	2.957848000
H	3.956619000	-3.383897000	3.113231000
H	5.053032000	-3.624012000	0.930140000

2i: E= -1793.098886

C	4.480794000	-1.923482000	-2.592403000
C	2.389959000	-1.796977000	-0.397521000
C	3.344040000	-1.993192000	-3.296380000
C	1.594411000	-2.140814000	-1.472011000
C	1.949816000	-1.619875000	-2.851988000
H	5.393161000	-2.261071000	-3.099435000
H	3.422684000	-2.355515000	-4.328008000
H	0.995667000	-3.055474000	-1.409154000
H	1.823225000	-0.521741000	-2.914599000
H	1.217290000	-2.022021000	-3.567775000
C	4.700206000	-1.436785000	-1.191706000
H	5.531292000	-0.709442000	-1.197276000
C	3.489312000	-0.789434000	-0.523074000
H	3.744302000	-0.415361000	0.481613000
O	2.515101000	-2.496530000	0.766947000
C	1.570066000	-3.351842000	1.285888000

O	0.477162000	-3.468209000	0.814801000
C	2.113615000	-4.027276000	2.493412000
H	2.415729000	-3.273678000	3.236672000
H	1.357099000	-4.697570000	2.916458000
H	3.017997000	-4.596530000	2.230466000
H	5.065727000	-2.272322000	-0.563568000
H	3.149539000	0.076166000	-1.116093000
Au	0.282259000	-0.636510000	-0.388373000
C	-0.971427000	0.789469000	0.389649000
C	-1.651937000	2.724718000	1.303187000
C	-2.756685000	1.974691000	1.048953000
H	-1.534825000	3.719891000	1.728808000
H	-3.816158000	2.178705000	1.192485000
N	-0.564116000	1.975298000	0.891022000
N	-2.315556000	0.781530000	0.503828000
C	0.804430000	2.421721000	0.884493000
C	1.270822000	3.090927000	-0.260974000
C	1.617668000	2.146641000	1.996591000
C	2.615094000	3.472840000	-0.277287000
C	2.953449000	2.552386000	1.926549000
C	3.448612000	3.204106000	0.802464000
H	3.015675000	3.998757000	-1.149957000
H	3.619525000	2.355886000	2.772547000
H	4.496493000	3.515369000	0.771948000
C	-3.176936000	-0.250846000	-0.014418000
C	-3.466192000	-0.214385000	-1.391052000
C	-3.698039000	-1.229404000	0.853310000
C	-4.329414000	-1.190476000	-1.896163000
C	-4.555728000	-2.177170000	0.286727000
C	-4.873815000	-2.160157000	-1.066003000
H	-4.580474000	-1.187588000	-2.961540000
H	-4.979848000	-2.952203000	0.933121000
H	-5.550030000	-2.915078000	-1.476027000
C	-2.891506000	0.823431000	-2.333964000
H	-2.215871000	1.484459000	-1.761556000
C	-3.437516000	-1.324354000	2.347870000
H	-3.815638000	-2.326152000	2.621974000
C	-1.973891000	-1.298010000	2.773972000
H	-1.889277000	-1.642854000	3.817637000
H	-1.350473000	-1.960237000	2.149589000
H	-1.543797000	-0.282199000	2.744785000
C	-4.266800000	-0.322604000	3.147859000
H	-5.327966000	-0.343973000	2.852738000
H	-4.213174000	-0.554278000	4.224009000
H	-3.896009000	0.708765000	3.024973000
C	-2.053642000	0.165966000	-3.426072000
H	-1.578186000	0.925716000	-4.068155000
H	-1.256226000	-0.467122000	-2.996224000
H	-2.668434000	-0.475902000	-4.078632000
C	-3.987130000	1.704145000	-2.925044000
H	-3.554122000	2.485204000	-3.571134000
H	-4.687333000	1.117230000	-3.542678000
H	-4.576183000	2.202145000	-2.137601000
C	1.108498000	1.414957000	3.220571000
H	0.008421000	1.346867000	3.143597000
C	1.650175000	-0.011687000	3.261359000
H	1.249666000	-0.556396000	4.132958000
H	1.375837000	-0.575629000	2.351692000
H	2.751920000	-0.017444000	3.340885000
C	1.425105000	2.158674000	4.512832000
H	2.507675000	2.178605000	4.721231000

