

Supporting information

Computational Study on the NHC-Catalyzed Synthesis of 2,3-Disubstituted Indoles: Mechanism, Key Intermediate and Role of Catalyst

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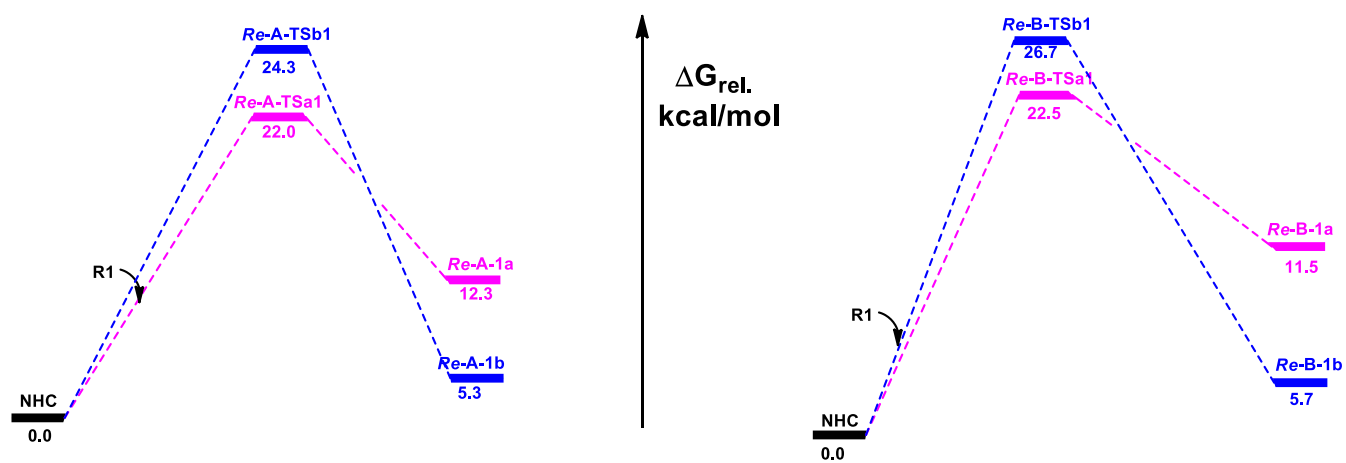


Figure S1. Energy profiles for the *Re* face of path **a** and **b**, the relative energies are given in kcal/mol.

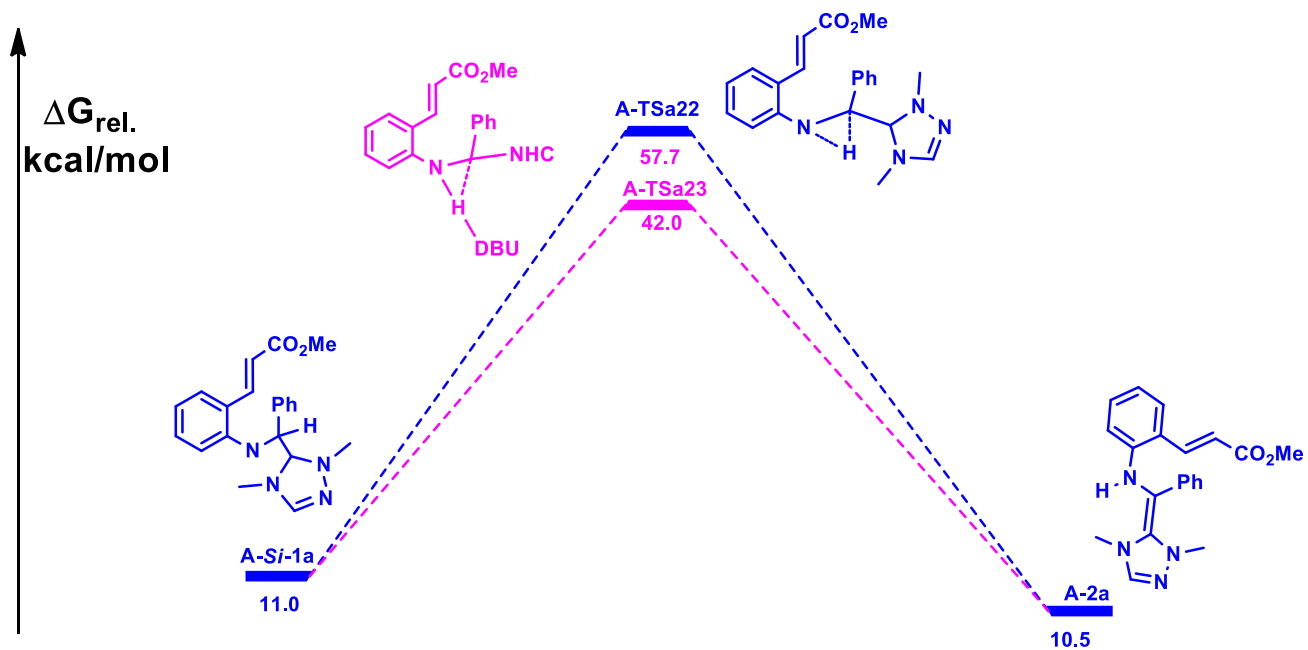


Figure S2 Energy profiles for the first direct [1,2] proton migration and assisted by DBU of path **a** for series **A**; the relative energies are given in kcal/mol.

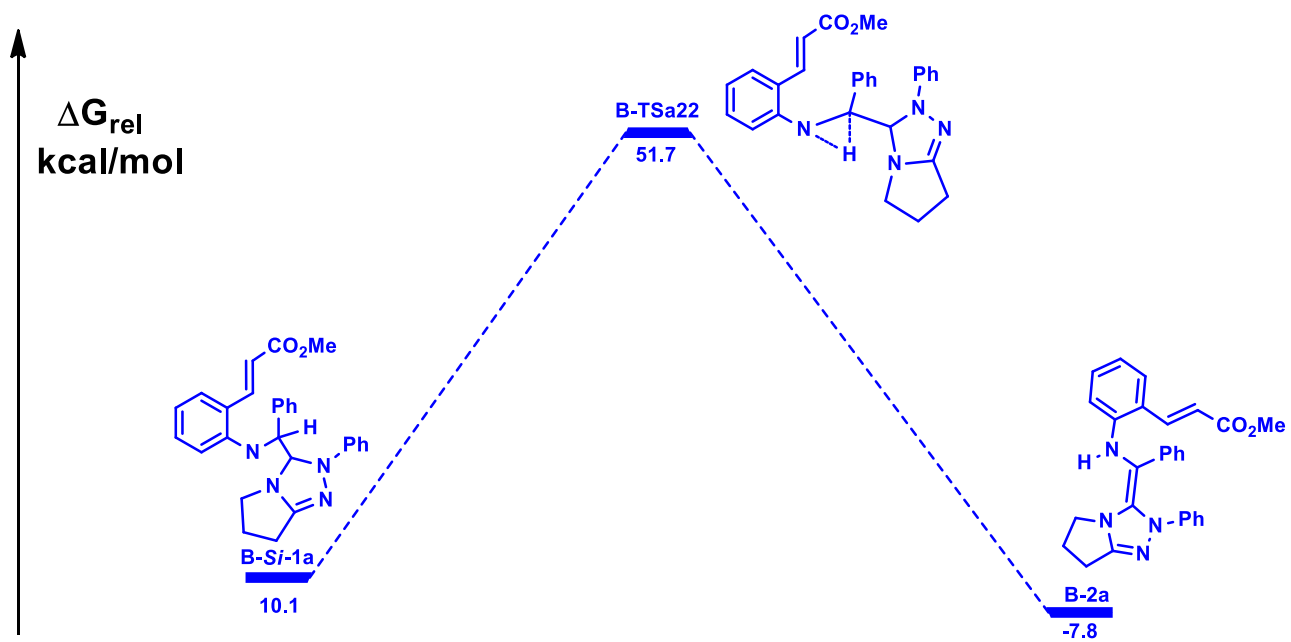


Figure S3. Energy profiles for the first direct [1,2] proton migration of path **a** for series **B**; the relative energies are given in kcal/mol.

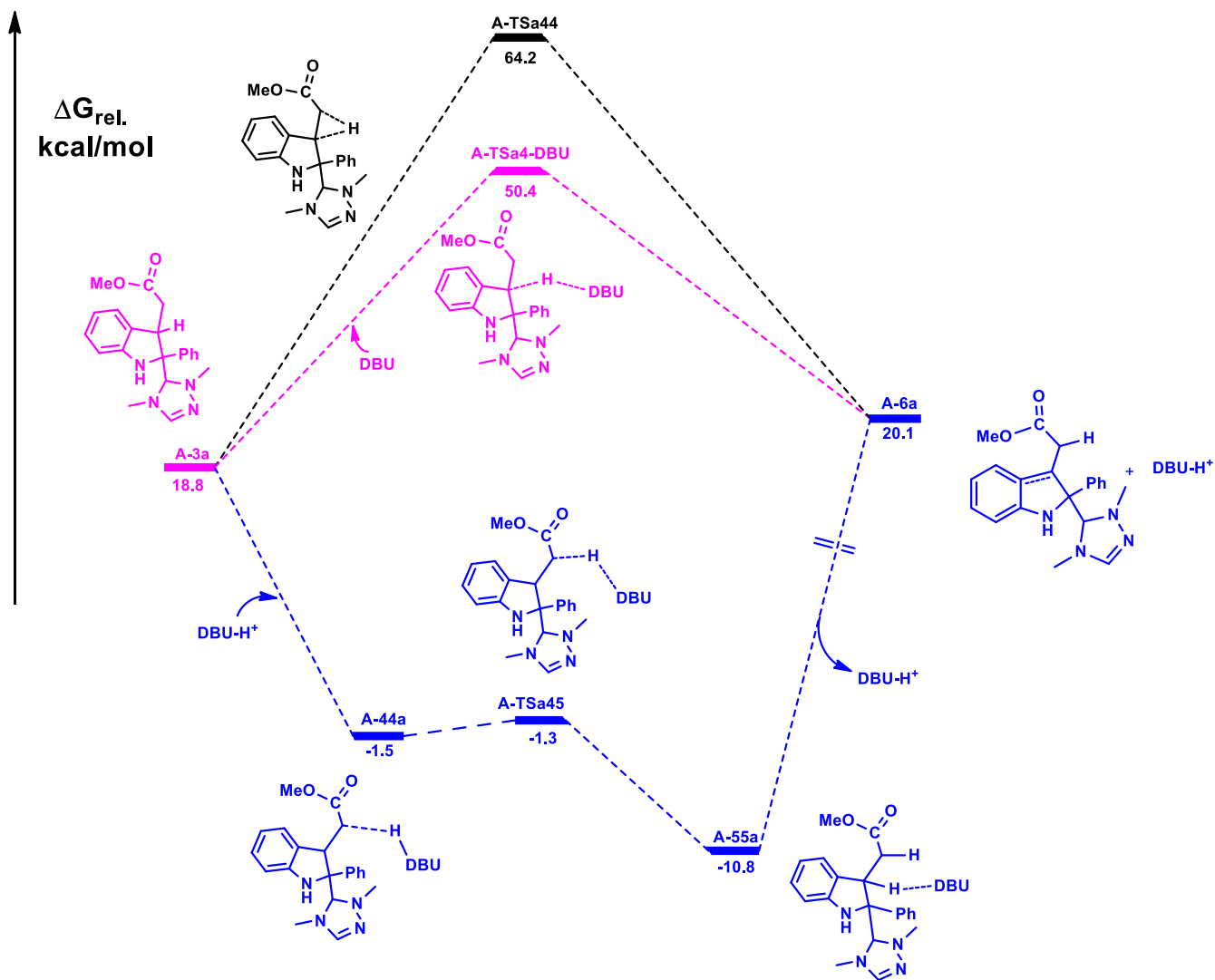


Figure S4 Energy profiles for the second direct [1,2] proton migration and assisted by DBU, DBU-H⁺ of path **a** for series **A**; the relative energies are given in kcal/mol.

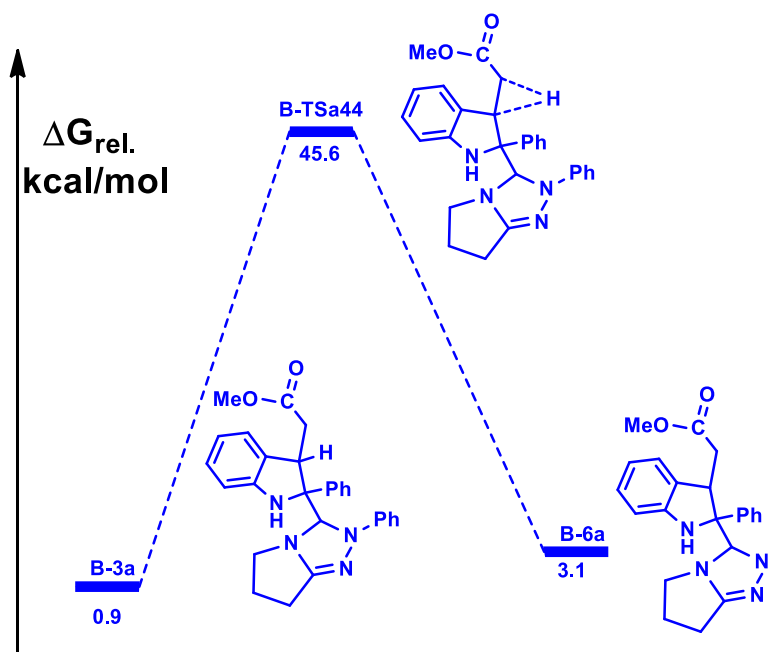


Figure S5. Energy profiles for the second direct [1,2] proton migration of path **a** for series **B**; the relative energies are given in kcal/mol.

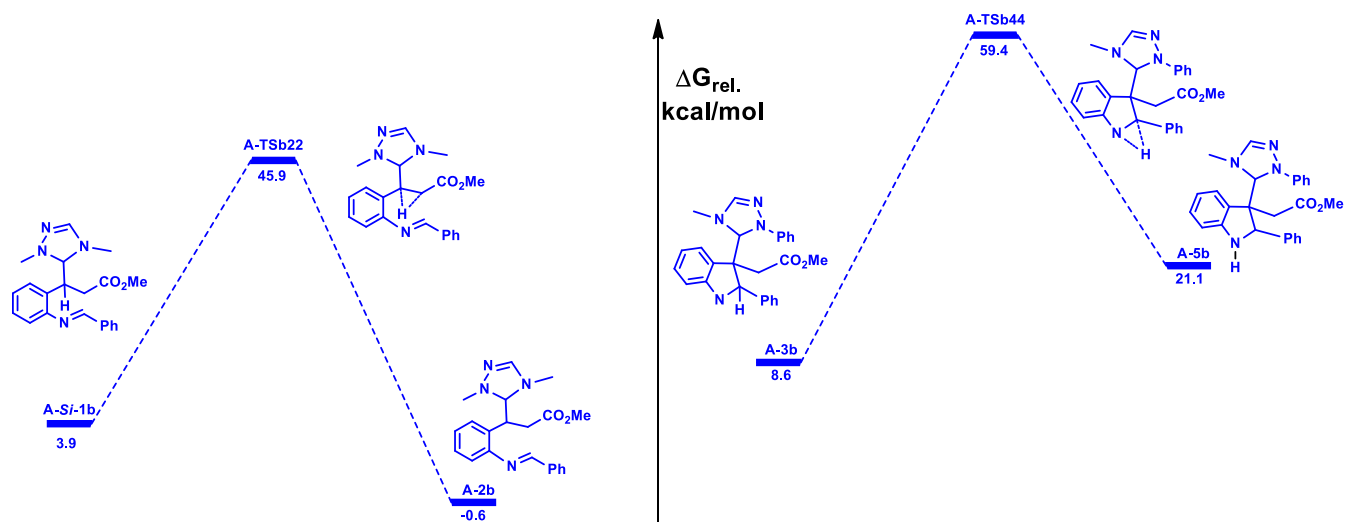


Figure S6. Energy profiles for the first and second direct [1,2] proton migration of path **b** for series **A**; the relative energies are given in kcal/mol.

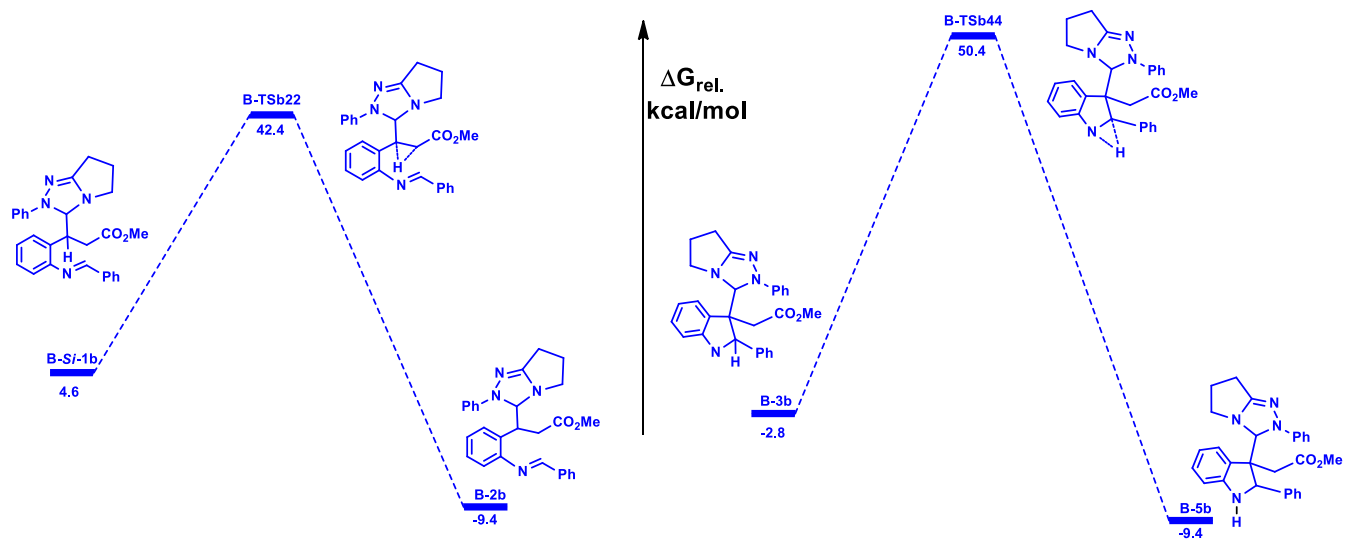


Figure S7. Energy profiles for the first and second direct [1,2] proton migration of path **b** for series **B**; the relative energies are given in kcal/mol.

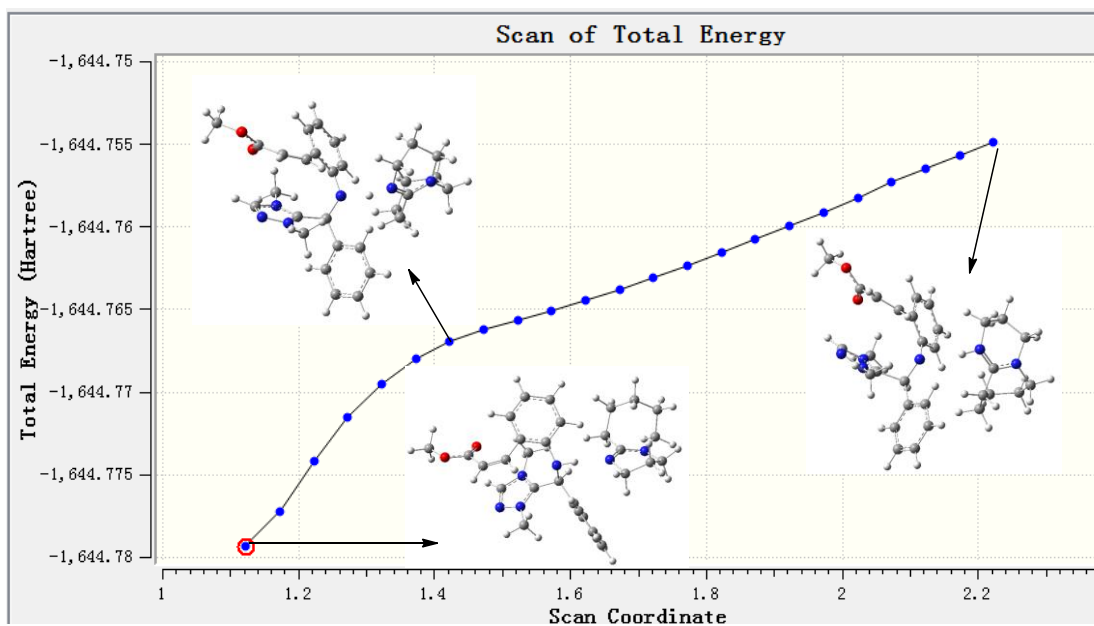


Figure S8. The calculation results of flexible scan to the N–H bond of **A-11a**.