H	1.071640000	3.201399000	4.481210000
H	0.942119000	1.662489000	5.369613000
C	0.381442000	3.396092000	-1.447371000
H	-0.643051000	3.061642000	-1.203784000
C	0.311116000	4.894297000	-1.722099000
H	-0.014735000	5.455603000	-0.831398000
H	1.290520000	5.297584000	-2.029088000
H	-0.399670000	5.106902000	-2.536562000
C	0.826505000	2.623123000	-2.684265000
H	0.132831000	2.795956000	-3.523913000
H	1.831117000	2.935201000	-3.017587000
H	0.858669000	1.535119000	-2.491075000

1j: E= -1439.522225

C	-1.869598000	2.612801000	-0.192694000
C	0.490348000	1.058324000	0.278985000
C	-0.576689000	3.241736000	-0.514334000
C	0.709225000	2.406033000	-0.281906000
C	0.277184000	2.810430000	-1.654798000
H	-2.203227000	2.746260000	0.845633000
H	-0.460346000	4.280475000	-0.181551000
H	1.549544000	2.947277000	0.167108000
H	-0.102460000	2.047167000	-2.341755000
H	0.887108000	3.568999000	-2.152062000
C	-2.596348000	1.840817000	-1.017655000
H	-2.309328000	1.789290000	-2.079078000
C	-0.135333000	0.019683000	-0.395960000
C	-0.883395000	-1.128197000	0.119692000
C	-0.786702000	-1.633223000	1.428963000
C	-1.802543000	-1.720669000	-0.763871000
C	-1.603305000	-2.680763000	1.836506000
C	-2.628119000	-2.756652000	-0.347375000
C	-2.531441000	-3.237701000	0.955991000
H	-0.064771000	-1.212868000	2.132136000
H	-1.885171000	-1.341440000	-1.788181000
H	-1.515882000	-3.068630000	2.854894000
H	-3.354171000	-3.185438000	-1.042966000
H	-3.176016000	-4.056256000	1.287295000
O	0.434371000	1.051752000	1.661451000
C	1.581944000	1.163121000	2.389660000
O	2.666600000	1.087949000	1.877733000
C	1.280710000	1.354922000	3.831422000
H	0.762356000	2.315687000	3.972571000
H	0.593296000	0.570852000	4.183482000
H	2.208656000	1.343060000	4.413906000
C	-3.750207000	1.023138000	-0.643131000
C	-3.959378000	0.603676000	0.680787000
C	-4.640147000	0.581451000	-1.633430000
C	-5.040155000	-0.206667000	1.005089000
C	-5.723944000	-0.228686000	-1.308742000
C	-5.927853000	-0.623578000	0.012075000
H	-3.241422000	0.888552000	1.457985000
H	-4.481253000	0.893033000	-2.671765000
H	-5.186061000	-0.528803000	2.040180000
H	-6.415436000	-0.553492000	-2.091105000
H	-6.777578000	-1.262104000	0.269104000
H	-0.274438000	0.201649000	-1.468185000
Au	2.198655000	-0.336210000	-0.494672000
P	4.220809000	-1.393681000	-1.073141000
H	4.712632000	-1.204112000	-2.386094000