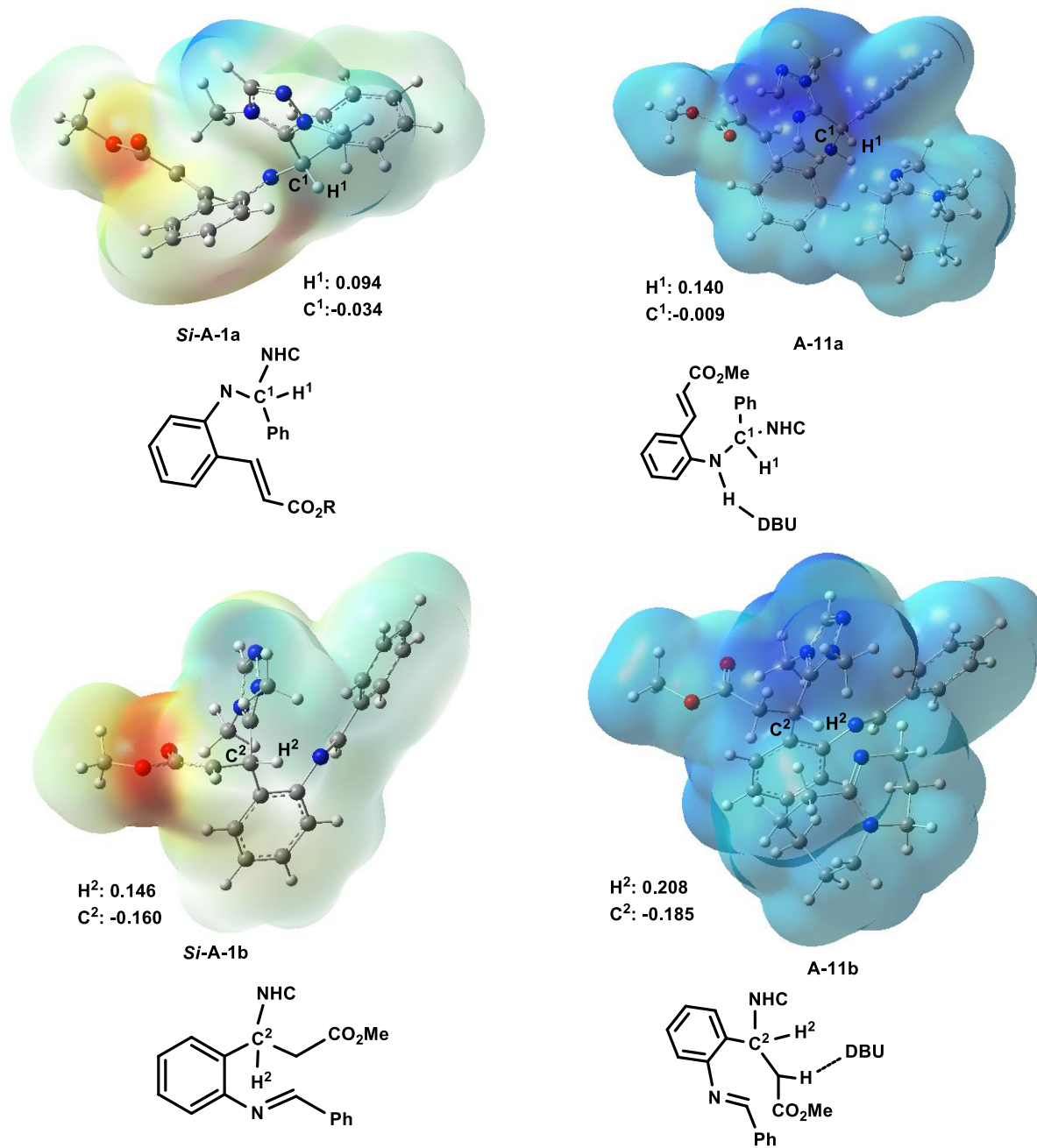


Figure S9 The electrostatic potential analysis and the NPA charge distributions for intermediate **Si-A-1a**, **A-11a**, **Si-A-1b** and **A-11b**.

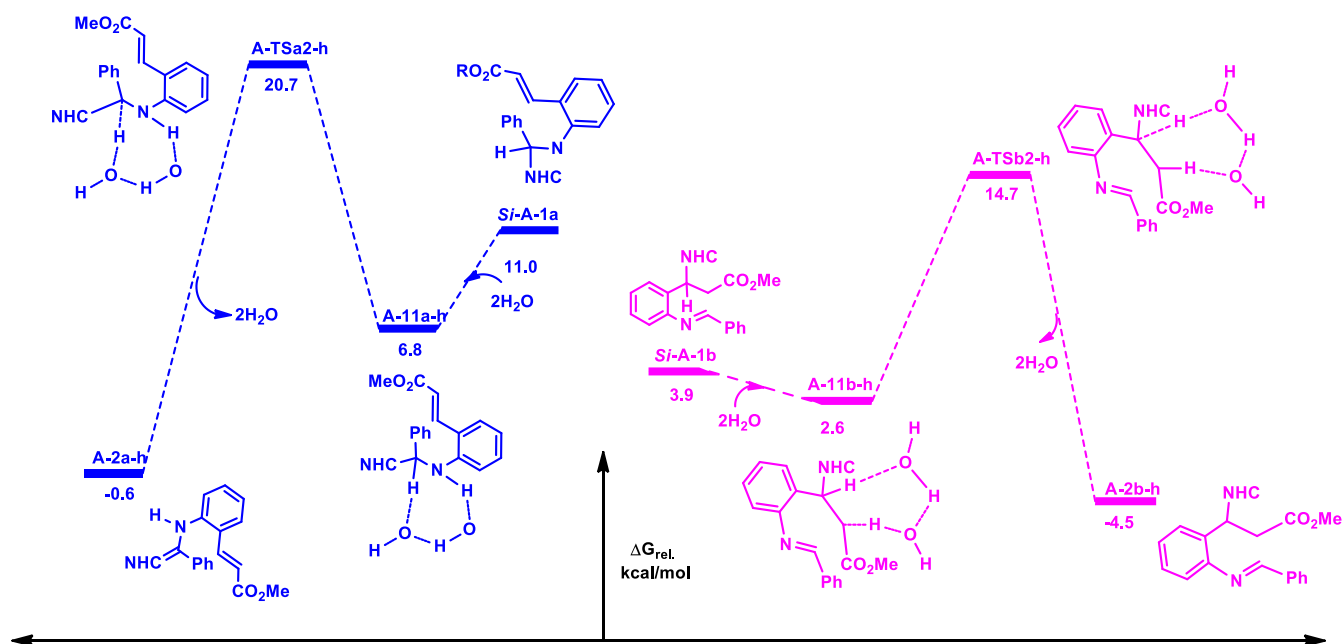


Figure S10 Energy profiles for water assisted [1,2]-H shift for the first step t of path **a** and **b** for series **A**; the relative energies are given in kcal/mol.

Table S1: The energies for species of path a in series A

	E	G
Si-A-TS _{a1}	-1181.975453	-1182.031670
Re-A-TS _{a1}	-1181.972795	-1182.029289
Si-A-1a	-1181.987267	-1182.042849
Re-A-1a	-1181.984410	-1182.040442
A-11a	-1644.109521	-1644.178613
A-TS _{a2}	-1644.087562	-1644.155847
A-2a	-1182.017490	-1182.070367
A-TS _{a3}	-1181.998623	-1182.049603
A-3a	-1181.999703	-1182.051214
A-4a	-1334.758132	-1334.816149
A-TS _{a4}	-1334.751057	-1334.806319
A-5a	-1334.751311	-1334.807516
A-TS _{a5}	-1334.747342	-1334.805181
A-6a	-1181.998402	-1182.049782
A-TS _{a6}	-1181.995945	-1182.047027

Table S2 The energies for species of path b in series A

	E	G
Si-A-TSb1	-1181.973010	-1182.028981
Re-A-TSb1	-1181.969491	-1182.026852
Si-A-1b	-1182.002927	-1182.057623
Re- A-1b	-1182.000265	-1182.056827
A-11b	-1644.132205	-1644.201357
A-TSb2	-1644.120892	-1644.187643
A-2b	-1182.026987	-1182.081648
A-TSb3	-1181.998545	-1182.053108
A-3b	-1182.004937	-1182.056810
A-4b	-1334.773827	-1334.831595
A-TSb4	-1334.744884	-1334.802745
A-5b	-1181.982588	-1182.034293
A-TSb5	-1181.975060	-1182.028398

Cartesian coordinates of the optimized species for series A

Si-A-TSa1

C	-2.817627000	-2.739161000	-1.467361000
C	-1.506029000	-3.191145000	-1.368729000
C	-0.439960000	-2.294925000	-1.341239000
C	-0.662235000	-0.904390000	-1.425272000
C	-2.007841000	-0.457186000	-1.510241000
C	-3.057611000	-1.367645000	-1.531645000
C	-2.241697000	0.994392000	-1.587647000
N	0.295087000	0.073637000	-1.275003000
C	-3.088936000	1.726496000	-0.849341000
C	-3.823529000	1.237112000	0.338767000
C	1.540000000	-0.326725000	-1.062899000
O	-3.561162000	0.273188000	1.024593000
C	2.572045000	0.748634000	-0.910251000
C	3.881674000	0.542971000	-1.343435000
C	4.841735000	1.542506000	-1.195653000
C	4.495527000	2.754217000	-0.606544000
C	3.184369000	2.968499000	-0.179839000
C	2.227332000	1.973687000	-0.333265000
O	-4.847815000	2.067437000	0.628680000
C	-5.593618000	1.713757000	1.788787000
H	-3.644009000	-3.441144000	-1.488975000
H	-1.305207000	-4.257044000	-1.305528000
H	0.568158000	-2.680979000	-1.240434000
H	-4.074999000	-0.992308000	-1.598833000
H	-1.659387000	1.519730000	-2.342619000
H	-3.242443000	2.775946000	-1.077944000
H	1.940775000	-1.228496000	-1.549528000
H	4.146420000	-0.398999000	-1.819118000
H	5.855330000	1.376647000	-1.547159000
H	5.241499000	3.533374000	-0.486686000
H	2.910237000	3.917721000	0.270073000
H	1.195233000	2.126992000	-0.032847000
H	-6.364595000	2.475314000	1.893555000
H	-6.043447000	0.725565000	1.669264000
H	-4.948513000	1.696749000	2.670314000
N	0.713364000	-0.735728000	1.746715000
N	2.547005000	-1.290926000	2.843183000
N	2.692945000	-1.411365000	1.493627000
C	1.605632000	-1.087206000	0.783005000
C	1.320599000	-0.879590000	2.963436000

H	0.827378000	-0.679707000	3.902886000
C	3.978891000	-1.822945000	0.965355000
H	4.362996000	-2.634120000	1.583525000
H	3.831785000	-2.167755000	-0.057430000
H	4.674274000	-0.981047000	0.971876000
C	-0.684038000	-0.327593000	1.563825000
H	-0.733116000	0.520151000	0.880768000
H	-1.265781000	-1.146732000	1.140768000
H	-1.087692000	-0.056728000	2.539345000

Re-A-TS_{a1}

C	2.813474000	-2.726855000	-1.508136000
C	1.501291000	-3.175131000	-1.403424000
C	0.439361000	-2.275054000	-1.356678000
C	0.665531000	-0.884619000	-1.427422000
C	2.011748000	-0.441552000	-1.516416000
C	3.057718000	-1.355594000	-1.557281000
C	2.250208000	1.010215000	-1.579794000
N	-0.289734000	0.095678000	-1.267979000
C	3.099434000	1.732292000	-0.834360000
C	3.834123000	1.226496000	0.347067000
C	-1.533940000	-0.305753000	-1.053133000
O	3.583472000	0.242747000	1.007360000
C	-2.566770000	0.769250000	-0.897585000
C	-3.869614000	0.573911000	-1.355737000
C	-4.830696000	1.572559000	-1.205527000
C	-4.491986000	2.772467000	-0.588246000
C	-3.187665000	2.975949000	-0.135656000
C	-2.229576000	1.982454000	-0.292012000
O	4.844289000	2.066071000	0.662170000
C	5.586399000	1.696272000	1.819621000
H	3.637116000	-3.431481000	-1.544408000
H	1.296875000	-4.240947000	-1.350549000
H	-0.569322000	-2.659186000	-1.252460000
H	4.075848000	-0.982811000	-1.626418000
H	1.667474000	1.545045000	-2.327809000
H	3.252115000	2.784780000	-1.048974000
H	-1.936391000	-1.202886000	-1.547832000
H	-4.127351000	-0.359694000	-1.851873000
H	-5.838265000	1.416063000	-1.578211000
H	-5.238222000	3.551195000	-0.466985000
H	-2.919600000	3.915603000	0.337274000
H	-1.202887000	2.127179000	0.030349000
H	6.351069000	2.461457000	1.942889000
H	4.936446000	1.657903000	2.696944000

H	6.044026000	0.713685000	1.684542000
N	-2.714689000	-1.440304000	1.479751000
N	-1.231127000	-0.911097000	3.007673000
N	-0.737595000	-0.754236000	1.744951000
C	-1.607060000	-1.074914000	0.780299000
C	-2.445560000	-1.325081000	2.815936000
H	-3.151973000	-1.555402000	3.599506000
C	0.655580000	-0.327419000	1.596152000
H	1.268582000	-1.155242000	1.237553000
H	0.708216000	0.484321000	0.870727000
H	0.993074000	-0.005473000	2.578583000
C	-3.981755000	-1.850450000	0.897188000
H	-4.637554000	-0.987887000	0.762024000
H	-3.785994000	-2.309009000	-0.071883000
H	-4.454832000	-2.584702000	1.550857000

Si-A-1a

C	2.617345000	2.687128000	-1.567839000
C	1.287036000	3.089227000	-1.474176000
C	0.254840000	2.164651000	-1.364996000
C	0.511608000	0.762868000	-1.351097000
C	1.887671000	0.372802000	-1.470146000
C	2.898268000	1.321422000	-1.562733000
C	2.165540000	-1.064000000	-1.499254000
N	-0.380498000	-0.223700000	-1.124868000
C	3.095966000	-1.742837000	-0.804517000
C	3.879874000	-1.197716000	0.320943000
C	-1.672253000	0.213603000	-0.759044000
O	3.620576000	-0.234007000	1.011629000
C	-2.638679000	-0.958645000	-0.594646000
C	-3.971187000	-0.859366000	-0.992143000
C	-4.847562000	-1.927647000	-0.807863000
C	-4.393215000	-3.104052000	-0.221594000
C	-3.056676000	-3.215096000	0.159976000
C	-2.183116000	-2.150356000	-0.028456000
O	4.955968000	-1.979579000	0.567775000
C	5.750302000	-1.568600000	1.673763000
H	3.414630000	3.416409000	-1.653851000
H	1.044080000	4.149242000	-1.486136000
H	-0.765790000	2.534768000	-1.307942000
H	3.925628000	0.974848000	-1.642844000
H	1.531769000	-1.638965000	-2.174416000
H	3.276918000	-2.791517000	-1.016175000
H	-2.157584000	0.940563000	-1.448247000
H	-4.320058000	0.046928000	-1.482164000
H	-5.879350000	-1.843425000	-1.134400000

H	-5.073045000	-3.937759000	-0.077854000
H	-2.692933000	-4.140677000	0.595308000
H	-1.128834000	-2.233975000	0.215266000
H	6.557886000	-2.295260000	1.750089000
H	6.151389000	-0.565814000	1.509060000
H	5.157312000	-1.556781000	2.591463000
N	-0.690409000	0.845942000	1.565866000
N	-2.274510000	2.169616000	2.360377000
N	-2.568733000	1.741235000	1.108727000
C	-1.628011000	0.942083000	0.599706000
C	-1.125793000	1.613957000	2.607234000
H	-0.564818000	1.737022000	3.521064000
C	-3.822241000	2.152520000	0.496068000
H	-4.133264000	3.066464000	0.998226000
H	-3.659154000	2.341605000	-0.565217000
H	-4.573988000	1.371858000	0.623020000
C	0.630482000	0.184844000	1.559530000
H	0.576797000	-0.719881000	0.960136000
H	1.370838000	0.847861000	1.109907000
H	0.887076000	-0.027221000	2.597467000

Re- A-1a

C	2.629943000	-2.619773000	-1.663010000
C	1.306041000	-3.035611000	-1.549153000
C	0.269625000	-2.122738000	-1.390277000
C	0.514193000	-0.719512000	-1.346349000
C	1.884376000	-0.315635000	-1.478525000
C	2.899752000	-1.252459000	-1.622230000
C	2.153879000	1.123438000	-1.469957000
N	-0.384594000	0.255093000	-1.085836000
C	3.096263000	1.783516000	-0.773972000
C	3.905519000	1.203588000	0.316209000
C	-1.663430000	-0.214355000	-0.715449000
O	3.668197000	0.211656000	0.972356000
C	-2.660308000	0.930431000	-0.561501000
C	-3.892115000	0.903794000	-1.212607000
C	-4.797601000	1.953332000	-1.061185000
C	-4.473773000	3.036332000	-0.251250000
C	-3.237252000	3.074119000	0.393066000
C	-2.334521000	2.029185000	0.236124000
O	4.979229000	1.986778000	0.573614000
C	5.794284000	1.541349000	1.650792000
H	3.430857000	-3.339619000	-1.786342000
H	1.071339000	-4.097060000	-1.583149000
H	-0.745304000	-2.505530000	-1.315820000
H	3.922388000	-0.894623000	-1.711873000

H	1.502077000	1.715865000	-2.111761000
H	3.266567000	2.840048000	-0.952790000
H	-2.132477000	-0.955513000	-1.402679000
H	-4.133883000	0.066306000	-1.863931000
H	-5.748812000	1.926743000	-1.583450000
H	-5.176533000	3.854377000	-0.130205000
H	-2.974796000	3.926109000	1.012272000
H	-1.354480000	2.064490000	0.703305000
H	6.598695000	2.270080000	1.740377000
H	5.216433000	1.492202000	2.576921000
H	6.198326000	0.547549000	1.443749000
N	-2.579312000	-1.738855000	1.142914000
N	-1.014869000	-1.623707000	2.677270000
N	-0.675717000	-0.885352000	1.590056000
C	-1.606110000	-0.945493000	0.638606000
C	-2.173004000	-2.130566000	2.385335000
H	-2.751255000	-2.774379000	3.030654000
C	0.655169000	-0.252421000	1.595278000
H	1.382521000	-0.940552000	1.161086000
H	0.623774000	0.645718000	0.983246000
H	0.889969000	-0.051085000	2.638236000
C	-3.821329000	-2.107182000	0.474766000
H	-4.368214000	-2.786065000	1.128457000
H	-4.415153000	-1.212215000	0.284167000
H	-3.597606000	-2.610606000	-0.467320000

A-11a

C	1.712326000	-3.603741000	1.239317000
C	0.340954000	-3.348823000	1.211605000
C	-0.123687000	-2.039461000	1.236116000
C	2.608987000	-2.547891000	1.319491000
C	5.025002000	-0.803816000	0.119813000
C	0.164338000	0.979242000	-0.026032000
O	4.481570000	-1.444101000	-0.761613000
C	-0.549883000	2.319840000	0.044644000
C	-0.700552000	3.012252000	1.244762000
C	-1.369290000	4.234712000	1.264360000
C	-1.884935000	4.771765000	0.088381000
C	-1.737106000	4.079043000	-1.113056000
C	-1.075725000	2.856068000	-1.131816000
O	6.346047000	-0.751069000	0.272033000
C	7.113536000	-1.515728000	-0.664588000
H	2.079149000	-4.624210000	1.232879000
H	-0.364909000	-4.173060000	1.184829000
H	-1.188051000	-1.814739000	1.218575000
H	3.671559000	-2.748894000	1.398601000

H	2.700470000	0.671932000	2.233756000
H	4.947111000	0.889009000	1.484173000
H	-0.295204000	2.595531000	2.161708000
H	-1.487320000	4.766224000	2.202898000
H	-2.405201000	5.723514000	0.106430000
H	-2.144366000	4.487319000	-2.031935000
H	-0.979732000	2.306527000	-2.065990000
H	6.809542000	-2.563169000	-0.636987000
H	6.968349000	-1.127107000	-1.674662000
H	8.150264000	-1.403822000	-0.356354000
N	2.050993000	0.210766000	-1.556500000
N	3.441864000	1.911226000	-1.441807000
N	2.361401000	2.121048000	-0.658689000
C	1.503014000	1.105320000	-0.709337000
C	4.345581000	0.063212000	1.117288000
C	3.091800000	-0.096087000	1.567092000
C	2.162512000	-1.218849000	1.345523000
C	0.779490000	-0.973173000	1.291844000
N	0.294509000	0.375166000	1.306643000
N	-4.751792000	-0.459600000	-0.594293000
C	-5.449702000	-1.403343000	-1.461424000
C	-5.661868000	-2.767943000	-0.794580000
C	-4.392854000	-3.260809000	-0.093042000
C	-3.120054000	-3.098941000	-0.931446000
C	-2.691682000	-1.628497000	-1.199595000
C	-3.407969000	-0.589143000	-0.360604000
C	-3.444307000	1.107463000	1.254055000
C	-4.862799000	0.658927000	1.584860000
C	-5.592969000	0.352711000	0.287655000
H	-6.405528000	-0.951081000	-1.740307000
H	-4.888644000	-1.524113000	-2.391567000
H	-6.479502000	-2.709358000	-0.067574000
H	-5.975184000	-3.482599000	-1.564166000
H	-4.263291000	-2.718331000	0.851997000
H	-4.514400000	-4.314497000	0.174775000
H	-3.243612000	-3.621699000	-1.886424000
H	-2.300347000	-3.604414000	-0.410670000
H	-2.827465000	-1.374362000	-2.256072000
H	-1.628815000	-1.511903000	-0.979804000
H	-2.886433000	1.313238000	2.174641000
H	-3.466314000	2.053610000	0.690691000
H	-5.402855000	1.425274000	2.145992000
H	-4.817243000	-0.243130000	2.205043000
H	-5.873881000	1.280382000	-0.227032000
H	-6.515142000	-0.203014000	0.489950000

H	-0.453823000	0.343704000	-0.677297000
C	1.589210000	-1.139725000	-1.893156000
H	1.681341000	-1.274873000	-2.970709000
H	2.217844000	-1.851794000	-1.355161000
H	0.550069000	-1.252617000	-1.591254000
C	2.309631000	3.338410000	0.150034000
H	1.553541000	4.018295000	-0.244146000
H	2.071887000	3.072621000	1.179499000
H	3.301129000	3.781489000	0.084184000
C	3.233495000	0.743643000	-1.976802000
H	3.907400000	0.234063000	-2.647542000
N	-2.716080000	0.103114000	0.484124000
H	-0.676571000	0.339537000	1.627151000

A-TSa2

C	3.572438000	-0.504179000	3.626429000
C	2.272632000	-0.616917000	4.118127000
C	1.196782000	-0.277682000	3.318162000
C	3.753403000	-0.035791000	2.337260000
C	4.319353000	-1.093347000	-0.596963000
C	-0.049109000	0.850835000	-0.064439000
O	3.657404000	-2.027099000	-0.192573000
C	-0.189106000	2.335437000	-0.263903000
C	0.437318000	3.251843000	0.588115000
C	0.246145000	4.620285000	0.416752000
C	-0.582592000	5.094448000	-0.597804000
C	-1.238451000	4.190440000	-1.430057000
C	-1.053723000	2.822411000	-1.253346000
O	5.565636000	-1.219535000	-1.055429000
C	6.102725000	-2.545805000	-1.024748000
H	4.425642000	-0.765463000	4.241024000
H	2.095092000	-0.972035000	5.127982000
H	0.185663000	-0.381457000	3.704904000
H	4.757721000	0.088313000	1.942158000
H	2.672872000	1.899460000	-0.035248000
H	4.201933000	0.862688000	-1.577475000
H	1.067536000	2.886668000	1.395240000
H	0.745396000	5.319009000	1.080263000
H	-0.728906000	6.161237000	-0.728854000
H	-1.905330000	4.550817000	-2.206931000
H	-1.589698000	2.115010000	-1.885292000
H	6.116719000	-2.923664000	-0.000951000
H	5.497350000	-3.212338000	-1.642109000
H	7.111975000	-2.464720000	-1.421591000
N	0.839163000	-1.274984000	-1.027330000
N	1.657342000	-0.617044000	-2.963694000

N	1.118686000	0.437670000	-2.284584000
C	0.628632000	0.070401000	-1.085093000
C	3.849707000	0.315614000	-0.707493000
C	3.029302000	0.890790000	0.180945000
C	2.680951000	0.328272000	1.504921000
C	1.368192000	0.197388000	2.004010000
N	0.197344000	0.411783000	1.278499000
N	-4.770715000	-0.588459000	-0.080003000
C	-5.590287000	-1.676542000	-0.616282000
C	-5.357756000	-2.988053000	0.138501000
C	-3.863754000	-3.274886000	0.323421000
C	-3.040281000	-3.016805000	-0.943284000
C	-2.880544000	-1.520020000	-1.338886000
C	-3.458759000	-0.513939000	-0.367487000
C	-3.209916000	1.441316000	0.987014000
C	-4.317876000	0.863540000	1.857823000
C	-5.382157000	0.254503000	0.956580000
H	-6.634453000	-1.360076000	-0.556866000
H	-5.364858000	-1.800036000	-1.678739000
H	-5.852049000	-2.955317000	1.115299000
H	-5.832267000	-3.795414000	-0.429400000
H	-3.467527000	-2.661502000	1.143205000
H	-3.731693000	-4.315169000	0.632580000
H	-3.487858000	-3.563406000	-1.779926000
H	-2.043556000	-3.443566000	-0.803467000
H	-3.345648000	-1.329827000	-2.312186000
H	-1.824207000	-1.266578000	-1.459169000
H	-2.386203000	1.848136000	1.582012000
H	-3.590336000	2.267871000	0.372670000
H	-4.765799000	1.634378000	2.488165000
H	-3.901198000	0.092194000	2.514679000
H	-5.979011000	1.036397000	0.472827000
H	-6.063838000	-0.374876000	1.537068000
H	-1.390982000	0.501629000	-0.144355000
C	0.556045000	-2.197022000	0.070017000
H	0.612261000	-3.207181000	-0.336525000
H	1.307073000	-2.080151000	0.851985000
H	-0.446247000	-2.006839000	0.456339000
C	1.340519000	1.762782000	-2.855125000
H	0.425174000	2.160147000	-3.293259000
H	1.697149000	2.448423000	-2.087350000
H	2.096702000	1.627799000	-3.625874000
C	1.483428000	-1.629646000	-2.178591000
H	1.814480000	-2.637070000	-2.380248000
N	-2.668035000	0.402468000	0.117430000

H -0.639442000 0.191514000 1.801752000

A-2a

C 2.683748000 3.487556000 -0.556180000
C 1.911625000 4.042011000 0.463454000
C 0.753946000 3.411143000 0.885342000
C 2.252848000 2.311394000 -1.151001000
C 2.508655000 -1.046750000 -0.982964000
C -1.289381000 0.290111000 0.596127000
O 3.159222000 -0.371099000 -0.219781000
C -2.676474000 0.169403000 0.140305000
C -3.533937000 -0.842237000 0.611029000
C -4.855094000 -0.923358000 0.185148000
C -5.372168000 0.021485000 -0.697656000
C -4.548138000 1.055768000 -1.140414000
C -3.225174000 1.133350000 -0.726410000
O 2.789423000 -2.347089000 -1.221078000
C 3.872345000 -2.861346000 -0.448011000
H 3.601969000 3.962929000 -0.881241000
H 2.220333000 4.964496000 0.945885000
H 0.173830000 3.829101000 1.704673000
H 2.831490000 1.861075000 -1.951674000
H -0.326166000 0.605083000 -2.069740000
H 0.904141000 -1.409749000 -2.408589000
H -1.296917000 2.153302000 1.519418000
H -3.156970000 -1.553343000 1.342610000
H -5.492650000 -1.715480000 0.567069000
H -6.405937000 -0.035662000 -1.021658000

H	-4.940807000	1.808182000	-1.818086000
H	-2.591714000	1.947445000	-1.067886000
H	3.644259000	-2.766734000	0.616479000
H	3.974055000	-3.907021000	-0.736183000
H	4.791505000	-2.313267000	-0.666026000
N	-0.596382000	-2.081426000	0.387676000
N	1.253694000	-2.095836000	1.607459000
N	0.658642000	-0.860958000	1.666559000
C	-0.490290000	-0.794108000	0.912400000
C	1.300268000	-0.650793000	-1.741385000
C	0.625866000	0.493030000	-1.548058000
C	1.073249000	1.667019000	-0.763474000
C	0.313466000	2.214533000	0.290639000
N	-0.816253000	1.610225000	0.814632000
C	1.339668000	0.178459000	2.413666000
H	2.049087000	0.710010000	1.772769000
H	0.606204000	0.870851000	2.823440000
H	1.873763000	-0.315350000	3.224963000
C	-1.380041000	-2.470113000	-0.768775000
H	-2.397398000	-2.761070000	-0.499235000
H	-1.437940000	-1.623107000	-1.456950000
H	-0.870184000	-3.301679000	-1.258630000
C	0.485273000	-2.793615000	0.847758000
H	0.657425000	-3.826200000	0.581938000

A-TSa3

C	2.242503000	3.751312000	-0.735614000
C	1.689841000	4.213175000	0.456480000

C	0.702506000	3.478217000	1.113002000
C	1.791391000	2.556070000	-1.296704000
C	2.071005000	-0.931940000	-1.112482000
C	-0.893136000	0.215034000	0.339434000
O	2.516053000	-0.535247000	-0.027698000
C	-2.343535000	0.063400000	-0.016208000
C	-3.139356000	-1.005561000	0.414407000
C	-4.491566000	-1.069049000	0.090088000
C	-5.085184000	-0.051989000	-0.650705000
C	-4.314630000	1.036287000	-1.054990000
C	-2.962620000	1.094292000	-0.740388000
O	2.654851000	-2.005761000	-1.741378000
C	3.770314000	-2.550679000	-1.061125000
H	3.026608000	4.318401000	-1.226146000
H	2.041146000	5.143207000	0.892720000
H	0.288943000	3.816375000	2.059156000
H	2.205535000	2.174243000	-2.225204000
H	0.595599000	-0.979673000	-2.674622000
H	-1.493167000	1.829307000	1.506903000
H	-2.701865000	-1.792035000	1.023722000
H	-5.084980000	-1.911234000	0.432153000
H	-6.140010000	-0.099276000	-0.899949000
H	-4.768925000	1.844699000	-1.619186000
H	-2.373140000	1.954981000	-1.047138000
H	3.477500000	-2.954435000	-0.086918000
H	4.150393000	-3.352016000	-1.696072000
H	4.544441000	-1.795584000	-0.901593000
N	0.630406000	-1.031562000	1.958521000

N	0.684266000	-3.010083000	0.974624000
N	-0.165380000	-2.170579000	0.326448000
C	-0.227282000	-0.958154000	0.900344000
C	0.938304000	-0.440845000	-1.801317000
C	0.793664000	1.828414000	-0.664991000
C	0.267820000	2.287800000	0.538983000
N	-0.654239000	1.401631000	1.134361000
C	0.146112000	0.594559000	-1.239467000
H	-0.681894000	0.866069000	-1.901436000
C	-0.861929000	-2.699169000	-0.838123000
H	-1.650677000	-3.382915000	-0.512113000
H	-1.283516000	-1.876771000	-1.407592000
H	-0.118669000	-3.222768000	-1.438138000
C	1.239528000	0.057138000	2.723928000
H	1.801542000	0.683624000	2.028896000
H	0.480453000	0.632828000	3.243917000
H	1.921054000	-0.405932000	3.438788000
C	1.168858000	-2.281038000	1.930324000
H	1.915385000	-2.612517000	2.635532000

A-3a

C	2.817857000	3.392926000	-0.669686000
C	2.285567000	3.959535000	0.487004000
C	1.157745000	3.407840000	1.098063000
C	2.213396000	2.277187000	-1.253632000
C	1.844989000	-1.214354000	-1.144541000
C	-0.757381000	0.389133000	0.142119000
O	2.302996000	-0.944980000	-0.009548000

C	-2.257941000	0.326303000	-0.145131000
C	-3.121517000	-0.549931000	0.520055000
C	-4.495769000	-0.509678000	0.297880000
C	-5.037258000	0.422808000	-0.579818000
C	-4.192917000	1.324340000	-1.222260000
C	-2.820791000	1.279958000	-1.002970000
O	2.311290000	-2.343080000	-1.803390000
C	3.293932000	-3.067368000	-1.093455000
H	3.710539000	3.819320000	-1.115564000
H	2.762661000	4.826588000	0.933020000
H	0.755847000	3.824045000	2.017509000
H	2.612635000	1.812005000	-2.150225000
H	0.503801000	-0.890195000	-2.788256000
H	-1.353246000	2.080917000	1.208155000
H	-2.727809000	-1.274791000	1.226491000
H	-5.142340000	-1.205410000	0.823085000
H	-6.107659000	0.454679000	-0.753715000
H	-4.602212000	2.068412000	-1.897841000
H	-2.183282000	2.009779000	-1.492204000
H	2.898983000	-3.456947000	-0.148531000
H	3.587388000	-3.896750000	-1.739907000
H	4.164299000	-2.446478000	-0.862898000
N	0.457697000	-0.958549000	1.975088000
N	0.162399000	-3.011771000	1.219089000
N	-0.448282000	-2.107932000	0.417053000
C	-0.271827000	-0.856850000	0.839673000
C	0.842851000	-0.538563000	-1.824067000
C	1.077105000	1.744385000	-0.669669000

C	0.573706000	2.299120000	0.500240000
N	-0.513674000	1.547032000	1.016985000
C	0.193161000	0.623373000	-1.189793000
H	-0.483058000	1.065093000	-1.930147000
C	-1.126741000	-2.626016000	-0.766939000
H	-1.961834000	-3.250419000	-0.440414000
H	-1.468557000	-1.797451000	-1.377478000
H	-0.391800000	-3.204509000	-1.326384000
C	1.258487000	0.074909000	2.641646000
H	1.947392000	0.476676000	1.895534000
H	0.616919000	0.848482000	3.050185000
H	1.816607000	-0.425302000	3.433458000
C	0.722103000	-2.283711000	2.135691000
H	1.330922000	-2.666806000	2.939678000

A-4a

C	-3.577955000	-2.509358000	-1.320713000
C	-2.890970000	-3.709341000	-1.139447000
C	-1.552301000	-3.715876000	-0.743636000
C	-2.936288000	-1.284910000	-1.118545000
C	-2.159780000	1.832766000	-0.062048000
C	0.660248000	-0.822660000	-0.040131000
O	-2.523508000	1.952533000	-1.244295000
C	1.913435000	-0.487818000	-0.847386000
C	3.051462000	-1.283080000	-0.645802000
C	4.241640000	-1.001705000	-1.305412000
C	4.310120000	0.087856000	-2.173771000
C	3.184241000	0.877895000	-2.373339000

C	1.985021000	0.598909000	-1.715797000
O	-2.702247000	2.662671000	0.894833000
C	-3.659066000	3.583442000	0.400409000
H	-4.618920000	-2.527655000	-1.626482000
H	-3.401800000	-4.653418000	-1.300851000
H	-1.017051000	-4.647729000	-0.585927000
H	-3.443625000	-0.337539000	-1.273635000
H	-1.259201000	0.760322000	1.515056000
H	1.092992000	-2.761103000	-0.665039000
H	3.016950000	-2.113863000	0.057066000
H	5.113955000	-1.625075000	-1.136227000
H	5.238121000	0.315396000	-2.688495000
H	3.221689000	1.730279000	-3.043831000
H	1.139690000	1.263237000	-1.890518000
H	-4.495649000	3.068907000	-0.079604000
H	-4.010680000	4.146817000	1.266095000
H	-3.215731000	4.261558000	-0.334747000
N	0.281572000	-1.040216000	2.478180000
N	1.730566000	0.380314000	3.322944000
N	1.812161000	0.361946000	1.969812000
C	0.936635000	-0.490837000	1.429208000
C	-1.168980000	0.971641000	0.451776000
C	-1.601434000	-1.287183000	-0.737061000
C	-0.928151000	-2.488750000	-0.559707000
N	0.400581000	-2.283592000	-0.098750000
C	-0.683547000	-0.104539000	-0.486761000
H	-0.514833000	0.378309000	-1.455482000
C	2.744009000	1.326027000	1.359047000

H	3.227741000	1.810422000	2.204448000
H	3.476994000	0.804888000	0.746814000
H	2.176064000	2.059435000	0.781931000
C	-0.851741000	-1.969746000	2.473698000
H	-1.638444000	-1.575067000	1.828845000
H	-0.529226000	-2.942298000	2.110056000
H	-1.214295000	-2.034367000	3.499237000
C	0.794218000	-0.472380000	3.604127000
H	0.455693000	-0.715405000	4.599603000
O	0.545044000	3.267875000	0.274650000
H	0.068201000	3.930391000	0.786936000
H	-0.014769000	2.436760000	0.380843000
O	-0.118189000	2.791603000	-2.449338000
H	0.137590000	3.213339000	-1.612397000
H	-1.039315000	2.524720000	-2.288053000

A-TSa4

C	-3.287429000	-2.862175000	-1.101091000
C	-2.550657000	-3.939424000	-0.612413000
C	-1.268881000	-3.750408000	-0.096608000
C	-2.755436000	-1.571213000	-1.087654000
C	-2.505832000	1.590848000	-0.269372000
C	0.716292000	-0.623808000	0.125278000
O	-2.777492000	1.578013000	-1.460069000
C	1.944315000	-0.466673000	-0.777158000
C	3.104600000	-1.165116000	-0.406137000
C	4.272394000	-1.059930000	-1.149864000
C	4.298500000	-0.243186000	-2.280006000
C	3.153815000	0.453203000	-2.646874000

C	1.975496000	0.349839000	-1.904788000
O	-3.296306000	2.236223000	0.618934000
C	-4.405289000	2.919457000	0.045329000
H	-4.280889000	-3.027880000	-1.504319000
H	-2.975276000	-4.938167000	-0.632205000
H	-0.688502000	-4.583292000	0.289092000
H	-3.313779000	-0.731419000	-1.486946000
H	-1.526823000	0.795945000	1.409923000
H	1.267979000	-2.635625000	0.051858000
H	3.111327000	-1.773296000	0.497528000
H	5.159312000	-1.606299000	-0.845123000
H	5.208316000	-0.152405000	-2.864871000
H	3.161039000	1.096940000	-3.520286000
H	1.117717000	0.939193000	-2.220471000
H	-5.072490000	2.217922000	-0.461315000
H	-4.920311000	3.403472000	0.874272000
H	-4.067732000	3.661425000	-0.681727000
N	0.410805000	-0.335905000	2.638762000
N	1.893639000	1.201009000	3.153707000
N	1.923887000	0.940136000	1.824419000
C	1.023846000	0.016257000	1.481678000
C	-1.308793000	1.029569000	0.366589000
C	-1.477336000	-1.373440000	-0.576910000
C	-0.752320000	-2.460599000	-0.100498000
N	0.506958000	-2.069999000	0.409741000
C	-0.671047000	-0.097145000	-0.450734000
H	-0.501367000	0.331312000	-1.442793000
C	2.839247000	1.754311000	1.004188000

H	3.276810000	2.460783000	1.706591000
H	3.609347000	1.118172000	0.570107000
H	2.210946000	2.264888000	0.252666000
C	-0.654539000	-1.315943000	2.863116000
H	-1.403839000	-1.240445000	2.076213000
H	-0.236760000	-2.320745000	2.865803000
H	-1.111693000	-1.076799000	3.823608000
C	0.968555000	0.419888000	3.622050000
H	0.669600000	0.364043000	4.657579000
O	0.520482000	2.761337000	-0.301585000
H	0.373282000	3.668479000	-0.008602000
H	-0.468541000	1.964230000	0.223666000
O	-0.262948000	2.333342000	-2.798569000
H	0.025965000	2.633977000	-1.893597000
H	-1.197559000	2.121705000	-2.681478000

A-5a

C	2.833925000	3.464006000	-0.764008000
C	1.924588000	4.380557000	-0.237971000
C	0.695448000	3.960372000	0.270233000
C	2.528969000	2.101766000	-0.799085000
C	2.589729000	-1.383860000	-0.119142000
C	-0.748510000	0.554514000	0.263112000
O	3.050156000	-1.004103000	-1.173737000
C	-1.838945000	0.367241000	-0.799276000
C	-3.143352000	0.727566000	-0.424304000
C	-4.204207000	0.600121000	-1.310354000
C	-3.971444000	0.107600000	-2.594375000

C	-2.681702000	-0.248636000	-2.967174000
C	-1.608833000	-0.124480000	-2.080928000
O	3.003301000	-2.499060000	0.495091000
C	3.826229000	-3.333845000	-0.315786000
H	3.783902000	3.813170000	-1.154520000
H	2.173095000	5.437064000	-0.220882000
H	-0.014019000	4.670626000	0.683813000
H	3.218504000	1.372789000	-1.212037000
H	2.135642000	-0.045062000	1.470173000
H	-1.614649000	2.442134000	0.416085000
H	-3.339792000	1.085830000	0.586572000
H	-5.206642000	0.876299000	-0.999205000
H	-4.794556000	-0.001223000	-3.293452000
H	-2.488009000	-0.644103000	-3.959022000
H	-0.630271000	-0.460736000	-2.422263000
H	4.735492000	-2.809225000	-0.616172000
H	4.066102000	-4.204130000	0.293175000
H	3.271940000	-3.627253000	-1.211259000
N	-0.752282000	0.006607000	2.752251000
N	-1.799696000	-1.927476000	2.802627000
N	-1.724275000	-1.463314000	1.532287000
C	-1.092411000	-0.292799000	1.474639000
C	1.585793000	-0.625747000	0.716455000
C	1.302484000	1.678027000	-0.304597000
C	0.404696000	2.602289000	0.221433000
N	-0.764389000	1.974322000	0.712252000
C	0.740223000	0.280218000	-0.201870000
H	0.724403000	-0.221355000	-1.169568000

C	-2.198231000	-2.330144000	0.438959000
H	-2.494897000	-3.253996000	0.932311000
H	-3.055375000	-1.862598000	-0.044958000
H	-1.312974000	-2.478902000	-0.244300000
C	0.007016000	1.148590000	3.269830000
H	0.847132000	1.367000000	2.612482000
H	-0.630659000	2.027801000	3.327600000
H	0.374140000	0.864525000	4.256619000
C	-1.202224000	-1.024469000	3.520343000
H	-1.071907000	-1.069519000	4.590771000
O	0.335618000	-2.492677000	-0.762471000
H	0.547400000	-3.431373000	-0.696158000
H	0.989377000	-1.400811000	1.193779000
O	0.877757000	-1.610024000	-3.074921000
H	0.655689000	-2.069455000	-2.181043000
H	1.785327000	-1.314882000	-2.942962000

A-TSa5

C	-3.158808000	2.957956000	0.484460000
C	-3.083570000	3.128589000	-0.895703000
C	-2.164865000	2.397764000	-1.654844000
C	-2.313474000	2.057194000	1.137257000
C	-2.128681000	-1.511598000	0.481973000
C	0.477063000	0.157041000	-0.450767000
O	-1.911346000	-2.269104000	-0.446551000
C	1.752966000	1.021427000	-0.405067000
C	2.818982000	0.749439000	-1.268671000
C	3.936335000	1.579234000	-1.310637000