H	5.349055000	-1.026993000	-0.302063000
H	4.265736000	-2.803926000	-0.968390000

TS1j: E= -1439.497232

C	1.684396000	-2.539437000	-1.057914000
C	-0.428624000	-0.965528000	-0.115966000
C	0.438370000	-3.083250000	-1.433344000
C	-0.817069000	-2.166381000	-0.859606000
C	-0.574833000	-2.381520000	-2.294278000
H	2.299729000	-3.161247000	-0.395179000
H	0.283572000	-4.149374000	-1.244331000
H	-1.544511000	-2.815639000	-0.359156000
H	-0.218638000	-1.548887000	-2.909441000
H	-1.271787000	-3.037801000	-2.822673000
C	2.101750000	-1.221639000	-1.309891000
H	1.927297000	-0.874087000	-2.338687000
C	0.528660000	-0.081675000	-0.761023000
C	1.130030000	1.122829000	-0.156338000
C	1.553257000	1.209900000	1.179527000
C	1.332105000	2.229928000	-0.996085000
C	2.137940000	2.378381000	1.655756000
C	1.916716000	3.397210000	-0.518326000
C	2.322241000	3.473040000	0.812418000
H	1.436729000	0.353360000	1.844800000
H	1.019640000	2.172364000	-2.045644000
H	2.463643000	2.432368000	2.698066000
H	2.058878000	4.249295000	-1.188061000
H	2.785424000	4.387043000	1.193816000
O	-0.022237000	-1.301914000	1.200304000
C	-0.936860000	-1.562925000	2.162238000
O	-2.122813000	-1.516170000	1.964807000
C	-0.272751000	-1.877116000	3.458909000
H	0.535358000	-2.608721000	3.317319000
H	0.184977000	-0.959441000	3.862444000
H	-1.012118000	-2.253357000	4.175325000
C	3.360346000	-0.722157000	-0.718911000
C	3.777710000	-1.120949000	0.557738000
C	4.141708000	0.198852000	-1.425613000
C	4.963260000	-0.634505000	1.098268000
C	5.324658000	0.691874000	-0.883416000
C	5.740313000	0.271832000	0.378204000
H	3.157861000	-1.806875000	1.147129000
H	3.817520000	0.527552000	-2.419755000
H	5.281761000	-0.958912000	2.092816000
H	5.929010000	1.403592000	-1.452030000
H	6.671402000	0.655126000	0.804413000
H	0.201884000	0.128779000	-1.786911000
Au	-2.261119000	0.258555000	-0.186008000
P	-4.175666000	1.619205000	-0.297931000
H	-4.968584000	1.561585000	-1.469535000
H	-5.166240000	1.414975000	0.692770000
H	-3.988936000	3.018468000	-0.188906000

2j: E= -1439.532665

C	1.824538000	-1.733431000	-2.417124000
C	0.219950000	-0.642905000	-0.101182000
C	0.692054000	-2.440781000	-2.517247000
C	-0.587812000	-1.712817000	-0.458170000
C	-0.657685000	-2.142957000	-1.912802000

H	2.705075000	-2.141932000	-2.929450000
H	0.734275000	-3.349047000	-3.129547000
H	-0.749420000	-2.491706000	0.298949000
H	-1.189474000	-1.395226000	-2.533615000
H	-1.289701000	-3.041617000	-1.968582000
C	2.113808000	-0.433872000	-1.712765000
H	2.457064000	0.273993000	-2.492883000
C	0.831897000	0.252083000	-1.134588000
C	0.986536000	1.693210000	-0.704080000
C	1.807218000	2.109380000	0.355681000
C	0.270605000	2.666136000	-1.413145000
C	1.903594000	3.459633000	0.682284000
C	0.368555000	4.016728000	-1.086082000
C	1.187541000	4.416609000	-0.034343000
H	2.385476000	1.377820000	0.926666000
H	-0.369125000	2.360049000	-2.250094000
H	2.552927000	3.768451000	1.506378000
H	-0.192272000	4.758419000	-1.661361000
H	1.272184000	5.475313000	0.225085000
O	0.702742000	-0.423341000	1.130104000
C	0.139887000	-0.810673000	2.333392000
O	-0.969392000	-1.249462000	2.401554000
C	1.099830000	-0.530741000	3.427435000
H	2.081658000	-0.965836000	3.182534000
H	1.247388000	0.558909000	3.501343000
H	0.718326000	-0.921838000	4.377358000
C	3.257125000	-0.584151000	-0.733272000
C	3.305220000	-1.660377000	0.160672000
C	4.285354000	0.362920000	-0.696686000
C	4.330289000	-1.762120000	1.097750000
C	5.315839000	0.261539000	0.234879000
C	5.334081000	-0.794929000	1.142835000
H	2.536124000	-2.440101000	0.109981000
H	4.271093000	1.199630000	-1.404136000
H	4.359139000	-2.613459000	1.784553000
H	6.112588000	1.010142000	0.248277000
H	6.143809000	-0.878257000	1.872868000
H	0.133059000	0.257939000	-1.987630000
Au	-2.312220000	-0.347969000	0.012675000
P	-4.313648000	0.843450000	0.318833000
H	-5.477489000	0.280546000	-0.255776000
H	-4.739078000	1.045522000	1.652799000
H	-4.370836000	2.161622000	-0.191490000