C	3.994510000	2.703967000	-0.493732000
C	2.930799000	2.990010000	0.357957000
C	1.816671000	2.156519000	0.407718000
O	-3.347935000	-1.013763000	0.725146000
C	-4.343414000	-1.330006000	-0.242829000
H	-3.875358000	3.535951000	1.059242000
H	-3.740813000	3.836788000	-1.390201000
H	-2.106195000	2.521374000	-2.732432000
H	-2.360589000	1.928640000	2.214930000
H	-0.369553000	-1.731251000	1.685212000
H	0.192101000	1.118877000	-2.275974000
H	2.787106000	-0.126205000	-1.916189000
H	4.759096000	1.344343000	-1.978435000
H	4.863963000	3.352664000	-0.519846000
H	2.966966000	3.868154000	0.994868000
H	0.998519000	2.380935000	1.082958000
H	-4.074149000	-0.899005000	-1.211061000
H	-4.448972000	-2.411633000	-0.349845000
H	-5.267363000	-0.885381000	0.122493000
N	0.567586000	-2.091451000	-1.732563000
N	1.883970000	-3.233890000	-0.379567000
N	1.687433000	-1.978553000	0.082064000
C	0.881673000	-1.271854000	-0.707112000
C	-1.091475000	-0.955358000	1.414670000
C	-1.390571000	1.327920000	0.396625000
C	-1.335147000	1.509472000	-0.988789000
N	-0.366935000	0.646652000	-1.569792000
C	-0.400443000	0.304645000	0.842733000

H	0.303311000	0.633109000	1.955378000
C	2.389806000	-1.549194000	1.291934000
H	3.432620000	-1.361172000	1.029119000
H	1.919991000	-0.650071000	1.694838000
H	2.289729000	-2.336736000	2.036874000
C	-0.331134000	-1.881454000	-2.871105000
H	-1.301871000	-1.566741000	-2.501655000
H	0.086869000	-1.134488000	-3.543603000
H	-0.409235000	-2.840455000	-3.384415000
C	1.185916000	-3.279845000	-1.473401000
H	1.093272000	-4.144030000	-2.112736000
O	0.946534000	-1.816028000	3.791064000
H	0.342661000	-1.947440000	4.527025000
H	-1.570621000	-0.645289000	2.347300000
O	0.799809000	0.696875000	3.094892000
H	0.928454000	-0.827283000	3.618264000
H	1.600347000	1.232009000	3.114463000

A-6a

C	4.540887000	0.112958000	-1.026467000
C	4.765711000	0.963312000	0.047650000
C	3.670527000	1.430452000	0.803837000
C	3.250119000	-0.286486000	-1.394602000
C	-0.375526000	-2.180802000	-1.264860000
C	0.066703000	0.777666000	0.302911000
O	0.257322000	-2.838388000	-0.470212000
C	-0.942142000	1.885624000	-0.020015000
C	-1.754558000	2.412538000	0.986951000

C	-2.619699000	3.468701000	0.715691000
C	-2.680986000	4.001161000	-0.570646000
C	-1.864316000	3.485091000	-1.574379000
C	-0.989755000	2.437047000	-1.297753000
O	-1.546003000	-2.603387000	-1.783619000
C	-1.966936000	-3.900772000	-1.358028000
H	5.387332000	-0.259860000	-1.596900000
H	5.773963000	1.255690000	0.318774000
H	3.821043000	2.076945000	1.664914000
H	3.108512000	-0.961474000	-2.234034000
H	-0.881769000	-0.348537000	-2.228170000
H	1.037807000	2.306406000	1.335774000
H	-1.709280000	1.985089000	1.988351000
H	-3.245001000	3.876016000	1.504237000
H	-3.359165000	4.820350000	-0.787526000
H	-1.906319000	3.903931000	-2.575043000
H	-0.321342000	2.032601000	-2.053526000
H	-2.203168000	-3.886573000	-0.290881000
H	-2.854884000	-4.134316000	-1.944021000
H	-1.181079000	-4.636156000	-1.541008000
N	-0.011058000	-1.238991000	1.925541000
N	-2.029314000	-2.054206000	1.547616000
N	-1.846131000	-0.873745000	0.884053000
C	-0.623878000	-0.347303000	1.101444000
C	0.022328000	-0.805490000	-1.797346000
C	2.146166000	0.199715000	-0.679669000
C	2.406820000	1.046773000	0.429572000
N	1.178455000	1.332613000	1.095178000

C	0.739861000	0.058931000	-0.826882000
C	-2.955393000	-0.385867000	0.074403000
H	-3.535168000	0.359288000	0.621909000
H	-2.577393000	0.054857000	-0.846556000
H	-3.565251000	-1.257682000	-0.155698000
C	1.423820000	-1.367439000	2.181298000
H	1.906205000	-1.614338000	1.232006000
H	1.822838000	-0.436937000	2.573761000
H	1.553323000	-2.180075000	2.896379000
C	-0.897868000	-2.249056000	2.147531000
H	-0.661183000	-3.113574000	2.748611000
H	0.684453000	-1.007666000	-2.651261000

A-TSa6

C	-4.336696000	-1.225506000	-0.996028000
C	-4.317844000	-2.183053000	0.014344000
C	-3.122270000	-2.458930000	0.699493000
C	-3.182576000	-0.529183000	-1.366712000
C	-0.326685000	2.117501000	-1.262282000
C	0.173276000	-0.920986000	0.182705000
O	-1.211790000	2.489242000	-0.527239000
C	1.531721000	-1.544961000	-0.077378000
C	2.398922000	-1.819686000	0.982243000
C	3.610239000	-2.467033000	0.756049000
C	3.970791000	-2.833667000	-0.538973000
C	3.105262000	-2.570294000	-1.598276000
C	1.883486000	-1.943424000	-1.366537000
O	0.640570000	2.938908000	-1.714611000

C	0.517364000	4.304286000	-1.311815000
H	-5.271133000	-1.007391000	-1.504970000
H	-5.226730000	-2.708490000	0.286521000
H	-3.093917000	-3.185026000	1.507665000
H	-3.225979000	0.229693000	-2.142820000
H	0.868866000	0.583160000	-2.138070000
H	-0.307615000	-2.704858000	1.175879000
H	2.117829000	-1.507247000	1.986585000
H	4.273888000	-2.682708000	1.587800000
H	4.919548000	-3.328780000	-0.719852000
H	3.378370000	-2.861913000	-2.607565000
H	1.178642000	-1.764910000	-2.173468000
H	0.641000000	4.386682000	-0.230227000
H	1.310961000	4.840068000	-1.830933000
H	-0.460934000	4.697398000	-1.596424000
N	-0.414248000	1.115563000	1.958597000
N	1.135933000	2.624410000	1.534724000
N	1.453368000	1.406410000	0.994486000
C	0.533886000	0.449972000	1.240797000
C	-0.172350000	0.705544000	-1.812988000
C	-1.972807000	-0.818223000	-0.723769000
C	-1.985196000	-1.781381000	0.317473000
N	-0.699306000	-1.818468000	0.890671000
C	-0.629593000	-0.363926000	-0.887222000
C	2.713222000	1.301341000	0.273847000
H	3.427859000	0.696129000	0.833732000
H	2.550670000	0.848614000	-0.704882000
H	3.081578000	2.318245000	0.153790000

C	-1.761514000	0.657621000	2.285558000
H	-2.383651000	0.742110000	1.391610000
H	-1.729231000	-0.377786000	2.614767000
H	-2.149312000	1.298256000	3.078650000
C	-0.011984000	2.410878000	2.096166000
H	-0.595137000	3.161103000	2.608327000
H	-0.777985000	0.685713000	-2.730822000

3) Cartesian coordinates of the optimized species in pathway A- b

Si-A-TSb1

C	1.901138000	-3.628202000	0.022878000
C	0.637769000	-4.125895000	0.324295000
C	-0.485705000	-3.330459000	0.119957000
C	-0.346008000	-2.029523000	-0.370359000
C	0.936013000	-1.507045000	-0.645821000
C	2.044230000	-2.331207000	-0.465511000
C	1.025265000	-0.106175000	-1.150954000
N	-1.468888000	-1.234620000	-0.658607000
C	2.164015000	0.594894000	-1.531467000
C	3.400981000	0.620184000	-0.801237000
C	-2.393114000	-1.108531000	0.205395000
O	3.657358000	0.070726000	0.266082000
C	-3.605932000	-0.318006000	-0.064563000
C	-3.802246000	0.286186000	-1.312619000
C	-4.942978000	1.039741000	-1.548112000
C	-5.900215000	1.196051000	-0.543709000

C	-5.712240000	0.595115000	0.697395000
C	-4.567457000	-0.159682000	0.935635000
O	4.330064000	1.404219000	-1.414731000
C	5.562270000	1.517235000	-0.721390000
H	2.779598000	-4.250073000	0.160761000
H	0.520724000	-5.138336000	0.697667000
H	-1.483369000	-3.723156000	0.293369000
H	3.029532000	-1.938497000	-0.681428000
H	2.063141000	1.351967000	-2.300268000
H	0.140911000	0.131277000	-1.742311000
H	-2.318953000	-1.568470000	1.202921000
H	-3.048521000	0.143598000	-2.080491000
H	-5.093713000	1.504859000	-2.517106000
H	-6.792611000	1.784272000	-0.732494000
H	-6.455719000	0.714968000	1.478539000
H	-4.414481000	-0.629158000	1.904201000
H	6.196077000	2.155441000	-1.336619000
H	5.416686000	1.965280000	0.265246000
H	6.026405000	0.536967000	-0.586488000
N	1.038036000	0.732927000	1.735881000
N	0.695761000	2.898469000	1.508748000
N	0.178518000	2.176880000	0.471776000
C	0.387519000	0.854972000	0.546684000
C	1.212760000	1.981665000	2.269567000
H	1.706613000	2.169044000	3.211147000
C	-0.399400000	2.864506000	-0.661992000
H	-1.206073000	2.251249000	-1.065400000
H	-0.789897000	3.821493000	-0.319369000

H	0.365742000	3.025780000	-1.427628000
C	1.483379000	-0.517046000	2.343197000
H	1.585845000	-0.358956000	3.418300000
H	0.733038000	-1.287217000	2.157740000
H	2.435406000	-0.810160000	1.900710000

Re-A-TSb1

C	2.227397000	3.559823000	-0.035271000
C	1.155657000	4.120093000	0.655466000
C	-0.026817000	3.405449000	0.792433000
C	-0.148041000	2.130507000	0.234515000
C	0.939765000	1.536584000	-0.437563000
C	2.112263000	2.285679000	-0.575873000
C	0.805527000	0.188282000	-1.066618000
N	-1.348746000	1.418523000	0.439010000
C	1.821856000	-0.570258000	-1.617461000
C	3.130724000	-0.713824000	-1.026521000
C	-2.176083000	1.337940000	-0.520811000
O	3.534156000	-0.226229000	0.019991000
C	-3.402826000	0.525883000	-0.428676000
C	-3.615070000	-0.328713000	0.659990000
C	-4.761708000	-1.111110000	0.711413000
C	-5.703036000	-1.045599000	-0.317333000
C	-5.493653000	-0.199634000	-1.402523000
C	-4.342279000	0.579676000	-1.459868000
O	3.922995000	-1.540740000	-1.762753000
C	5.207631000	-1.776546000	-1.206123000
H	3.152566000	4.113425000	-0.154790000

H	1.237529000	5.114183000	1.083600000
H	-0.876169000	3.819883000	1.325964000
H	2.946009000	1.848177000	-1.109934000
H	1.580144000	-1.279360000	-2.400804000
H	-0.160519000	0.051911000	-1.552002000
H	-1.998384000	1.844324000	-1.481845000
H	-2.863954000	-0.363745000	1.443928000
H	-4.926647000	-1.775255000	1.553961000
H	-6.598334000	-1.657592000	-0.272747000
H	-6.224027000	-0.148700000	-2.203391000
H	-4.168456000	1.238758000	-2.306800000
H	5.714195000	-2.453164000	-1.894079000
H	5.767661000	-0.842870000	-1.109319000
H	5.125543000	-2.229914000	-0.214927000
N	-0.074044000	-2.217671000	0.485862000
N	1.145645000	-2.179305000	2.312689000
N	0.964557000	-0.931183000	1.782321000
C	0.235901000	-0.902029000	0.660304000
C	0.502088000	-2.948727000	1.489800000
H	0.411807000	-4.020285000	1.588338000
C	1.566063000	0.215884000	2.449930000
H	0.809272000	0.990981000	2.576861000
H	1.921479000	-0.130856000	3.418860000
H	2.394301000	0.585163000	1.844113000
C	-0.818153000	-2.727784000	-0.648900000
H	-0.203461000	-2.660909000	-1.550777000
H	-1.083394000	-3.769842000	-0.466167000
H	-1.729484000	-2.140559000	-0.776984000

Si-A-1b

C	-2.257213000	3.573581000	-0.148543000
C	-1.007068000	4.183856000	-0.088668000
C	0.144825000	3.429535000	-0.284041000
C	0.044334000	2.058812000	-0.543239000
C	-1.218717000	1.449473000	-0.647906000
C	-2.358794000	2.213278000	-0.433375000
C	-1.314184000	-0.029680000	-1.029980000
N	1.170687000	1.221700000	-0.703047000
C	-2.661356000	-0.652311000	-1.218964000
C	-3.434860000	-0.894979000	-0.090057000
C	2.191398000	1.403059000	0.038256000
O	-3.111021000	-0.676883000	1.098506000
C	3.370042000	0.525693000	-0.019310000
C	3.377053000	-0.620708000	-0.823307000
C	4.484657000	-1.455979000	-0.832072000
C	5.596891000	-1.153911000	-0.044077000
C	5.596153000	-0.015640000	0.757125000
C	4.483060000	0.818757000	0.772288000
O	-4.673509000	-1.436844000	-0.362206000
C	-5.474545000	-1.666220000	0.778355000
H	-3.156061000	4.159827000	0.012978000
H	-0.926426000	5.249172000	0.102939000
H	1.122661000	3.902481000	-0.271665000
H	-3.321006000	1.716470000	-0.509469000
H	-3.044564000	-0.818283000	-2.214911000
H	-0.760252000	-0.110419000	-1.976415000

H	2.223780000	2.206695000	0.790371000
H	2.500821000	-0.835847000	-1.427301000
H	4.485571000	-2.347266000	-1.450942000
H	6.462245000	-1.808701000	-0.054048000
H	6.459656000	0.220757000	1.370059000
H	4.474228000	1.706561000	1.399611000
H	-6.410808000	-2.089872000	0.410449000
H	-4.995768000	-2.363612000	1.472446000
H	-5.673924000	-0.737833000	1.322489000
N	-0.203094000	-0.767882000	1.205299000
N	0.661138000	-2.692197000	0.546092000
N	0.017061000	-2.065682000	-0.467928000
C	-0.521255000	-0.901116000	-0.098634000
C	0.514751000	-1.879584000	1.548560000
H	0.896504000	-2.051129000	2.542954000
C	-0.134527000	-2.695411000	-1.765511000
H	0.439048000	-2.150392000	-2.519479000
H	0.238757000	-3.712898000	-1.672378000
H	-1.199154000	-2.676251000	-2.018983000
C	-0.588847000	0.302701000	2.122876000
H	-0.420532000	-0.065936000	3.135090000
H	0.020625000	1.190387000	1.941697000
H	-1.650490000	0.495096000	1.962540000

Re- A-1b

C	2.678816000	3.347539000	-0.256483000
C	1.640685000	4.120295000	0.255736000
C	0.377052000	3.563698000	0.437713000

C	0.159178000	2.232302000	0.091700000
C	1.199260000	1.444445000	-0.430295000
C	2.454788000	2.015348000	-0.597352000
C	0.914976000	-0.003512000	-0.838144000
N	-1.079732000	1.596201000	0.360352000
C	1.993974000	-0.840095000	-1.447631000
C	3.063594000	-1.235358000	-0.648281000
C	-1.949620000	1.517636000	-0.561541000
O	3.229547000	-0.976904000	0.560536000
C	-3.160019000	0.687344000	-0.406627000
C	-3.361983000	-0.061186000	0.759802000
C	-4.462892000	-0.900093000	0.862129000
C	-5.368902000	-1.001037000	-0.196186000
C	-5.172034000	-0.259372000	-1.357109000
C	-4.067975000	0.582767000	-1.462234000
O	4.004538000	-1.994733000	-1.313789000
C	5.107650000	-2.381488000	-0.520168000
H	3.665164000	3.780314000	-0.386842000
H	1.811873000	5.158802000	0.521193000
H	-0.440992000	4.144916000	0.851479000
H	3.243049000	1.386846000	-0.999722000
H	1.967567000	-1.064206000	-2.504037000
H	0.097376000	0.049727000	-1.571350000
H	-1.810103000	2.009167000	-1.536090000
H	-2.639256000	0.027882000	1.566335000
H	-4.621649000	-1.475841000	1.768730000
H	-6.228354000	-1.658718000	-0.113422000
H	-5.875660000	-0.337135000	-2.179326000

H	-3.904273000	1.160416000	-2.368692000
H	5.754830000	-2.974596000	-1.168843000
H	5.654286000	-1.511809000	-0.142303000
H	4.793739000	-2.977371000	0.341986000
N	-0.553577000	-1.817010000	0.097577000
N	-0.225792000	-1.689425000	2.265839000
N	0.491089000	-0.738388000	1.610279000
C	0.313698000	-0.795158000	0.292522000
C	-0.844173000	-2.334371000	1.324176000
H	-1.507864000	-3.171665000	1.476069000
C	1.285408000	0.208291000	2.386108000
H	0.733360000	1.145450000	2.481862000
H	1.430732000	-0.252033000	3.361536000
H	2.238059000	0.335180000	1.873206000
C	-1.015584000	-2.284139000	-1.197832000
H	-0.137602000	-2.400121000	-1.840116000
H	-1.517434000	-3.241250000	-1.059072000
H	-1.718822000	-1.563650000	-1.624923000

A-11b

C	-2.351728000	-0.530114000	2.961634000
C	-1.441911000	0.352617000	3.534049000
C	-0.258272000	0.656113000	2.870478000
C	0.025776000	0.080852000	1.627356000
C	-0.924880000	-0.761668000	1.014117000
C	-2.095145000	-1.074033000	1.704182000
C	-0.687719000	-1.186306000	-0.424610000
N	1.230351000	0.291360000	0.923712000

C	-1.838447000	-1.966820000	-1.073923000
C	-2.036232000	-3.354492000	-0.505311000
C	2.311045000	0.507168000	1.573260000
O	-1.142984000	-4.036296000	-0.054130000
C	3.611924000	0.674087000	0.918784000
C	3.775010000	0.420214000	-0.449119000
C	5.022698000	0.554531000	-1.039633000
C	6.118996000	0.949573000	-0.270243000
C	5.966467000	1.199342000	1.091054000
C	4.717522000	1.054407000	1.686113000
O	-3.303781000	-3.742725000	-0.582736000
C	-3.570968000	-5.079125000	-0.128080000
H	-3.272158000	-0.778844000	3.478539000
H	-1.653232000	0.809721000	4.494829000
H	0.439190000	1.364976000	3.305724000
H	-2.836987000	-1.732197000	1.260166000
H	-2.767886000	-1.399218000	-0.991642000
H	-0.613924000	-0.225712000	-0.973616000
H	2.324818000	0.546105000	2.672229000
H	2.913420000	0.106074000	-1.029417000
H	5.147687000	0.348775000	-2.097514000
H	7.094277000	1.057320000	-0.733295000
H	6.819819000	1.501641000	1.688210000
H	4.594666000	1.242139000	2.749703000
H	-4.636427000	-5.232957000	-0.280250000
H	-2.987258000	-5.794462000	-0.709205000
H	-3.310128000	-5.173179000	0.927267000
N	1.412159000	-2.604272000	0.119070000

N	2.452143000	-2.449415000	-1.820130000
N	1.281216000	-1.769853000	-1.838745000
C	0.631725000	-1.849658000	-0.678228000
C	2.512668000	-2.939326000	-0.618373000
H	3.323123000	-3.541230000	-0.235610000
C	0.888426000	-1.052728000	-3.050921000
H	0.247933000	-0.205031000	-2.785919000
H	1.806369000	-0.695796000	-3.516419000
H	0.381125000	-1.738232000	-3.732521000
C	1.187780000	-2.983495000	1.514293000
H	1.818818000	-3.846084000	1.725491000
H	1.456770000	-2.150367000	2.166346000
H	0.144439000	-3.258697000	1.641748000
N	-1.745102000	3.608686000	-1.058331000
C	-3.030917000	4.177105000	-0.668156000
C	-3.490789000	3.688408000	0.710425000
C	-3.313477000	2.174887000	0.860801000
C	-3.803528000	1.379808000	-0.353636000
C	-2.964061000	1.566624000	-1.649699000
C	-1.655131000	2.306524000	-1.468573000
C	0.683550000	2.420921000	-1.554286000
C	0.597777000	3.382709000	-0.375116000
C	-0.554827000	4.342661000	-0.620311000
H	-2.930575000	5.265911000	-0.686296000
H	-3.778773000	3.928177000	-1.425369000
H	-2.931197000	4.202439000	1.500007000
H	-4.543680000	3.963945000	0.839772000
H	-2.254576000	1.939532000	1.035127000