1k: E= -2214.600152

C	-4.030587000	2.444606000	-0.184969000
C	-1.494109000	1.327069000	0.567693000
C	-2.856122000	3.333073000	-0.231441000
C	-1.476771000	2.742189000	0.148637000
C	-1.771730000	3.190352000	-1.244128000
H	-4.570540000	2.436212000	0.771870000
H	-3.010787000	4.337344000	0.181869000
H	-0.835534000	3.391046000	0.756911000
H	-1.885769000	2.444831000	-2.037202000
H	-1.264456000	4.098103000	-1.581783000
C	-4.424116000	1.612664000	-1.163013000
H	-3.939708000	1.693653000	-2.147961000
C	-1.751754000	0.268907000	-0.284223000
O	-1.871061000	1.173501000	1.899056000
C	-0.981701000	1.372895000	2.902446000

O	0.191914000	1.542903000	2.702356000
C	-1.657830000	1.314432000	4.227344000
H	-2.433734000	2.092053000	4.286552000
H	-2.171219000	0.347289000	4.343481000
H	-0.923570000	1.451128000	5.029096000
H	-1.668097000	0.519370000	-1.348537000
Au	0.579989000	0.238174000	0.157823000
P	2.471485000	-1.226420000	-0.006814000
C	2.683141000	-1.994992000	1.716644000
C	2.067166000	-2.467968000	-1.398258000
C	4.084622000	-0.484401000	-0.475253000
C	5.189767000	-1.342526000	-0.621166000
C	4.232164000	0.872942000	-0.837803000
C	6.406098000	-0.895707000	-1.120718000
C	5.465253000	1.299700000	-1.356866000
C	6.541732000	0.435510000	-1.501484000
H	5.104081000	-2.396574000	-0.352185000
H	7.242705000	-1.592241000	-1.218059000
H	5.572680000	2.353465000	-1.631835000
H	7.489050000	0.804880000	-1.903289000
C	3.199153000	1.932455000	-0.700975000
C	2.768508000	2.369107000	0.560051000
C	2.763072000	2.624452000	-1.839481000
C	1.957157000	3.496180000	0.678686000
C	1.938987000	3.740331000	-1.719824000
C	1.551097000	4.190047000	-0.458654000
H	3.115639000	1.854116000	1.461659000
H	3.099693000	2.292310000	-2.827733000
H	1.658282000	3.838350000	1.673679000
H	1.620149000	4.278460000	-2.617484000
H	0.938496000	5.092050000	-0.361681000
C	1.378946000	-2.689140000	2.100602000
H	0.508212000	-2.016084000	2.013206000
H	1.181094000	-3.589556000	1.496283000
H	1.443702000	-3.012702000	3.153702000
C	3.843011000	-2.976722000	1.860110000
H	3.789986000	-3.823246000	1.159691000
H	4.820379000	-2.483647000	1.751025000
H	3.812422000	-3.397034000	2.880187000
C	2.929140000	-0.818191000	2.663527000
H	3.846834000	-0.263420000	2.401800000
H	2.085355000	-0.108103000	2.694955000
H	3.069405000	-1.210171000	3.685906000
C	2.829533000	-3.788354000	-1.337081000
H	2.566948000	-4.380570000	-2.230964000
H	3.922209000	-3.665347000	-1.353303000
H	2.552169000	-4.396969000	-0.461448000
C	0.568508000	-2.773268000	-1.368476000
H	-0.037465000	-1.882982000	-1.603689000
H	0.346513000	-3.532238000	-2.138653000
H	0.218979000	-3.174564000	-0.402997000
C	2.387493000	-1.743251000	-2.706761000
H	1.919053000	-0.743321000	-2.752507000
H	3.469813000	-1.620684000	-2.870042000
H	1.986382000	-2.334837000	-3.547794000
C	-2.367220000	-1.034250000	-0.020139000
C	-2.922620000	-1.703441000	-1.124182000
C	-2.464315000	-1.640449000	1.244400000
C	-3.569450000	-2.923606000	-0.974854000
C	-3.101895000	-2.866684000	1.389947000
C	-3.662269000	-3.509101000	0.285671000