H	-3.847427000	1.833054000	1.752985000
H	-4.849027000	1.635516000	-0.558400000
H	-3.800954000	0.319398000	-0.079703000
H	-3.550552000	2.089651000	-2.411840000
H	-2.699885000	0.601615000	-2.087936000
H	1.494908000	1.704289000	-1.399526000
H	0.911866000	2.982017000	-2.472161000
H	1.530221000	3.936660000	-0.239926000
H	0.408768000	2.802777000	0.536284000
H	-0.284633000	5.088119000	-1.378982000
H	-0.806538000	4.884708000	0.298104000
N	-0.556807000	1.676207000	-1.730491000
H	-1.645985000	-2.084103000	-2.147646000

A-TSb2

C	-2.281793000	1.732584000	2.756865000
C	-1.042815000	1.703612000	3.391861000
C	0.003834000	1.000283000	2.809611000
C	-0.173433000	0.313869000	1.601734000
C	-1.416677000	0.370210000	0.924688000
C	-2.456688000	1.087345000	1.535941000
C	-1.549163000	-0.228156000	-0.438283000
N	0.845643000	-0.461648000	1.002214000
C	-2.858844000	0.079546000	-1.158577000
C	-4.057493000	-0.633056000	-0.554273000
C	1.720367000	-1.038999000	1.733911000
O	-3.996671000	-1.694169000	0.025053000
C	2.772374000	-1.895964000	1.167942000

C	2.604217000	-2.509056000	-0.079991000
C	3.601751000	-3.320944000	-0.601596000
C	4.778653000	-3.528109000	0.118771000
C	4.945776000	-2.936888000	1.368853000
C	3.940757000	-2.133226000	1.897598000
O	-5.190515000	0.038243000	-0.754588000
C	-6.378246000	-0.596491000	-0.259597000
H	-3.111440000	2.271341000	3.202643000
H	-0.889894000	2.228930000	4.328345000
H	0.981614000	1.003926000	3.282149000
H	-3.429589000	1.149655000	1.057597000
H	-3.061079000	1.154113000	-1.180208000
H	-0.500172000	0.512931000	-1.102671000
H	1.721331000	-0.939465000	2.829063000
H	1.669390000	-2.366492000	-0.612967000
H	3.458942000	-3.805232000	-1.562120000
H	5.557921000	-4.164065000	-0.287945000
H	5.855363000	-3.109299000	1.934096000
H	4.065194000	-1.678168000	2.876799000
H	-7.197752000	0.072023000	-0.512792000
H	-6.510123000	-1.569712000	-0.734852000
H	-6.307231000	-0.732661000	0.820929000
N	-1.117849000	-2.621896000	0.367290000
N	-0.566109000	-3.566779000	-1.549711000
N	-0.840547000	-2.246021000	-1.713451000
C	-1.188030000	-1.635635000	-0.565493000
C	-0.732552000	-3.763302000	-0.278961000
H	-0.589184000	-4.709244000	0.221639000

C	-0.789543000	-1.687295000	-3.054454000
H	-0.703005000	-0.603124000	-2.985733000
H	0.083417000	-2.103616000	-3.556750000
H	-1.691660000	-1.961035000	-3.605811000
C	-1.554238000	-2.563986000	1.760629000
H	-1.706136000	-3.589129000	2.097542000
H	-0.799662000	-2.077905000	2.379972000
H	-2.498273000	-2.024127000	1.805002000
N	1.823442000	3.078820000	-1.553033000
C	1.950476000	4.502726000	-1.237590000
C	2.095065000	4.741516000	0.269428000
C	1.105613000	3.885431000	1.063896000
C	-0.322922000	3.917251000	0.510688000
C	-0.524119000	3.244181000	-0.876557000
C	0.654600000	2.437338000	-1.361981000
C	1.628062000	0.362340000	-2.022959000
C	2.915098000	0.882520000	-1.401140000
C	3.076379000	2.346192000	-1.777650000
H	2.813520000	4.883300000	-1.789924000
H	1.076343000	5.029828000	-1.625946000
H	3.118446000	4.520689000	0.592079000
H	1.925282000	5.805962000	0.463943000
H	1.453432000	2.844410000	1.086100000
H	1.087701000	4.217422000	2.106253000
H	-0.667432000	4.955541000	0.455196000
H	-0.972387000	3.408137000	1.225865000
H	-0.754209000	3.989189000	-1.645203000
H	-1.379636000	2.567748000	-0.840071000

H	1.441035000	-0.665192000	-1.707550000
H	1.699984000	0.381398000	-3.119323000
H	3.778432000	0.307979000	-1.744361000
H	2.842464000	0.771671000	-0.314044000
H	3.370995000	2.453059000	-2.828487000
H	3.850306000	2.819846000	-1.165167000
N	0.489275000	1.162492000	-1.590097000
H	-2.820533000	-0.233015000	-2.209358000

A-2b

C	-2.260476000	3.694101000	-0.190228000
C	-0.994948000	4.282332000	-0.239869000
C	0.124096000	3.471824000	-0.356577000
C	-0.001098000	2.077799000	-0.435604000
C	-1.279921000	1.463818000	-0.382997000
C	-2.394909000	2.316071000	-0.256680000
C	-1.437477000	0.015710000	-0.515894000
N	1.112890000	1.244629000	-0.626092000
C	-2.608157000	-0.505371000	-1.332618000
C	-3.539222000	-1.284864000	-0.437886000
C	2.196964000	1.464032000	0.004233000
O	-3.482213000	-2.478145000	-0.247297000
C	3.352132000	0.559350000	-0.106919000
C	3.225356000	-0.678582000	-0.749742000
C	4.303829000	-1.550747000	-0.796892000
C	5.519997000	-1.195025000	-0.211985000
C	5.651807000	0.033963000	0.429222000
C	4.568182000	0.904475000	0.487678000

O	-4.417326000	-0.486658000	0.198472000
C	-5.249067000	-1.149764000	1.148476000
H	-3.145514000	4.315913000	-0.095785000
H	-0.885084000	5.361069000	-0.203506000
H	1.112778000	3.912348000	-0.450569000
H	-3.382111000	1.867692000	-0.183421000
H	-3.139675000	0.343452000	-1.765908000
H	-2.318559000	-1.165376000	-2.154177000
H	2.306508000	2.308876000	0.703867000
H	2.267100000	-0.936196000	-1.192058000
H	4.196357000	-2.514938000	-1.283342000
H	6.361709000	-1.879222000	-0.250821000
H	6.595845000	0.311304000	0.887149000
H	4.662544000	1.861704000	0.994805000
H	-5.915592000	-0.387287000	1.547950000
H	-5.818960000	-1.946884000	0.666934000
H	-4.642457000	-1.586643000	1.945197000
N	0.162626000	-0.665538000	1.259469000
N	0.684001000	-2.714142000	0.601395000
N	-0.212517000	-2.146310000	-0.267046000
C	-0.553957000	-0.866109000	0.085279000
C	0.886798000	-1.806439000	1.493910000
H	1.554938000	-1.913716000	2.335492000
C	-0.507734000	-2.820733000	-1.509588000
H	0.127292000	-3.704449000	-1.543058000
H	-1.559904000	-3.116039000	-1.546491000
H	-0.266946000	-2.162240000	-2.350460000
C	-0.102591000	0.376372000	2.227681000

H	0.256843000	0.040190000	3.201323000
H	0.384813000	1.318866000	1.964233000
H	-1.182236000	0.546235000	2.271148000

A-TSb3

C	3.966582000	-0.002333000	-1.053162000
C	3.827687000	0.904919000	-2.106028000
C	2.590179000	1.429148000	-2.461183000
C	1.435035000	1.033354000	-1.765183000
C	1.578277000	0.066054000	-0.719883000
C	2.831082000	-0.402511000	-0.343946000
C	0.279918000	-0.162513000	-0.001791000
N	0.179380000	1.548115000	-1.908564000
C	0.145014000	0.831257000	1.139959000
C	1.175026000	0.543378000	2.208544000
C	-0.719231000	0.631887000	-1.513281000
O	1.267279000	-0.512688000	2.798982000
C	-2.051053000	1.055360000	-1.007664000
C	-2.278707000	2.382847000	-0.637004000
C	-3.497429000	2.751101000	-0.076826000
C	-4.494872000	1.797740000	0.125159000
C	-4.276985000	0.473173000	-0.250655000
C	-3.060564000	0.106512000	-0.818826000
O	1.999781000	1.570772000	2.418310000
C	3.050639000	1.322361000	3.352172000
H	4.944587000	-0.386432000	-0.784052000
H	4.709523000	1.213536000	-2.661051000
H	2.494868000	2.142829000	-3.272387000

H	2.917454000	-1.090751000	0.496197000
H	0.318548000	1.823187000	0.710691000
H	-0.851104000	0.839737000	1.588843000
H	-0.777394000	-0.330346000	-2.056312000
H	-1.482694000	3.101160000	-0.809348000
H	-3.673058000	3.784840000	0.204678000
H	-5.443523000	2.088157000	0.565820000
H	-5.055143000	-0.270108000	-0.106896000
H	-2.886134000	-0.926254000	-1.119212000
H	3.616518000	2.249557000	3.416071000
H	2.639971000	1.048467000	4.326178000
H	3.684555000	0.508675000	2.992603000
N	-0.073986000	-2.478729000	-0.828428000
N	-1.602997000	-3.227300000	0.579016000
N	-1.191299000	-1.977848000	0.940336000
C	-0.249420000	-1.473662000	0.099814000
C	-0.913220000	-3.501095000	-0.477164000
H	-0.975019000	-4.425509000	-1.031248000
C	-1.765396000	-1.407631000	2.150437000
H	-2.311150000	-2.218703000	2.629136000
H	-0.961171000	-1.063077000	2.801508000
H	-2.457576000	-0.599383000	1.901582000
C	0.898272000	-2.575345000	-1.916984000
H	0.681330000	-3.498941000	-2.455649000
H	0.815672000	-1.727822000	-2.594847000
H	1.911769000	-2.601179000	-1.516192000

A-3b

C	3.572251000	-1.969720000	0.302064000
C	3.110710000	-3.179411000	-0.244473000
C	1.877349000	-3.296000000	-0.862423000
C	1.022499000	-2.164468000	-0.952691000
C	1.528744000	-0.935113000	-0.421195000
C	2.757767000	-0.837469000	0.209621000
C	0.395927000	0.068850000	-0.488627000
N	-0.247859000	-2.143718000	-1.370444000
C	0.822358000	1.385380000	-1.149594000
C	1.832428000	2.164006000	-0.338882000
C	-0.605813000	-0.761889000	-1.472736000
O	1.760823000	2.355041000	0.856687000
C	-2.062134000	-0.450952000	-1.207875000
C	-2.792939000	-1.210263000	-0.290613000
C	-4.097533000	-0.857905000	0.039718000
C	-4.700185000	0.247719000	-0.559245000
C	-3.996860000	0.984828000	-1.507628000
C	-2.686394000	0.633368000	-1.829001000
O	2.822525000	2.640278000	-1.094898000
C	3.821471000	3.382061000	-0.390462000
H	4.545935000	-1.912601000	0.774853000
H	3.746311000	-4.059611000	-0.178987000
H	1.535835000	-4.245629000	-1.261083000
H	3.076650000	0.096467000	0.669908000
H	1.277117000	1.123016000	-2.105362000
H	-0.026913000	2.042639000	-1.369879000
H	-0.361363000	-0.348497000	-2.473169000
H	-2.319440000	-2.094834000	0.126384000

H	-4.655246000	-1.454558000	0.755465000
H	-5.720309000	0.517715000	-0.305250000
H	-4.470608000	1.826452000	-2.004092000
H	-2.141607000	1.197272000	-2.584880000
H	3.371134000	4.233489000	0.123405000
H	4.312971000	2.742868000	0.346014000
H	4.530672000	3.715001000	-1.145275000
N	-0.330365000	-0.741060000	1.823465000
N	-1.569111000	0.935695000	2.538883000
N	-1.031147000	1.213200000	1.329164000
C	-0.261434000	0.217840000	0.863474000
C	-1.134863000	-0.254338000	2.810265000
H	-1.369173000	-0.807537000	3.706237000
C	-1.348772000	2.519858000	0.761280000
H	-2.052150000	2.972735000	1.456282000
H	-0.439760000	3.116296000	0.702453000
H	-1.825991000	2.393911000	-0.209390000
C	0.210846000	-2.112634000	1.882123000
H	-0.153645000	-2.538224000	2.817555000
H	-0.171139000	-2.674075000	1.029694000
H	1.300774000	-2.096142000	1.868725000

A-4b

C	-3.470404000	1.087032000	1.718267000
C	-3.194607000	2.453453000	1.590175000
C	-2.069496000	2.923501000	0.924448000
C	-1.154840000	2.002557000	0.362094000
C	-1.474955000	0.618338000	0.466759000

C	-2.593664000	0.160557000	1.141333000
C	-0.329592000	-0.154454000	-0.162075000
N	0.035761000	2.284047000	-0.204537000
C	-0.817216000	-1.116167000	-1.253762000
C	-1.599624000	-2.295270000	-0.733855000
C	0.479699000	1.067162000	-0.848933000
O	-1.473191000	-2.788584000	0.368817000
C	1.976761000	0.851610000	-0.841583000
C	2.769609000	1.322962000	0.207379000
C	4.127907000	1.024203000	0.258913000
C	4.718084000	0.261490000	-0.747389000
C	3.946080000	-0.177177000	-1.819487000
C	2.585805000	0.122357000	-1.865957000
O	-2.442030000	-2.772876000	-1.650624000
C	-3.216378000	-3.901525000	-1.239935000
H	-4.358090000	0.751218000	2.241746000
H	-3.883771000	3.173316000	2.024552000
H	-1.867320000	3.987598000	0.849956000
H	-2.778506000	-0.905047000	1.248700000
H	-1.451163000	-0.520811000	-1.920866000
H	0.003202000	-1.500799000	-1.872458000
H	0.144036000	1.041874000	-1.900428000
H	2.303259000	1.957408000	0.955916000
H	4.733706000	1.398317000	1.078924000
H	5.778185000	0.032256000	-0.708589000
H	4.405581000	-0.739248000	-2.627039000
H	1.987698000	-0.193309000	-2.719358000
H	-2.563960000	-4.730709000	-0.958248000

H	-3.841106000	-3.637724000	-0.384409000
H	-3.830219000	-4.166759000	-2.097924000
N	0.730611000	-0.266428000	2.157530000
N	2.082174000	-1.996477000	1.976193000
N	1.375115000	-1.812088000	0.836654000
C	0.532920000	-0.773073000	0.913915000
C	1.677851000	-1.043909000	2.755085000
H	2.034408000	-0.873299000	3.758963000
C	1.619814000	-2.762861000	-0.243707000
H	2.436128000	-3.392171000	0.103582000
H	0.726621000	-3.363380000	-0.407146000
H	1.927635000	-2.229787000	-1.141497000
C	0.181830000	0.932479000	2.815557000
H	0.720294000	1.033743000	3.758244000
H	0.363159000	1.799142000	2.179623000
H	-0.885911000	0.813164000	2.997045000
O	-2.281244000	1.418109000	-2.525607000
H	-1.717984000	2.211844000	-2.645790000
H	-2.683840000	1.559449000	-1.660000000
O	-0.572857000	3.605411000	-2.451142000
H	-0.236951000	3.292941000	-1.557647000
H	-1.049666000	4.421332000	-2.271722000
A-TSb4			
C	-3.580607000	1.104085000	1.585533000
C	-3.295193000	2.469327000	1.507010000
C	-2.107297000	2.930330000	0.947985000
C	-1.193738000	1.993072000	0.458170000
C	-1.500770000	0.626403000	0.486252000

C	-2.678408000	0.172294000	1.066901000
C	-0.350487000	-0.149040000	-0.144525000
N	0.090823000	2.234353000	0.004857000
C	-0.858908000	-1.051928000	-1.283910000
C	-1.762883000	-2.169528000	-0.833586000
C	0.519289000	1.027805000	-0.750604000
O	-1.661880000	-2.767471000	0.219955000
C	1.991205000	0.783246000	-0.706447000
C	2.831441000	1.295777000	0.292955000
C	4.186583000	0.978567000	0.324493000
C	4.739272000	0.141838000	-0.642691000
C	3.927392000	-0.348006000	-1.663168000
C	2.575736000	-0.017648000	-1.699852000
O	-2.694138000	-2.459910000	-1.743200000
C	-3.584079000	-3.520140000	-1.390529000
H	-4.507193000	0.767132000	2.037345000
H	-4.010820000	3.187107000	1.897018000
H	-1.875873000	3.989916000	0.904153000
H	-2.892489000	-0.889977000	1.135238000
H	-1.368053000	-0.395345000	-1.996126000
H	-0.028667000	-1.493454000	-1.846616000
H	0.016428000	1.221608000	-1.997030000
H	2.405842000	1.968201000	1.032896000
H	4.818173000	1.389026000	1.107361000
H	5.795789000	-0.104547000	-0.616509000
H	4.353755000	-0.969070000	-2.445935000
H	1.953110000	-0.353208000	-2.527958000
H	-3.028200000	-4.442381000	-1.209181000

H	-4.140810000	-3.260685000	-0.487564000
H	-4.258190000	-3.634348000	-2.236885000
N	0.697517000	-0.388552000	2.176468000
N	1.972396000	-2.168190000	1.945816000
N	1.250688000	-1.938569000	0.820536000
C	0.457272000	-0.862968000	0.925669000
C	1.622617000	-1.212709000	2.745301000
H	2.003728000	-1.072802000	3.744912000
C	1.434288000	-2.894847000	-0.268195000
H	2.173096000	-3.605045000	0.095952000
H	0.492478000	-3.402196000	-0.466820000
H	1.823066000	-2.383076000	-1.146681000
C	0.188458000	0.804898000	2.867807000
H	0.708788000	0.850588000	3.824667000
H	0.416502000	1.689329000	2.273302000
H	-0.885611000	0.720066000	3.028678000
O	-0.677707000	1.506350000	-2.997955000
H	-0.801647000	3.045564000	-2.550760000
H	-0.105006000	1.489976000	-3.773891000
O	-0.823364000	3.945257000	-2.091930000
H	0.101111000	3.063438000	-0.602423000
H	-1.749656000	4.052123000	-1.853244000

A-5b

C	3.312376000	-1.723816000	1.235712000
C	3.010183000	-3.012519000	0.783034000
C	1.856126000	-3.272185000	0.053399000
C	0.994773000	-2.208609000	-0.235285000

C	1.335143000	-0.900920000	0.147490000
C	2.470369000	-0.659317000	0.914175000
C	0.288430000	0.076307000	-0.393491000
N	-0.256824000	-2.246344000	-0.804831000
C	0.936261000	1.004863000	-1.491869000
C	2.270529000	1.554572000	-1.064961000
C	-0.752251000	-0.880427000	-0.936475000
O	2.446609000	2.340301000	-0.152878000
C	-2.143531000	-0.653876000	-0.955019000
C	-3.084007000	-1.726899000	-0.888102000
C	-4.449923000	-1.497105000	-0.870138000
C	-4.978943000	-0.205485000	-0.917941000
C	-4.082712000	0.860919000	-1.009445000
C	-2.713965000	0.652158000	-1.036204000
O	3.278201000	1.004598000	-1.746111000
C	4.585824000	1.336008000	-1.278954000
H	4.202750000	-1.550735000	1.830586000
H	3.677851000	-3.834009000	1.024708000
H	1.606933000	-4.281708000	-0.257989000
H	2.702901000	0.346907000	1.253737000
H	1.074255000	0.355272000	-2.354600000
H	0.257255000	1.808633000	-1.783288000
H	-2.710366000	-2.744900000	-0.832409000
H	-5.122037000	-2.350299000	-0.811860000
H	-6.049585000	-0.036686000	-0.905596000
H	-4.459848000	1.878764000	-1.078400000
H	-2.056616000	1.505240000	-1.185102000
H	4.712867000	2.418483000	-1.225569000

H	4.741015000	0.904728000	-0.286446000
H	5.277326000	0.896829000	-1.995125000
N	-0.862109000	0.200492000	1.851056000
N	-1.343168000	2.328504000	2.119153000
N	-0.639053000	2.131391000	0.973234000
C	-0.330868000	0.840562000	0.777082000
C	-1.463439000	1.141098000	2.624874000
H	-1.975942000	0.910826000	3.546025000
C	-0.412094000	3.321770000	0.155293000
H	-0.676507000	4.162882000	0.792185000
H	0.635015000	3.375136000	-0.130160000
H	-1.073445000	3.305794000	-0.712946000
C	-0.924309000	-1.238515000	2.118007000
H	-1.518603000	-1.365299000	3.023110000
H	-1.402485000	-1.739774000	1.274475000
H	0.079858000	-1.633689000	2.270288000
H	-0.356831000	-2.841394000	-1.621102000

A-TSb5

C	3.693694000	-1.884046000	0.041034000
C	3.195256000	-3.137265000	-0.331865000
C	1.867180000	-3.302774000	-0.708098000
C	1.042436000	-2.177474000	-0.719917000
C	1.543426000	-0.905779000	-0.397005000
C	2.864978000	-0.763070000	0.013527000
C	0.412925000	0.085136000	-0.449835000
N	-0.318560000	-2.101948000	-0.921566000
C	0.782895000	1.436123000	-1.091080000

C	1.938809000	2.132234000	-0.418828000
C	-0.667419000	-0.700496000	-1.040711000
O	1.958668000	2.514536000	0.730589000
C	-2.067143000	-0.377649000	-1.088465000
C	-3.047205000	-1.346487000	-0.759046000
C	-4.400249000	-1.040775000	-0.762415000
C	-4.846529000	0.238839000	-1.089807000
C	-3.902723000	1.201432000	-1.443834000
C	-2.548223000	0.899833000	-1.458617000
O	2.985806000	2.274097000	-1.245948000
C	4.129009000	2.904148000	-0.669840000
H	4.727340000	-1.785799000	0.354413000
H	3.852886000	-4.000918000	-0.315039000
H	1.475958000	-4.281975000	-0.966884000
H	3.248632000	0.196816000	0.345377000
H	1.034057000	1.235114000	-2.132804000
H	-0.069517000	2.115458000	-1.070658000
H	-2.723344000	-2.336819000	-0.454482000
H	-5.118134000	-1.809531000	-0.489029000
H	-5.904923000	0.475557000	-1.085468000
H	-4.227387000	2.196335000	-1.737058000
H	-1.851235000	1.648716000	-1.820177000
H	3.869838000	3.895095000	-0.291657000
H	4.517377000	2.305510000	0.158421000
H	4.865057000	2.973749000	-1.468365000
N	-0.419083000	-0.663670000	1.987267000
N	-2.007033000	0.816588000	2.386576000
N	-1.122895000	1.273420000	1.444804000

C	-0.151302000	0.382811000	1.137226000
C	-1.553101000	-0.355534000	2.685534000
H	-1.990333000	-1.014498000	3.420927000
C	-1.228266000	2.685641000	1.098511000
H	-1.671637000	3.182688000	1.961087000
H	-0.228135000	3.078913000	0.925998000
H	-1.877051000	2.823965000	0.232856000
C	0.374845000	-1.859667000	2.263311000
H	0.222015000	-2.121815000	3.312312000
H	0.060081000	-2.682684000	1.623653000
H	1.430106000	-1.647096000	2.098093000
H	-0.724204000	-2.717664000	-1.616887000

Table S3: The energies for species of path a in series B

	E	G
B-TSa1- <i>Si</i>	-1450.954177	-1451.015226
B-TSa1- <i>Re</i>	-1450.944136	-1451.005971
B-1a- <i>Si</i>	-1450.963154	-1451.023688
B-1a- <i>Re</i>	-1450.955426	-1451.016396
B-11a	-1917.872872	-1917.949611
B-TSa2	-1917.847827	-1917.925504
B-2a	-1450.981446	-1451.044633
B-TSa3	-1450.953517	-1451.012490
B-3a	-1450.954909	-1451.014599
B-4a	-1917.864744	-1917.941482
B-TSa4	-1917.853883	-1917.929071
B-5a	-1917.872876	-1917.946959
B-TSa5	-1917.865292	-1917.939983
B-6a	-1450.957608	-1451.016649
B-TSa6	-1450.959283	-1451.016645

Table S4: The energies for species of path b in series B

	E	G
B-TSb1- <i>Si</i>	-1450.946589	-1451.006032
B-TSb1- <i>Re</i>	-1450.942048	-1451.001121
B-1b- <i>Si</i>	-1450.976905	-1451.037046
B-1b- <i>Re</i>	-1450.972046	-1451.032642
B-11b	-1917.879072	-1917.960072
B-TSb2	-1917.869539	-1917.948974
B-2b	-1451.001448	-1451.063427
B-TSb3	-1450.975991	-1451.033104
B-3b	-1450.981631	-1451.038548
B-4b	-1917.888860	-1917.961101
B-TSb4	-1917.875521	-1917.950217
B-5b	-1450.952772	-1451.010943
B-TSb5	-1450.947198	-1451.005782

Cartesian coordinates of the optimized species in series B

B-TSa1-Si

C	-1.696109000	-2.843714000	-1.952001000
C	-0.309599000	-2.742943000	-1.834781000
C	0.302132000	-1.511119000	-1.651879000
C	-0.457859000	-0.323822000	-1.570489000
C	-1.865538000	-0.435875000	-1.728230000
C	-2.461094000	-1.684832000	-1.909405000
C	-2.647382000	0.807451000	-1.787928000
N	0.021797000	0.930987000	-1.256351000
C	-3.837832000	1.083912000	-1.229137000
C	-4.528139000	0.244277000	-0.229923000
C	1.267143000	1.045218000	-0.796053000
O	-4.051021000	-0.645418000	0.444546000
C	1.733481000	2.438158000	-0.501018000
C	3.090346000	2.757104000	-0.545091000
C	3.522529000	4.049922000	-0.259348000
C	2.596996000	5.034713000	0.071861000
C	1.237663000	4.724648000	0.100707000
C	0.807346000	3.435195000	-0.189192000
O	-5.811353000	0.635818000	-0.092127000
C	-6.558702000	-0.082401000	0.884216000
H	-2.169805000	-3.809029000	-2.093135000
H	0.305489000	-3.637519000	-1.884884000
H	1.384061000	-1.473151000	-1.573377000
H	-3.539014000	-1.737478000	-2.029703000

H	-2.192379000	1.594403000	-2.386965000
H	-4.342264000	2.014944000	-1.464383000
H	2.084464000	0.406155000	-1.169482000
H	3.810261000	1.991216000	-0.825327000
H	4.580513000	4.289104000	-0.302606000
H	2.931010000	6.042844000	0.296054000
H	0.511939000	5.495687000	0.341305000
H	-0.247149000	3.177204000	-0.208233000
H	-7.566208000	0.328681000	0.851365000
H	-6.569721000	-1.149253000	0.650943000
H	-6.123271000	0.052058000	1.877658000
C	-2.017104000	0.099223000	2.658213000
C	-1.623310000	-1.384886000	2.455523000
C	-0.235592000	-1.247513000	1.920957000
N	-0.024300000	0.023409000	1.465604000
C	-1.197871000	0.882358000	1.607995000
N	0.797897000	-2.003848000	1.712291000
N	1.666308000	-1.139074000	1.075415000
C	1.188514000	0.110958000	0.882908000
C	2.927838000	-1.606106000	0.631340000
C	3.972315000	-0.695517000	0.488616000
C	5.197501000	-1.141743000	0.003440000
C	5.379890000	-2.485218000	-0.313053000
C	4.329579000	-3.386331000	-0.147477000
C	3.094035000	-2.954119000	0.320747000
H	-1.731289000	0.424372000	3.662932000
H	-3.087195000	0.249496000	2.521443000
H	-2.253708000	-1.836411000	1.681530000

H	-1.678645000	-1.983212000	3.365088000
H	-1.701659000	0.948116000	0.639372000
H	-0.899911000	1.880332000	1.932802000
H	3.814155000	0.340515000	0.772203000
H	6.014300000	-0.436829000	-0.111661000
H	6.338617000	-2.831438000	-0.684022000
H	4.469595000	-4.433968000	-0.392403000
H	2.257816000	-3.632357000	0.446309000

B-TSa1-Re

C	1.707110000	-2.852229000	-2.187991000
C	0.327475000	-2.882179000	-2.013774000
C	-0.373964000	-1.721908000	-1.704184000
C	0.284628000	-0.482842000	-1.556200000
C	1.704784000	-0.469605000	-1.718469000
C	2.384043000	-1.644128000	-2.040457000
C	2.367034000	0.833070000	-1.598115000
N	-0.311744000	0.700834000	-1.187587000
C	3.565975000	1.192702000	-1.101633000
C	4.538124000	0.349424000	-0.385389000
C	-1.627326000	0.752715000	-1.014502000
O	4.638027000	-0.857806000	-0.364433000
C	-2.201879000	2.107661000	-0.718271000
C	-3.574944000	2.329169000	-0.815626000
C	-4.114632000	3.578776000	-0.528252000
C	-3.277051000	4.621891000	-0.140768000
C	-1.902577000	4.409434000	-0.054671000
C	-1.364386000	3.159721000	-0.346479000

O	5.373794000	1.139474000	0.337877000
C	6.338277000	0.432366000	1.106514000
H	2.252743000	-3.756038000	-2.436094000
H	-0.212711000	-3.819686000	-2.118570000
H	-1.451309000	-1.784694000	-1.575421000
H	3.457519000	-1.605394000	-2.171573000
H	1.742785000	1.656658000	-1.938246000
H	3.822468000	2.246914000	-1.100167000
H	-2.297281000	0.155695000	-1.664859000
H	-4.224241000	1.516461000	-1.137230000
H	-5.184560000	3.742033000	-0.613005000
H	-3.693361000	5.599135000	0.082754000
H	-1.246944000	5.225384000	0.233770000
H	-0.296508000	2.967155000	-0.305845000
H	6.956881000	1.190745000	1.584682000
H	5.849027000	-0.190004000	1.862098000
H	6.944577000	-0.214641000	0.468800000
N	-3.085045000	-1.265465000	0.439195000
N	-1.530922000	-2.211295000	1.670125000
N	-1.184842000	-0.946486000	1.248718000
C	-2.104079000	-0.334378000	0.481688000
C	-2.703914000	-2.373353000	1.144852000
C	-4.366587000	-1.421189000	-0.235938000
H	-4.977920000	-0.525607000	-0.119416000
H	-4.197818000	-1.603443000	-1.303341000
C	0.089516000	-0.411032000	1.596541000
C	1.196237000	-1.251743000	1.600342000
C	0.194394000	0.948763000	1.860703000

C	2.443133000	-0.709112000	1.886879000
H	1.074970000	-2.297671000	1.341163000
C	1.449274000	1.480064000	2.133619000
H	-0.695388000	1.570974000	1.834363000
C	2.570369000	0.653773000	2.151393000
H	3.321809000	-1.343509000	1.853369000
H	1.550668000	2.542848000	2.327059000
H	3.551030000	1.079696000	2.341974000
C	-4.953592000	-2.654709000	0.494697000
H	-5.570155000	-2.312142000	1.329080000
H	-5.580361000	-3.255902000	-0.164040000
C	-3.738430000	-3.447331000	1.046898000
H	-3.401467000	-4.215702000	0.344005000
H	-3.943216000	-3.928480000	2.003538000

B-1a-Si

C	-1.605083000	-3.063272000	-1.913215000
C	-0.223380000	-2.923675000	-1.781585000
C	0.367522000	-1.674560000	-1.657903000
C	-0.402772000	-0.478182000	-1.661570000
C	-1.813587000	-0.643567000	-1.839324000
C	-2.383083000	-1.909828000	-1.945467000
C	-2.641607000	0.560944000	-1.940231000
N	0.045239000	0.781662000	-1.435863000
C	-3.784166000	0.815234000	-1.277638000
C	-4.259561000	0.038369000	-0.114837000
C	1.307408000	0.894417000	-0.787109000
O	-3.579095000	-0.564652000	0.691574000

C	1.710991000	2.354099000	-0.602570000
C	2.602218000	2.750054000	0.396675000
C	2.983180000	4.083781000	0.519297000
C	2.471502000	5.035620000	-0.358471000
C	1.573364000	4.646325000	-1.349375000
C	1.189674000	3.313678000	-1.468949000
O	-5.598495000	0.142606000	0.020470000
C	-6.140411000	-0.521987000	1.156260000
H	-2.060969000	-4.042255000	-2.008451000
H	0.412425000	-3.806546000	-1.779080000
H	1.449658000	-1.617236000	-1.584759000
H	-3.460683000	-1.981235000	-2.076282000
H	-2.297456000	1.310310000	-2.653202000
H	-4.401242000	1.667256000	-1.544415000
H	2.158637000	0.361207000	-1.254152000
H	2.989020000	2.017940000	1.103798000
H	3.672831000	4.379214000	1.303869000
H	2.765577000	6.076246000	-0.264804000
H	1.164606000	5.386312000	-2.030645000
H	0.475252000	2.983260000	-2.214747000
H	-7.216829000	-0.364594000	1.110791000
H	-5.905482000	-1.588177000	1.126089000
H	-5.732548000	-0.102848000	2.080080000
C	-1.817687000	1.153119000	2.616960000
C	-1.424178000	-0.300093000	2.995435000
C	-0.143792000	-0.473133000	2.245102000
N	0.008639000	0.519832000	1.330168000
C	-1.117365000	1.453064000	1.270579000

N	0.813963000	-1.350434000	2.163809000
N	1.579590000	-0.877110000	1.122753000
C	1.083235000	0.246071000	0.578066000
C	2.716088000	-1.623807000	0.697776000
C	3.866393000	-0.965906000	0.275432000
C	4.946396000	-1.722541000	-0.172698000
C	4.876251000	-3.111457000	-0.175780000
C	3.719660000	-3.753713000	0.265786000
C	2.628549000	-3.013990000	0.701423000
H	-1.462963000	1.846765000	3.384008000
H	-2.898359000	1.255250000	2.519947000
H	-2.155909000	-1.007145000	2.594228000
H	-1.313521000	-0.457591000	4.068652000
H	-1.715492000	1.194856000	0.395449000
H	-0.749947000	2.475438000	1.171722000
H	3.919684000	0.117607000	0.301911000
H	5.846405000	-1.219154000	-0.508697000
H	5.722738000	-3.695779000	-0.520374000
H	3.661922000	-4.836796000	0.259377000
H	1.706808000	-3.483963000	1.024863000

B-1a-Re

C	-1.766338000	-3.247864000	1.671556000
C	-0.372267000	-3.233928000	1.646874000
C	0.334333000	-2.042123000	1.573449000
C	-0.326965000	-0.778315000	1.512261000
C	-1.773370000	-0.813614000	1.577137000
C	-2.447304000	-2.033628000	1.647357000

C	-2.433100000	0.482839000	1.615133000
N	0.258845000	0.415861000	1.330497000
C	-3.628084000	0.936506000	1.173013000
C	-4.630695000	0.231109000	0.370006000
C	1.653575000	0.425810000	1.124562000
O	-4.745868000	-0.957729000	0.148481000
C	2.185675000	1.849541000	0.940563000
C	3.555323000	2.109789000	0.982631000
C	4.038073000	3.399910000	0.783190000
C	3.146621000	4.441905000	0.540663000
C	1.777340000	4.186816000	0.509002000
C	1.294770000	2.895977000	0.709674000
O	-5.491517000	1.129428000	-0.182360000
C	-6.504966000	0.552900000	-0.993845000
H	-2.311310000	-4.183108000	1.731304000
H	0.177187000	-4.172040000	1.692022000
H	1.421301000	-2.084614000	1.596041000
H	-3.528996000	-2.020994000	1.686859000
H	-1.794212000	1.248798000	2.053062000
H	-3.856353000	1.986552000	1.321308000
H	2.271274000	-0.054802000	1.920437000
H	4.251950000	1.301678000	1.201612000
H	5.105308000	3.593612000	0.826321000
H	3.518541000	5.450108000	0.387916000
H	1.079332000	4.999850000	0.333978000
H	0.235440000	2.660046000	0.703211000
H	-7.139284000	1.378099000	-1.315476000
H	-6.067879000	0.048996000	-1.861119000

H	-7.084415000	-0.181030000	-0.428825000
N	3.120364000	-1.128071000	-0.316620000
N	1.911416000	-1.396494000	-2.132793000
N	1.318995000	-0.530196000	-1.248694000
C	2.031545000	-0.365832000	-0.129731000
C	3.006218000	-1.743633000	-1.531810000
C	4.309514000	-1.533043000	0.432672000
H	5.063444000	-0.744075000	0.368728000
H	4.059557000	-1.711832000	1.480014000
C	0.013190000	-0.003781000	-1.557957000
C	-1.065707000	-0.875253000	-1.505547000
C	-0.118240000	1.331121000	-1.917030000
C	-2.330936000	-0.378437000	-1.799203000
H	-0.919582000	-1.904426000	-1.191140000
C	-1.389997000	1.815246000	-2.198727000
H	0.755256000	1.974289000	-1.945423000
C	-2.493139000	0.964326000	-2.130457000
H	-3.192209000	-1.031307000	-1.711493000
H	-1.521017000	2.859868000	-2.460064000
H	-3.488777000	1.355369000	-2.318299000
C	4.723023000	-2.812596000	-0.334151000
H	5.801939000	-2.965400000	-0.310137000
H	4.243915000	-3.675429000	0.134527000
C	4.173993000	-2.643594000	-1.775326000
H	3.881656000	-3.587828000	-2.234424000
H	4.897181000	-2.150608000	-2.432399000

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C	-2.298841000	-1.950073000	-3.088149000
C	-1.009342000	-2.282071000	-2.675995000
C	-0.325309000	-1.504641000	-1.748873000
C	-0.911805000	-0.346856000	-1.170532000
C	-2.203254000	0.016661000	-1.667055000
C	-2.874039000	-0.785776000	-2.583484000
C	-2.752406000	1.297483000	-1.210499000
N	-0.431211000	0.385596000	-0.125187000
C	-3.979782000	1.575518000	-0.740611000
C	-5.005042000	0.570451000	-0.399760000
C	0.666647000	-0.165615000	0.618355000
O	-4.845076000	-0.618135000	-0.209768000
C	0.911960000	0.652097000	1.883136000
C	2.201722000	1.017535000	2.268004000
C	2.403234000	1.735884000	3.445495000
C	1.320491000	2.098485000	4.240928000
C	0.027421000	1.759575000	3.843993000
C	-0.175443000	1.043131000	2.669124000
O	-6.212435000	1.157356000	-0.257491000
C	-7.267651000	0.275647000	0.108357000
H	-2.828491000	-2.560630000	-3.810549000
H	-0.518100000	-3.158627000	-3.092005000
H	0.696324000	-1.772575000	-1.492217000
H	-3.861648000	-0.475090000	-2.913768000
H	-2.053470000	2.129451000	-1.291406000
H	-4.263089000	2.604646000	-0.544395000
H	1.627738000	-0.243553000	0.079469000
H	3.032752000	0.803854000	1.602188000

H	3.408437000	2.032245000	3.728234000
H	1.479853000	2.661138000	5.155402000
H	-0.823588000	2.063638000	4.445696000
H	-1.178911000	0.819212000	2.318832000
H	-8.164924000	0.889685000	0.166458000
H	-7.388674000	-0.510375000	-0.640458000
H	-7.061278000	-0.193083000	1.073755000
N	-0.938034000	-2.041054000	1.273905000
N	0.292208000	-3.855808000	1.015706000
N	1.034084000	-2.708738000	0.897689000
C	0.295285000	-1.593483000	1.010137000
C	-0.906608000	-3.406804000	1.238339000
C	-2.310647000	-1.512739000	1.413318000
H	-2.448580000	-0.632272000	0.787959000
H	-2.467401000	-1.261305000	2.466885000
O	3.032914000	1.715593000	-0.577223000
H	2.134269000	2.098331000	-0.671475000
O	0.464797000	2.799140000	-0.911400000
H	0.005199000	2.017627000	-0.478753000
C	2.395213000	-2.780397000	0.470561000
C	2.702576000	-3.563049000	-0.638635000
C	3.360924000	-2.039986000	1.140456000
C	4.015225000	-3.581487000	-1.096691000
H	1.915771000	-4.127704000	-1.127599000
C	4.667203000	-2.056886000	0.661783000
H	3.085768000	-1.461824000	2.015995000
C	4.992665000	-2.822409000	-0.455531000
H	4.271369000	-4.177824000	-1.965437000

H	5.429670000	-1.472270000	1.165315000
H	6.011695000	-2.827582000	-0.827539000
C	-3.129350000	-2.735204000	0.960959000
H	-4.130807000	-2.730675000	1.389242000
H	-3.227212000	-2.686366000	-0.127741000
C	-2.284169000	-3.968197000	1.372311000
H	-2.470935000	-4.267157000	2.409363000
H	-2.432853000	-4.835377000	0.729074000
C	3.499331000	1.401404000	-1.884383000
C	4.987141000	1.105738000	-1.736985000
C	2.753496000	0.170629000	-2.402013000
C	3.268725000	2.597013000	-2.809809000
H	5.508930000	1.986314000	-1.352033000
H	5.129368000	0.281089000	-1.031095000
H	5.428067000	0.823744000	-2.697916000
H	1.673617000	0.358276000	-2.391787000
H	3.050702000	-0.084227000	-3.424668000
H	2.966041000	-0.692965000	-1.757072000
H	3.655775000	2.401736000	-3.814819000
H	2.197983000	2.814077000	-2.879516000
H	3.775120000	3.479274000	-2.405256000
C	0.274927000	4.031058000	-0.218558000
C	-1.175960000	4.152055000	0.249590000
C	1.220386000	4.117865000	0.981855000
C	0.607908000	5.124457000	-1.229178000
H	-1.856841000	4.211117000	-0.606186000
H	-1.448614000	3.280087000	0.855634000
H	-1.312086000	5.052443000	0.856924000

H	2.243648000	3.887318000	0.668235000
H	1.202359000	5.122905000	1.416688000
H	0.927850000	3.405336000	1.757968000
H	0.458898000	6.117906000	-0.795293000
H	1.651623000	5.034677000	-1.545805000
H	-0.029253000	5.021665000	-2.112023000