H	-2.860386000	-1.242364000	-2.116572000
H	-2.034717000	-1.153015000	2.121530000
H	-4.013187000	-3.413855000	-1.845588000
H	-3.167586000	-3.326619000	2.379869000
H	-4.169564000	-4.469722000	0.409288000
C	-5.455661000	0.580242000	-1.059517000
C	-6.064946000	0.089864000	-2.224069000
C	-6.795247000	-0.971834000	0.241175000
C	-7.037671000	-0.902892000	-2.157646000
C	-7.409729000	-1.433125000	-0.923512000
H	-7.070507000	-1.398273000	1.210222000
H	-7.511741000	-1.263795000	-3.074782000
H	-8.174618000	-2.212657000	-0.868409000
H	-5.776452000	0.510019000	-3.194068000
C	-5.823105000	0.019040000	0.174235000
H	-5.312982000	0.342331000	1.088619000

TS1k: -2214.573568

C	-3.849905000	2.632204000	-0.355774000
C	-1.493240000	1.260356000	0.277914000
C	-2.736135000	3.488249000	-0.421422000
C	-1.319921000	2.671815000	-0.014450000
C	-1.554733000	3.288921000	-1.327700000
H	-4.605737000	2.879950000	0.400112000
H	-2.807966000	4.444407000	0.105137000
H	-0.775865000	3.256390000	0.734686000
H	-1.704404000	2.645511000	-2.200911000
H	-0.973613000	4.187820000	-1.554239000
C	-3.962085000	1.400424000	-1.026345000
H	-3.700863000	1.428869000	-2.094796000
C	-2.190870000	0.474809000	-0.715008000
O	-2.024484000	1.050552000	1.577243000
C	-1.279769000	1.258433000	2.683812000
O	-0.136753000	1.633134000	2.651216000
C	-2.051547000	0.914103000	3.913697000
H	-2.123426000	-0.183745000	3.990864000
H	-1.533047000	1.297611000	4.800303000
H	-3.077257000	1.305626000	3.863610000
H	-1.781367000	0.697102000	-1.707968000
Au	0.538437000	0.351314000	0.100061000
P	2.338637000	-1.209664000	0.125734000
C	2.314614000	-2.017337000	1.853441000
C	2.000754000	-2.434381000	-1.285290000
C	4.037688000	-0.576014000	-0.170422000
C	5.112542000	-1.478323000	-0.081863000
C	4.306982000	0.755427000	-0.558032000
C	6.414648000	-1.103808000	-0.385013000
C	5.626050000	1.107277000	-0.886592000
C	6.671145000	0.197638000	-0.805595000
H	4.933544000	-2.509943000	0.225310000
H	7.224649000	-1.832588000	-0.298803000
H	5.824738000	2.140326000	-1.189030000
H	7.688114000	0.508458000	-1.059315000
C	3.321717000	1.868287000	-0.616218000
C	2.803200000	2.428767000	0.559380000
C	3.026850000	2.477792000	-1.841891000
C	2.034028000	3.589718000	0.511125000
C	2.251737000	3.634675000	-1.890778000
C	1.767877000	4.201612000	-0.712498000
H	3.042194000	1.973442000	1.526877000