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C	-2.332995000	-1.036315000	-3.431241000
C	-1.124568000	-1.568029000	-3.000342000
C	-0.540060000	-1.137077000	-1.811744000
C	-1.142161000	-0.140665000	-1.030810000
C	-2.374386000	0.392692000	-1.470751000
C	-2.948462000	-0.057371000	-2.655165000
C	-3.032805000	1.457925000	-0.681900000
N	-0.673395000	0.249559000	0.230176000
C	-4.219524000	1.362466000	-0.071890000
C	-5.001565000	0.107285000	0.038035000
C	0.665789000	-0.190461000	0.644625000
O	-4.584702000	-1.027948000	-0.051633000
C	1.047058000	0.555818000	1.918509000
C	2.189546000	1.361267000	1.961776000
C	2.514916000	2.060650000	3.122582000
C	1.696971000	1.978708000	4.245950000
C	0.546741000	1.192889000	4.206534000
C	0.228097000	0.486521000	3.050501000
O	-6.291645000	0.380186000	0.310694000
C	-7.126489000	-0.762390000	0.472132000

H	-2.790143000	-1.372764000	-4.355205000
H	-0.616768000	-2.323907000	-3.592231000
H	0.416698000	-1.554543000	-1.520138000
H	-3.893892000	0.377096000	-2.967815000
H	-2.486760000	2.401394000	-0.629998000
H	-4.666505000	2.229105000	0.404063000
H	1.458456000	0.308148000	-0.298345000
H	2.785991000	1.450268000	1.057366000
H	3.401741000	2.686871000	3.139964000
H	1.948072000	2.531239000	5.145883000
H	-0.101171000	1.132851000	5.075578000
H	-0.680112000	-0.110622000	3.010824000
H	-8.124669000	-0.377223000	0.673068000
H	-7.123992000	-1.370329000	-0.435071000
H	-6.777360000	-1.377152000	1.305300000
N	-0.558849000	-2.369330000	1.048006000
N	1.022522000	-3.873177000	0.732835000
N	1.521316000	-2.594604000	0.684313000
C	0.569190000	-1.648549000	0.860030000
C	-0.243575000	-3.693930000	0.945688000
C	-1.994509000	-2.154395000	1.311466000
H	-2.384144000	-1.308250000	0.753867000
H	-2.123561000	-1.983799000	2.384847000
O	1.877931000	1.345643000	-0.962354000
H	0.681493000	2.376462000	-0.760440000
O	-0.174133000	2.899372000	-0.600456000
H	-0.751935000	1.262582000	0.345346000
C	2.881274000	-2.407357000	0.291927000

C	3.389541000	-3.216936000	-0.721496000
C	3.661380000	-1.444035000	0.917036000
C	4.707538000	-3.040128000	-1.121881000
H	2.751341000	-3.964628000	-1.178205000
C	4.974470000	-1.264241000	0.490487000
H	3.250419000	-0.855384000	1.727828000
C	5.498317000	-2.059912000	-0.523726000
H	5.113748000	-3.660759000	-1.913200000
H	5.587170000	-0.504021000	0.963142000
H	6.522933000	-1.917458000	-0.850415000
C	-2.578015000	-3.502893000	0.851991000
H	-3.507882000	-3.738325000	1.369289000
H	-2.791007000	-3.427269000	-0.217707000
C	-1.460837000	-4.547388000	1.098666000
H	-1.501758000	-4.957563000	2.113201000
H	-1.473166000	-5.378262000	0.393017000
C	2.459013000	1.310141000	-2.240520000
C	3.707492000	2.202208000	-2.220836000
C	2.886532000	-0.116358000	-2.602781000
C	1.455073000	1.832901000	-3.275400000
H	3.434165000	3.223897000	-1.942410000
H	4.412412000	1.821945000	-1.473066000
H	4.209283000	2.228341000	-3.194821000
H	2.012853000	-0.769289000	-2.686878000
H	3.419845000	-0.142031000	-3.559610000
H	3.549607000	-0.510767000	-1.826121000
H	1.879952000	1.843280000	-4.285504000
H	0.559449000	1.202331000	-3.274672000

H	1.145476000	2.849727000	-3.012503000
C	0.058140000	4.135386000	0.055393000
C	-0.373242000	4.009238000	1.520062000
C	1.534898000	4.516940000	-0.038002000
C	-0.801246000	5.183916000	-0.651306000
H	-1.419339000	3.685025000	1.568260000
H	0.240957000	3.267728000	2.039466000
H	-0.284778000	4.965088000	2.047524000
H	1.821353000	4.648151000	-1.086667000
H	1.731659000	5.452495000	0.495007000
H	2.158687000	3.724699000	0.386920000
H	-0.679788000	6.172523000	-0.196945000
H	-0.522063000	5.240954000	-1.707125000
H	-1.858963000	4.905854000	-0.593569000

B-2a

C	0.639631000	4.626027000	-0.790405000
C	-0.109913000	4.701185000	0.382024000
C	-0.622807000	3.550988000	0.961343000
C	0.837601000	3.386765000	-1.382132000
C	2.862314000	0.642627000	-1.665691000
C	-0.307349000	-0.113223000	0.967524000
O	3.285994000	1.674637000	-1.199398000
C	0.911482000	-0.345224000	1.773634000
C	0.987424000	-1.428683000	2.662332000
C	2.133691000	-1.665277000	3.416410000
C	3.224833000	-0.806609000	3.314723000
C	3.155511000	0.289507000	2.455741000

C	2.014816000	0.521125000	1.694126000
O	3.648784000	-0.443686000	-1.857226000
C	4.991984000	-0.283808000	-1.408690000
H	1.060371000	5.519433000	-1.237506000
H	-0.280721000	5.660457000	0.861042000
H	-1.175222000	3.609679000	1.895679000
H	1.409888000	3.301701000	-2.299938000
H	1.358572000	-0.581239000	-2.650397000
H	-1.365688000	1.389386000	1.900228000
H	0.127616000	-2.088529000	2.754717000
H	2.167570000	-2.512584000	4.094918000
H	4.118339000	-0.985515000	3.904489000
H	3.998505000	0.968789000	2.368296000
H	1.988654000	1.369195000	1.016526000
H	5.500590000	-1.217321000	-1.644836000
H	5.469923000	0.555426000	-1.918272000
H	5.009643000	-0.097834000	-0.331885000
N	-0.221358000	-2.280424000	-0.202985000
N	-2.154264000	-2.300123000	-1.306417000
N	-2.037819000	-1.133563000	-0.532520000
C	-0.833969000	-1.097933000	0.181013000
C	-3.448730000	0.874269000	-0.557995000
C	-4.657345000	1.492351000	-0.258535000
H	1.785724000	-4.551889000	-1.388239000
H	0.725685000	-4.918789000	-0.023656000
H	-0.962757000	-4.989390000	-1.720150000
H	-0.095701000	-3.848487000	-2.753776000
H	1.566119000	-2.852610000	0.782497000

H	1.788120000	-2.167373000	-0.835520000
C	1.476171000	0.323333000	-2.061391000
C	0.385967000	0.953932000	-1.598889000
C	0.298211000	2.216774000	-0.837042000
C	-0.420228000	2.292182000	0.375884000
C	-3.256505000	-0.461704000	-0.211822000
C	-4.277497000	-1.185040000	0.400190000
C	-5.489898000	-0.564186000	0.685636000
C	-5.678517000	0.776436000	0.363652000
C	-1.045762000	-2.913567000	-1.101918000
C	-0.349380000	-4.087492000	-1.716321000
C	0.913926000	-4.206789000	-0.831326000
C	1.142112000	-2.805181000	-0.220558000
N	-0.942380000	1.162213000	1.008429000
H	-0.573465000	0.496994000	-1.849453000
H	-2.651975000	1.422699000	-1.048758000
H	-4.804685000	2.534403000	-0.522615000
H	-6.622681000	1.262105000	0.588264000
H	-6.285210000	-1.128367000	1.161892000
H	-4.111340000	-2.231386000	0.634795000

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C	1.051080000	4.544668000	-0.667468000
C	0.133904000	4.776480000	0.354703000
C	-0.580110000	3.724260000	0.929453000
C	1.262161000	3.248547000	-1.142410000
C	2.977523000	0.341952000	-1.527101000
C	-0.168816000	0.114488000	0.573872000

O	3.541583000	1.239297000	-0.896960000
C	0.847156000	-0.239145000	1.633132000
C	0.463948000	-1.074769000	2.692945000
C	1.353287000	-1.389095000	3.715208000
C	2.643039000	-0.861396000	3.693589000
C	3.023240000	-0.016697000	2.655565000
C	2.135169000	0.301670000	1.628732000
O	3.740205000	-0.580628000	-2.221646000
C	5.133048000	-0.337664000	-2.170010000
H	1.608738000	5.372568000	-1.092207000
H	-0.020805000	5.785957000	0.723267000
H	-1.286003000	3.899953000	1.736076000
H	1.985923000	3.039847000	-1.922380000
H	1.337991000	-0.712850000	-2.376432000
H	-1.225469000	1.302199000	1.907732000
H	-0.542056000	-1.492058000	2.710083000
H	1.040565000	-2.040476000	4.525544000
H	3.344269000	-1.106199000	4.485376000
H	4.024923000	0.400460000	2.629417000
H	2.463735000	0.955333000	0.826267000
H	5.603760000	-1.139303000	-2.741545000
H	5.383435000	0.632392000	-2.609440000
H	5.499267000	-0.342481000	-1.139416000
N	-0.235948000	-2.207503000	-0.240857000
N	-2.273646000	-2.430121000	-1.060992000
N	-2.108138000	-1.198661000	-0.456680000
C	-0.864773000	-1.045430000	0.067483000
C	-3.279479000	0.932682000	-0.869228000

C	-4.450758000	1.677491000	-0.791783000
H	1.617590000	-4.804375000	-0.890342000
H	0.527715000	-4.846507000	0.500724000
H	-1.137194000	-5.139537000	-1.205330000
H	-0.204056000	-4.215796000	-2.393377000
H	1.455903000	-2.700038000	0.936638000
H	1.791564000	-2.364991000	-0.776203000
C	1.596442000	0.077293000	-1.680078000
C	0.528159000	0.766195000	-1.039970000
C	0.552125000	2.197917000	-0.582755000
C	-0.350364000	2.438918000	0.455898000
C	-3.274230000	-0.363874000	-0.364748000
C	-4.420520000	-0.931075000	0.182741000
C	-5.588919000	-0.179117000	0.245810000
C	-5.603225000	1.126449000	-0.236248000
C	-1.120439000	-2.997831000	-0.917596000
C	-0.479877000	-4.279716000	-1.336138000
C	0.768501000	-4.308773000	-0.419824000
C	1.094601000	-2.835405000	-0.081777000
N	-0.980177000	1.262581000	0.923562000
H	-0.400761000	0.612673000	-1.606048000
H	-2.381766000	1.359330000	-1.299995000
H	-4.459738000	2.691841000	-1.175357000
H	-6.514284000	1.713579000	-0.186201000
H	-6.485821000	-0.615484000	0.672049000
H	-4.387609000	-1.953598000	0.542759000

B-3a

C	-1.423897000	-4.489415000	-0.544894000
C	-0.442547000	-4.779806000	0.399670000
C	0.396186000	-3.779682000	0.899017000
C	-1.586296000	-3.185823000	-1.024943000
C	-3.040889000	-0.155236000	-1.462544000
C	0.121611000	-0.186788000	0.403883000
O	-3.665006000	-0.975764000	-0.766975000
C	-0.775548000	0.226721000	1.564451000
C	-0.206813000	0.971714000	2.607132000
C	-0.955936000	1.324442000	3.724070000
C	-2.288767000	0.926163000	3.811784000
C	-2.851212000	0.174820000	2.784950000
C	-2.106080000	-0.181289000	1.659814000
O	-3.767710000	0.738741000	-2.249041000
C	-5.164940000	0.546437000	-2.198149000
H	-2.075371000	-5.279413000	-0.903504000
H	-0.332644000	-5.795214000	0.767867000
H	1.154904000	-4.001045000	1.643910000
H	-2.364103000	-2.928529000	-1.734870000
H	-1.356993000	0.723227000	-2.386170000
H	1.228557000	-1.317736000	1.757278000
H	0.834254000	1.289173000	2.542078000
H	-0.501722000	1.905146000	4.520977000
H	-2.881951000	1.200670000	4.678474000
H	-3.888499000	-0.139152000	2.843596000
H	-2.581438000	-0.750835000	0.862307000
H	-5.556461000	0.691558000	-1.186195000
H	-5.599792000	1.284670000	-2.875573000

H	-5.444239000	-0.462118000	-2.517793000
N	0.318647000	2.197099000	-0.292166000
N	2.412642000	2.415963000	-0.942435000
N	2.162992000	1.148910000	-0.470564000
C	0.889022000	1.000700000	-0.059911000
C	3.216367000	-0.993586000	-1.072885000
C	4.338491000	-1.813414000	-1.050816000
H	-1.395604000	4.926468000	-0.751601000
H	-0.390046000	4.769650000	0.694429000
H	1.383990000	5.173506000	-0.874968000
H	0.490973000	4.424887000	-2.208577000
H	-1.425534000	2.620159000	0.829516000
H	-1.659644000	2.482098000	-0.922349000
C	-1.668115000	0.050234000	-1.594439000
C	-0.609860000	-0.745104000	-0.953223000
C	-0.755157000	-2.193430000	-0.537511000
C	0.215164000	-2.491043000	0.420615000
C	3.279207000	0.239502000	-0.434963000
C	4.436720000	0.677463000	0.197478000
C	5.554559000	-0.150660000	0.207262000
C	5.504454000	-1.395616000	-0.412942000
C	1.269297000	3.017391000	-0.824093000
C	0.703812000	4.363015000	-1.136863000
C	-0.595469000	4.346289000	-0.292172000
C	-0.998082000	2.861690000	-0.142797000
N	0.955589000	-1.331502000	0.779308000
H	0.246552000	-0.751321000	-1.650051000
H	2.304043000	-1.312664000	-1.562062000

H	4.297459000	-2.781009000	-1.538597000
H	6.377008000	-2.040214000	-0.403824000
H	6.462658000	0.180160000	0.699445000
H	4.454595000	1.656635000	0.663501000

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C	-0.990616000	-1.625907000	-3.968223000
C	-1.230942000	-0.350651000	-4.473555000
C	-0.925643000	0.792530000	-3.728585000
C	-0.437167000	-1.792064000	-2.692920000
C	2.048002000	-2.508390000	-0.467426000
C	0.983936000	0.986551000	-0.642530000
O	2.237720000	-2.777629000	-1.657833000
C	2.407296000	1.140773000	-1.164586000
C	3.090685000	2.339356000	-0.921130000
C	4.363851000	2.553385000	-1.439535000
C	4.966585000	1.565693000	-2.215052000
C	4.285919000	0.379159000	-2.470256000
C	3.009577000	0.159501000	-1.954477000
O	2.759463000	-3.207794000	0.506464000
C	3.556654000	-4.259027000	-0.004562000
H	-1.225761000	-2.497258000	-4.569992000
H	-1.655107000	-0.236317000	-5.466252000
H	-1.107608000	1.786206000	-4.126480000
H	-0.206159000	-2.774238000	-2.294889000
H	1.239450000	-1.521125000	1.208145000
H	0.365525000	2.462462000	-1.981190000
H	2.623349000	3.118096000	-0.317819000

H	4.880496000	3.486990000	-1.240092000
H	5.961510000	1.723210000	-2.619432000
H	4.747744000	-0.396454000	-3.072632000
H	2.506622000	-0.781688000	-2.158824000
H	4.295238000	-3.886262000	-0.719549000
H	4.056850000	-4.708104000	0.855396000
H	2.946060000	-5.010170000	-0.514393000
N	1.801579000	1.100888000	1.703186000
N	0.256122000	2.239577000	2.781227000
N	-0.012458000	2.174508000	1.435418000
C	0.921566000	1.484578000	0.763620000
C	-2.273536000	2.265898000	0.464737000
C	-3.353381000	3.046864000	0.061119000
H	2.604824000	-0.922878000	3.416017000
H	4.118543000	-0.044923000	3.688996000
H	2.905815000	1.993199000	4.312774000
H	1.736964000	0.788909000	4.880889000
H	3.884898000	1.130462000	1.531123000
H	3.131626000	-0.447469000	1.129014000
C	1.174683000	-1.582036000	0.127373000
C	0.391192000	-0.520625000	-0.544233000
C	-0.129831000	-0.663108000	-1.954600000
C	-0.372570000	0.612331000	-2.469797000
C	-1.149032000	2.920490000	0.948686000
C	-1.076590000	4.304636000	1.052666000
C	-2.164376000	5.067251000	0.641941000
C	-3.301676000	4.436285000	0.144837000
C	1.359553000	1.567138000	2.906772000

C	2.280986000	1.148137000	4.006926000
C	3.105857000	0.042687000	3.295723000
C	3.104664000	0.411333000	1.798933000
N	0.014966000	1.616030000	-1.543939000
H	-0.521719000	-0.347989000	0.057130000
H	-2.324775000	1.179619000	0.401883000
H	-4.244844000	2.557494000	-0.317678000
H	-4.153519000	5.029312000	-0.171687000
H	-2.123107000	6.148592000	0.715437000
H	-0.183087000	4.767446000	1.459076000
C	-1.096031000	-1.214801000	2.824210000
C	-1.340942000	-2.657574000	2.355586000
H	-0.094504000	-0.872250000	2.538813000
H	-1.838272000	-0.545024000	2.377275000
H	-1.176635000	-1.144988000	3.914225000
C	-2.733520000	-3.100574000	2.792717000
C	-0.267841000	-3.603479000	2.895690000
H	-2.936808000	-4.105382000	2.412017000
H	-2.816137000	-3.110267000	3.883584000
H	-3.479044000	-2.410756000	2.385436000
H	-0.225681000	-3.563957000	3.989018000
H	-0.494082000	-4.629325000	2.591974000
H	0.718101000	-3.345566000	2.492605000
O	-1.348434000	-2.731322000	0.928611000
H	-0.430722000	-2.553492000	0.588663000
C	-4.158492000	-2.595085000	-0.875653000
C	-4.142448000	-1.091710000	-0.603975000
H	-3.201367000	-2.910179000	-1.304475000

H	-4.314284000	-3.151236000	0.054003000
H	-4.955878000	-2.853296000	-1.578858000
C	-5.460039000	-0.637993000	0.018581000
C	-3.859416000	-0.325758000	-1.895012000
H	-5.403016000	0.424058000	0.279015000
H	-6.295539000	-0.782826000	-0.672972000
H	-5.658659000	-1.200015000	0.935881000
H	-4.654408000	-0.478494000	-2.632472000
H	-3.776235000	0.746829000	-1.690003000
H	-2.913680000	-0.659844000	-2.327673000
O	-3.122024000	-0.786124000	0.345323000
H	-2.469748000	-1.519942000	0.383153000

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C	-1.103033000	-1.057844000	-4.201876000
C	-1.300788000	0.277696000	-4.541201000
C	-0.957988000	1.307086000	-3.659106000
C	-0.561854000	-1.402661000	-2.957909000
C	2.012860000	-2.353497000	-0.757325000
C	0.921892000	1.030530000	-0.552161000
O	2.081848000	-2.631325000	-1.938764000
C	2.362859000	1.198424000	-1.031662000
C	3.111034000	2.297916000	-0.591024000
C	4.394634000	2.531130000	-1.074621000
C	4.946577000	1.666694000	-2.016834000
C	4.199938000	0.587381000	-2.478409000
C	2.912323000	0.354192000	-1.999783000
O	2.958416000	-2.805585000	0.123028000

C	3.947061000	-3.649434000	-0.456127000
H	-1.368815000	-1.838662000	-4.906288000
H	-1.721071000	0.529902000	-5.509713000
H	-1.108279000	2.348416000	-3.926327000
H	-0.380504000	-2.436556000	-2.684949000
H	1.291268000	-1.395711000	0.964238000
H	0.406283000	2.689124000	-1.713253000
H	2.687006000	2.985172000	0.140841000
H	4.959442000	3.387179000	-0.719048000
H	5.949441000	1.839692000	-2.393681000
H	4.614976000	-0.086723000	-3.220688000
H	2.346360000	-0.486542000	-2.383816000
H	3.485149000	-4.525298000	-0.916743000
H	4.509835000	-3.111458000	-1.223500000
H	4.603474000	-3.949826000	0.360051000
N	1.699834000	0.939218000	1.831723000
N	0.111141000	1.968240000	2.955108000
N	-0.118671000	2.014115000	1.604110000
C	0.837074000	1.388852000	0.904995000
C	-2.401495000	2.115944000	0.690454000
C	-3.495891000	2.905280000	0.342752000
H	2.428169000	-1.233513000	3.374012000
H	3.937103000	-0.401153000	3.792498000
H	2.706813000	1.578603000	4.560857000
H	1.510168000	0.330818000	4.958049000
H	3.787328000	0.996748000	1.760682000
H	3.094902000	-0.537380000	1.170610000
C	0.965265000	-1.613075000	-0.052833000

C	0.269892000	-0.414398000	-0.657910000
C	-0.222139000	-0.387459000	-2.082353000
C	-0.414470000	0.950526000	-2.435472000
C	-1.267622000	2.768849000	1.153156000
C	-1.191653000	4.150224000	1.284553000
C	-2.292942000	4.918215000	0.923892000
C	-3.444958000	4.292554000	0.453825000
C	1.215714000	1.295093000	3.058115000
C	2.092646000	0.771766000	4.148639000
C	2.941702000	-0.266896000	3.369367000
C	3.003492000	0.250139000	1.918359000
N	0.005484000	1.814323000	-1.390417000
H	-0.661257000	-0.313421000	-0.074607000
H	-2.447556000	1.027874000	0.594349000
H	-4.399555000	2.421987000	-0.013666000
H	-4.308859000	4.888730000	0.178546000
H	-2.252100000	5.998033000	1.017807000
H	-0.286877000	4.606755000	1.673263000
C	-1.023384000	-1.449418000	2.794567000
C	-1.197779000	-2.847704000	2.161979000
H	-0.064013000	-1.014824000	2.484757000
H	-1.826233000	-0.788088000	2.450825000
H	-1.039244000	-1.485938000	3.890691000
C	-2.525930000	-3.439845000	2.649829000
C	-0.037151000	-3.757923000	2.590242000
H	-2.674676000	-4.421315000	2.189835000
H	-2.559029000	-3.549740000	3.740126000
H	-3.345892000	-2.785090000	2.336752000