H	3.435609000	2.049840000	-2.764068000
H	1.658392000	4.020428000	1.444467000
H	2.047430000	4.110030000	-2.854845000
H	1.191907000	5.132415000	-0.747109000
C	0.860380000	-2.099771000	2.330420000
H	0.411660000	-1.097152000	2.436517000
H	0.216984000	-2.699889000	1.667590000
H	0.844742000	-2.575895000	3.326425000
C	2.923204000	-3.414590000	1.924872000
H	2.390792000	-4.140338000	1.289733000
H	3.992904000	-3.440062000	1.670682000
H	2.841799000	-3.777086000	2.964326000
C	3.069372000	-1.066541000	2.781834000
H	4.143703000	-1.008030000	2.545958000
H	2.648816000	-0.045779000	2.752340000
H	2.973055000	-1.427822000	3.820331000
C	3.110040000	-3.447451000	-1.556249000
H	2.769459000	-4.123094000	-2.360060000
H	4.037329000	-2.971035000	-1.909997000
H	3.346416000	-4.078655000	-0.686081000
C	0.699596000	-3.172340000	-0.982925000
H	-0.129952000	-2.485591000	-0.742034000
H	0.395672000	-3.747616000	-1.875217000
H	0.808678000	-3.892170000	-0.155255000
C	1.823211000	-1.571494000	-2.536741000
H	0.951632000	-0.897911000	-2.460202000
H	2.715006000	-0.955074000	-2.746413000
H	1.665480000	-2.229956000	-3.408638000
C	-2.542742000	-0.957344000	-0.622562000
C	-2.586694000	-1.677589000	-1.826790000
C	-2.879859000	-1.625472000	0.565255000
C	-2.940896000	-3.021841000	-1.853211000
C	-3.227839000	-2.972615000	0.538568000
C	-3.260521000	-3.675710000	-0.665449000
H	-2.339345000	-1.165783000	-2.765194000
H	-2.879805000	-1.085849000	1.514166000
H	-2.967537000	-3.561063000	-2.804081000
H	-3.488464000	-3.479906000	1.471791000
H	-3.542735000	-4.731935000	-0.676863000
C	-5.091579000	0.502972000	-0.705173000
C	-5.543767000	0.356393000	0.613197000
C	-5.701656000	-0.254037000	-1.711927000
C	-6.595890000	-0.502672000	0.911255000
C	-6.749466000	-1.119989000	-1.414221000
C	-7.201835000	-1.243524000	-0.102309000
H	-5.043798000	0.904282000	1.420237000
H	-5.350382000	-0.156220000	-2.745451000
H	-6.941511000	-0.602739000	1.943981000
H	-7.220858000	-1.698726000	-2.213186000
H	-8.027091000	-1.921370000	0.131874000

2k: -2214.617452

C	3.718797000	-1.768922000	-2.336068000
C	1.895294000	-0.699090000	-0.151383000
C	2.617103000	-2.507238000	-2.520414000
C	1.200622000	-1.824823000	-0.547340000
C	1.224505000	-2.256965000	-1.998432000
H	4.647357000	-2.147178000	-2.783098000
H	2.730121000	-3.410015000	-3.132256000
H	0.984719000	-2.594793000	0.202252000

H	0.696558000	-1.529493000	-2.648056000
H	0.626914000	-3.177290000	-2.086514000
C	3.908588000	-0.459705000	-1.616036000
H	4.304854000	0.249484000	-2.369748000
C	2.566798000	0.196582000	-1.157747000
O	2.296033000	-0.431759000	1.114721000
C	1.797281000	-0.958371000	2.278555000
O	0.800312000	-1.619344000	2.319504000
C	2.655781000	-0.525143000	3.411629000
H	3.714111000	-0.721800000	3.175366000
H	2.554769000	0.565065000	3.539869000
H	2.354099000	-1.035896000	4.333164000
H	1.934321000	0.165946000	-2.060883000
Au	-0.569528000	-0.431991000	-0.190426000
P	-2.383193000	1.090275000	0.048181000
C	-1.912802000	2.200541000	1.517745000
C	-2.619383000	1.988199000	-1.611513000
C	-4.004666000	0.317034000	0.419120000
C	-5.108430000	1.160207000	0.638897000
C	-4.218255000	-1.078631000	0.373932000
C	-6.389983000	0.656808000	0.821173000
C	-5.521890000	-1.566024000	0.553269000
C	-6.598567000	-0.718030000	0.777422000
H	-4.972921000	2.242890000	0.655192000
H	-7.224425000	1.342171000	0.990103000
H	-5.678142000	-2.648737000	0.517340000
H	-7.600850000	-1.132428000	0.914856000
C	-3.179398000	-2.118129000	0.128867000
C	-2.318134000	-2.544280000	1.149623000
C	-3.159502000	-2.796200000	-1.098423000
C	-1.471673000	-3.635226000	0.951819000
C	-2.304841000	-3.877836000	-1.298203000
C	-1.466431000	-4.306493000	-0.268966000
H	-2.335012000	-2.035491000	2.119831000
H	-3.844887000	-2.482285000	-1.893613000
H	-0.816611000	-3.958063000	1.766183000
H	-2.310741000	-4.404304000	-2.257093000
H	-0.814242000	-5.172545000	-0.416874000
C	-0.590622000	2.896784000	1.195299000
H	0.208713000	2.194051000	0.896321000
H	-0.688744000	3.656229000	0.401354000
H	-0.237966000	3.424558000	2.098495000
C	-2.949288000	3.249089000	1.916249000
H	-3.235988000	3.918067000	1.091700000
H	-3.857907000	2.797538000	2.341324000
H	-2.511424000	3.881396000	2.707780000
C	-1.720405000	1.248519000	2.699253000
H	-2.649559000	0.707713000	2.946973000
H	-0.927346000	0.501191000	2.525464000
H	-1.437931000	1.837624000	3.589103000
C	-3.398765000	3.296247000	-1.530688000
H	-3.535370000	3.684737000	-2.554918000
H	-4.405661000	3.177129000	-1.101833000
H	-2.857824000	4.072110000	-0.965609000
C	-1.241178000	2.271151000	-2.204535000
H	-0.672109000	1.340824000	-2.377723000
H	-1.365251000	2.774472000	-3.179295000
H	-0.625946000	2.924788000	-1.566857000
C	-3.351798000	0.999760000	-2.519444000
H	-2.842244000	0.020265000	-2.562550000
H	-4.394899000	0.831493000	-2.206994000

H	-3.370773000	1.406405000	-3.545250000
C	2.685121000	1.657826000	-0.781243000
C	3.308857000	2.127892000	0.385128000
C	2.178762000	2.604019000	-1.681852000
C	3.384809000	3.493947000	0.647476000
C	2.257585000	3.970327000	-1.422807000
C	2.854183000	4.420006000	-0.248260000
H	3.756656000	1.427041000	1.091895000
H	1.715625000	2.261886000	-2.614855000
H	3.876870000	3.838614000	1.561550000
H	1.855861000	4.685419000	-2.146883000
H	2.920581000	5.491035000	-0.038061000
C	4.955976000	-0.560029000	-0.528090000
C	5.918979000	0.443804000	-0.385253000
C	4.970036000	-1.634259000	0.369433000
C	6.854325000	0.395157000	0.645598000
C	5.902673000	-1.685989000	1.402822000
C	6.842850000	-0.666054000	1.548088000
H	5.928733000	1.282214000	-1.090849000
H	4.244414000	-2.447621000	0.248993000
H	7.601873000	1.187562000	0.740656000
H	5.908864000	-2.538117000	2.089401000
H	7.581083000	-0.710667000	2.353568000