H	0.020805000	-3.863655000	3.680078000
H	-0.173133000	-4.749240000	2.148282000
H	0.918869000	-3.362704000	2.225128000
O	-1.238256000	-2.764850000	0.766696000
H	-0.011815000	-2.347105000	0.242797000
C	-3.709747000	-2.704197000	-1.198071000
C	-3.910916000	-1.288509000	-0.653449000
H	-2.799186000	-2.742573000	-1.803605000
H	-3.589407000	-3.415601000	-0.376095000
H	-4.559650000	-3.006586000	-1.818454000
C	-5.197742000	-1.217661000	0.174918000
C	-3.982808000	-0.291559000	-1.811754000
H	-5.299009000	-0.219154000	0.613784000
H	-6.084335000	-1.423794000	-0.434457000
H	-5.161091000	-1.944664000	0.991870000
H	-4.833550000	-0.504649000	-2.468101000
H	-4.092782000	0.728038000	-1.427447000
H	-3.063813000	-0.331596000	-2.402348000
O	-2.825061000	-0.922970000	0.176159000
H	-2.213783000	-1.736419000	0.396875000

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C	-3.503454000	1.597572000	3.274768000
C	-4.250827000	2.212534000	2.275897000
C	-3.891267000	2.100594000	0.928542000
C	-2.359487000	0.856724000	2.951598000
C	-0.666270000	-2.211892000	2.079585000
C	-1.336822000	-0.080060000	-0.508650000

O	-1.439204000	-2.302111000	3.004466000
C	-2.181539000	-1.326226000	-0.812308000
C	-2.338405000	-1.754436000	-2.137027000
C	-3.202401000	-2.796446000	-2.458661000
C	-3.943540000	-3.419391000	-1.458906000
C	-3.821343000	-2.979380000	-0.144596000
C	-2.953334000	-1.939047000	0.179876000
O	-0.318164000	-3.273108000	1.321789000
C	-0.948111000	-4.500320000	1.684875000
H	-3.810753000	1.686634000	4.311085000
H	-5.136508000	2.781261000	2.540701000
H	-4.480323000	2.574112000	0.149417000
H	-1.785991000	0.348043000	3.720247000
H	0.901771000	-1.165685000	1.023038000
H	-2.885530000	1.017430000	-1.395792000
H	-1.776992000	-1.274261000	-2.936051000
H	-3.298112000	-3.116653000	-3.491241000
H	-4.617497000	-4.233521000	-1.704494000
H	-4.408077000	-3.442195000	0.643018000
H	-2.892690000	-1.605137000	1.209166000
H	-2.029975000	-4.421608000	1.551067000
H	-0.536380000	-5.257256000	1.018926000
H	-0.735779000	-4.744295000	2.727425000
N	0.624349000	-1.028726000	-1.819809000
N	1.355225000	0.712171000	-2.951776000
N	0.284712000	1.035629000	-2.165503000
C	-0.166990000	-0.009569000	-1.462956000
C	0.447732000	3.158110000	-1.041779000

C	0.140301000	4.514344000	-0.974390000
H	2.414146000	-3.688499000	-2.382294000
H	1.106125000	-3.238407000	-3.488579000
H	2.729849000	-1.588220000	-4.183094000
H	3.409025000	-1.458977000	-2.531146000
H	-0.095760000	-2.979332000	-1.409742000
H	1.389081000	-2.472034000	-0.538369000
C	0.027478000	-0.953110000	1.641905000
C	-0.801149000	0.128288000	0.950518000
C	-1.995771000	0.748703000	1.622080000
C	-2.760853000	1.360366000	0.624513000
C	-0.085742000	2.426769000	-2.089736000
C	-0.874950000	2.983993000	-3.084681000
C	-1.170135000	4.340543000	-3.001915000
C	-0.667502000	5.100671000	-1.946536000
C	1.542358000	-0.547998000	-2.707645000
C	2.499866000	-1.609748000	-3.117946000
C	1.739485000	-2.881881000	-2.670461000
C	0.850671000	-2.445512000	-1.486124000
N	-2.202684000	1.107542000	-0.650300000
H	-0.033097000	0.919608000	0.854293000
H	1.079790000	2.633319000	-0.318075000
H	0.537739000	5.110854000	-0.158753000
H	-0.902595000	6.158530000	-1.888000000
H	-1.788948000	4.804994000	-3.762390000
H	-1.245056000	2.368827000	-3.898735000
C	4.444548000	-2.581956000	-0.261929000
C	3.971688000	-1.361509000	0.528917000

H	3.608656000	-3.266444000	-0.446136000
H	4.877518000	-2.284468000	-1.223047000
H	5.211210000	-3.131041000	0.293896000
C	5.141074000	-0.387240000	0.697934000
C	3.439158000	-1.824304000	1.890178000
H	4.802027000	0.509865000	1.220466000
H	5.968363000	-0.833104000	1.260118000
H	5.507169000	-0.082076000	-0.287244000
H	4.231981000	-2.240498000	2.520731000
H	2.979807000	-0.977760000	2.404773000
H	2.670660000	-2.594967000	1.747951000
O	2.936565000	-0.730574000	-0.196855000
H	0.427407000	-0.476606000	2.543716000
C	2.934158000	1.518629000	3.211871000
C	2.279987000	2.151380000	1.966934000
H	2.259332000	0.770396000	3.644227000
H	3.876815000	1.022491000	2.964074000
H	3.142789000	2.269979000	3.982300000
C	3.255920000	3.190865000	1.381151000
C	1.012638000	2.878096000	2.465663000
H	2.787737000	3.728115000	0.548781000
H	3.578561000	3.928628000	2.125218000
H	4.142800000	2.684447000	0.986834000
H	1.243383000	3.649232000	3.209811000
H	0.476028000	3.353598000	1.637922000
H	0.327202000	2.155506000	2.925814000
O	1.928739000	1.208988000	1.009696000
H	2.635384000	0.136396000	0.333742000

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C	-3.385213000	-1.086906000	-3.396175000
C	-4.197770000	-1.648475000	-2.420802000
C	-3.862848000	-1.533576000	-1.062753000
C	-2.203749000	-0.414085000	-3.049616000
C	-0.255646000	2.546867000	-2.029958000
C	-1.130596000	0.414386000	0.427128000
O	-1.035767000	2.829384000	-2.907834000
C	-1.760071000	1.778456000	0.782899000
C	-1.689176000	2.322062000	2.069611000
C	-2.377204000	3.489986000	2.395599000
C	-3.170832000	4.119715000	1.444270000
C	-3.275821000	3.567774000	0.168655000
C	-2.578842000	2.410411000	-0.161576000
O	0.231968000	3.474437000	-1.172434000
C	-0.261030000	4.796317000	-1.377926000
H	-3.670849000	-1.156144000	-4.440941000
H	-5.109659000	-2.164284000	-2.703201000
H	-4.501707000	-1.950070000	-0.289512000
H	-1.598597000	0.063643000	-3.814879000
H	1.243118000	1.229263000	-1.226149000
H	-2.866934000	-0.412267000	1.262109000
H	-1.094072000	1.837462000	2.840833000
H	-2.296902000	3.898730000	3.398103000
H	-3.711626000	5.026281000	1.695760000
H	-3.903463000	4.040067000	-0.580980000
H	-2.672041000	1.994034000	-1.158917000

H	-1.342537000	4.823348000	-1.228497000
H	0.240385000	5.422629000	-0.640538000
H	-0.033337000	5.135191000	-2.390824000
N	1.025619000	0.905540000	1.696623000
N	1.292392000	-0.879435000	2.956393000
N	0.162997000	-0.967984000	2.187620000
C	-0.009509000	0.105464000	1.401818000
C	-0.584960000	-3.092360000	1.287713000
C	-1.332566000	-4.255142000	1.421754000
H	3.435501000	3.049235000	2.096515000
H	2.098582000	3.025416000	3.257607000
H	3.232117000	1.047405000	4.034102000
H	3.842987000	0.661926000	2.404404000
H	0.777313000	2.956182000	1.235869000
H	2.073730000	2.098909000	0.351622000
C	0.282619000	1.167706000	-1.744529000
C	-0.630942000	0.177663000	-1.031523000
C	-1.840883000	-0.324805000	-1.711652000
C	-2.701692000	-0.861107000	-0.737882000
C	-0.623827000	-2.168377000	2.319029000
C	-1.339668000	-2.373051000	3.488665000
C	-2.074908000	-3.549551000	3.613393000
C	-2.076485000	-4.482377000	2.579592000
C	1.797038000	0.266522000	2.622465000
C	3.000212000	1.069083000	2.969324000
C	2.583614000	2.467552000	2.451386000
C	1.573344000	2.216834000	1.310432000
N	-2.174962000	-0.616402000	0.549338000

H	0.258665000	-0.894273000	-1.010335000
H	0.017915000	-2.854896000	0.414299000
H	-1.337352000	-4.984107000	0.617593000
H	-2.657060000	-5.394010000	2.678284000
H	-2.645424000	-3.734807000	4.517301000
H	-1.318984000	-1.628696000	4.278234000
C	5.198973000	-1.003874000	-0.166136000
C	4.313376000	0.140094000	-0.664647000
H	5.296726000	-0.955397000	0.923151000
H	4.746589000	-1.966862000	-0.421009000
H	6.199445000	-0.960095000	-0.608264000
C	4.194174000	0.105117000	-2.187966000
C	4.895165000	1.487088000	-0.238511000
H	3.504541000	0.884062000	-2.529488000
H	5.167102000	0.265314000	-2.662691000
H	3.808874000	-0.861034000	-2.519729000
H	5.887360000	1.636836000	-0.673767000
H	4.245475000	2.302273000	-0.575502000
H	4.994134000	1.545609000	0.850380000
O	3.031996000	0.042523000	-0.062141000
H	0.494800000	0.724952000	-2.724803000
C	1.176928000	-1.875020000	-3.406365000
C	1.215565000	-2.613054000	-2.060813000
H	0.199228000	-1.401543000	-3.542198000
H	1.947172000	-1.099828000	-3.444848000
H	1.334653000	-2.563522000	-4.243480000
C	2.487213000	-3.460213000	-1.957720000
C	-0.003835000	-3.550284000	-2.003138000

H	2.545455000	-3.907188000	-0.960185000
H	2.496778000	-4.262603000	-2.703494000
H	3.381898000	-2.848408000	-2.109531000
H	-0.082502000	-4.138823000	-2.923427000
H	0.083655000	-4.254830000	-1.169084000
H	-0.928503000	-2.972412000	-1.886919000
O	1.206474000	-1.700743000	-0.982827000
H	2.496746000	-0.700557000	-0.465154000

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C	-2.340151000	3.954238000	-0.899586000
C	-2.978385000	3.723414000	0.313348000
C	-2.575139000	2.639413000	1.118019000
C	-1.296075000	3.137683000	-1.349649000
C	2.279605000	1.592719000	-1.828109000
C	0.130457000	0.197791000	0.511358000
O	2.470562000	2.778229000	-1.938045000
C	1.370693000	0.234666000	1.422637000
C	1.591428000	-0.769012000	2.369719000
C	2.663088000	-0.686942000	3.255438000
C	3.517802000	0.412022000	3.207394000
C	3.284743000	1.428713000	2.283548000
C	2.214755000	1.343497000	1.396144000
O	3.273057000	0.733564000	-1.473929000
C	4.520992000	1.354745000	-1.179395000
H	-2.646744000	4.798180000	-1.511363000
H	-3.780784000	4.372824000	0.645764000
H	-3.072750000	2.425610000	2.060170000

H	-0.780877000	3.367930000	-2.277504000
H	1.122362000	-0.160863000	-2.241580000
H	-0.901157000	0.684931000	2.266138000
H	0.920917000	-1.627340000	2.409334000
H	2.827478000	-1.474327000	3.984705000
H	4.354270000	0.480912000	3.895544000
H	3.936437000	2.297128000	2.258465000
H	2.009018000	2.142053000	0.686353000
H	4.394212000	2.114563000	-0.405172000
H	5.178896000	0.560551000	-0.827325000
H	4.932919000	1.829750000	-2.072745000
N	0.850646000	-2.043665000	-0.490575000
N	-1.053618000	-3.086942000	-0.874564000
N	-1.261334000	-1.882418000	-0.239994000
C	-0.105251000	-1.220557000	0.004906000
C	-3.127504000	-0.351406000	-0.637154000
C	-4.464947000	-0.023634000	-0.442369000
H	3.412071000	-3.778115000	-1.509349000
H	2.660874000	-4.171784000	0.041184000
H	0.981761000	-5.139628000	-1.376373000
H	1.275112000	-3.968043000	-2.671507000
H	2.772224000	-1.816770000	0.370974000
H	2.677659000	-1.452776000	-1.356349000
C	0.945492000	0.887720000	-1.961573000
C	0.101955000	1.045426000	-0.735428000
C	-0.878950000	2.056153000	-0.559897000
C	-1.545503000	1.844177000	0.673954000
C	-2.625753000	-1.491331000	-0.022425000

C	-3.432573000	-2.333307000	0.735684000
C	-4.771694000	-2.003625000	0.906234000
C	-5.285780000	-0.845026000	0.326086000
C	0.230151000	-3.147307000	-1.010983000
C	1.226996000	-4.098472000	-1.585731000
C	2.526829000	-3.619957000	-0.892850000
C	2.320026000	-2.121327000	-0.572625000
N	-1.043891000	0.657277000	1.264437000
H	-2.474984000	0.275404000	-1.234648000
H	-4.852953000	0.887344000	-0.885437000
H	-6.328363000	-0.583560000	0.474762000
H	-5.411652000	-2.648016000	1.499792000
H	-3.008393000	-3.228510000	1.177615000
H	0.427035000	1.365576000	-2.800957000

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C	-2.940904000	2.636794000	-1.942923000
C	-3.547215000	2.741559000	-0.691142000
C	-2.886135000	2.274618000	0.451954000
C	-1.672253000	2.077009000	-2.092121000
C	2.589248000	1.316606000	-1.746758000
C	0.284326000	0.460478000	0.616132000
O	2.819822000	2.495708000	-1.842173000
C	1.525100000	0.472802000	1.485690000
C	1.688658000	-0.468760000	2.503219000
C	2.781585000	-0.401287000	3.362950000
C	3.717865000	0.619269000	3.216672000
C	3.546464000	1.576066000	2.218647000

C	2.452005000	1.508911000	1.359480000
O	3.561904000	0.413341000	-1.476809000
C	4.854823000	0.975864000	-1.261751000
H	-3.467560000	2.995832000	-2.822355000
H	-4.538495000	3.173066000	-0.600703000
H	-3.355823000	2.312087000	1.430465000
H	-1.219923000	2.015298000	-3.078104000
H	1.370773000	-0.414818000	-2.044893000
H	-0.573544000	1.665661000	2.084981000
H	0.947303000	-1.257532000	2.615373000
H	2.898432000	-1.139604000	4.150127000
H	4.571478000	0.674602000	3.884794000
H	4.263326000	2.384909000	2.112664000
H	2.299820000	2.263465000	0.592149000
H	4.836281000	1.638601000	-0.393173000
H	5.523697000	0.135115000	-1.083224000
H	5.172796000	1.546745000	-2.136129000
N	0.731289000	-1.928375000	-0.330308000
N	-1.257023000	-2.478551000	-1.123675000
N	-1.349222000	-1.492428000	-0.151401000
C	-0.127055000	-1.070310000	0.293658000
C	-3.681082000	-0.976428000	-0.573931000
C	-4.947318000	-0.658454000	-0.098069000
H	3.103773000	-3.703648000	-1.629767000
H	2.135006000	-4.454994000	-0.359826000
H	0.501189000	-4.613665000	-2.098847000
H	1.126222000	-3.183302000	-2.936917000
H	2.439690000	-2.423688000	0.797957000

H	2.767765000	-1.495711000	-0.676149000
C	1.224666000	0.664701000	-1.879433000
C	0.285151000	0.992960000	-0.764186000
C	-0.990492000	1.609587000	-0.960168000
C	-1.632675000	1.721244000	0.296079000
C	-2.640853000	-1.152160000	0.334449000
C	-2.853480000	-1.032923000	1.706476000
C	-4.120286000	-0.697947000	2.166716000
C	-5.170212000	-0.511847000	1.268844000
C	0.011176000	-2.711740000	-1.191555000
C	0.920474000	-3.618124000	-1.953000000
C	2.183572000	-3.611097000	-1.052229000
C	2.148635000	-2.285808000	-0.245730000
N	-0.834575000	1.103020000	1.285019000
H	-3.478960000	-1.067060000	-1.635101000
H	-5.757779000	-0.506640000	-0.803108000
H	-6.158479000	-0.253270000	1.634501000
H	-4.291277000	-0.593833000	3.233474000
H	-2.023436000	-1.179851000	2.388669000
H	0.797906000	1.074691000	-2.800269000

6) Cartesian coordinates of the optimized species in pathway B-b

B-TSb1-Si

C	3.270824000	-2.419964000	-1.692000000
C	2.198724000	-3.273527000	-1.939534000
C	0.904761000	-2.768499000	-1.957270000

C	0.679284000	-1.410431000	-1.719566000
C	1.758907000	-0.537711000	-1.468083000
C	3.050212000	-1.063961000	-1.469961000
C	1.490206000	0.924875000	-1.303084000
N	-0.614617000	-0.853841000	-1.715065000
C	2.439103000	1.920864000	-1.076666000
C	3.416378000	1.810542000	-0.040863000
C	-1.554774000	-1.471639000	-1.118825000
O	3.575550000	0.869844000	0.734356000
C	-2.879541000	-0.851768000	-0.943225000
C	-3.165580000	0.399793000	-1.503214000
C	-4.394645000	1.001744000	-1.267823000
C	-5.343919000	0.370537000	-0.460788000
C	-5.063186000	-0.871477000	0.100249000
C	-3.836115000	-1.481987000	-0.144746000
O	4.190108000	2.931628000	0.066565000
C	5.149811000	2.889683000	1.108632000
H	4.284807000	-2.806551000	-1.686611000
H	2.370105000	-4.327910000	-2.132125000
H	0.061078000	-3.412912000	-2.185981000
H	3.882744000	-0.399071000	-1.277856000
H	2.273383000	2.908696000	-1.489859000
H	0.691357000	1.219836000	-1.987556000
H	-1.394166000	-2.439486000	-0.623524000
H	-2.409531000	0.871561000	-2.124863000
H	-4.625741000	1.960896000	-1.722842000
H	-6.303178000	0.844668000	-0.278617000
H	-5.799367000	-1.364998000	0.726183000
H	-3.608756000	-2.451532000	0.292160000
H	5.859010000	2.071163000	0.958018000
H	5.669658000	3.847716000	1.078650000
H	4.670336000	2.748015000	2.080911000
C	-2.157220000	3.734816000	-0.093001000
C	-2.525319000	3.042608000	1.248368000
C	-1.621577000	1.853925000	1.228049000
N	-0.659397000	1.984831000	0.264334000
C	-0.737801000	3.242420000	-0.469084000
N	-1.488846000	0.738587000	1.872289000
N	-0.385100000	0.174094000	1.259167000
C	0.140542000	0.899234000	0.251545000
C	0.037739000	-1.132384000	1.636758000
C	1.380843000	-1.471289000	1.497880000
C	1.763714000	-2.780904000	1.772902000
C	0.829371000	-3.717478000	2.207752000
C	-0.502247000	-3.344765000	2.381392000

C	-0.909911000	-2.046700000	2.091815000
H	-2.205037000	4.822184000	-0.028263000
H	-2.859755000	3.408519000	-0.863199000
H	-3.576599000	2.753808000	1.295981000
H	-2.299888000	3.675083000	2.112128000
H	-0.615949000	3.075085000	-1.540786000
H	0.055949000	3.912041000	-0.127325000
H	2.104747000	-0.720358000	1.187174000
H	2.804989000	-3.060349000	1.651653000
H	1.139162000	-4.734666000	2.424781000
H	-1.228932000	-4.067509000	2.738603000
H	-1.941468000	-1.730755000	2.205056000

B-TSb1-Re

C	3.416217000	-1.513251000	2.257650000
C	2.616679000	-2.653582000	2.275132000
C	1.271945000	-2.558690000	1.944260000
C	0.718990000	-1.323133000	1.606874000
C	1.523297000	-0.165748000	1.547635000
C	2.869504000	-0.286898000	1.899813000
C	0.926192000	1.159178000	1.185213000
N	-0.630470000	-1.289325000	1.192256000
C	1.605428000	2.364336000	1.024125000
C	2.817602000	2.492849000	0.274843000
C	-1.528218000	-0.775309000	1.926945000
O	3.441251000	1.607451000	-0.303601000
C	-2.912387000	-0.624328000	1.429539000
C	-3.259091000	-1.090853000	0.154552000
C	-4.554051000	-0.924969000	-0.318194000
C	-5.513149000	-0.285315000	0.471460000
C	-5.170191000	0.191154000	1.734185000
C	-3.872001000	0.020818000	2.211842000
O	3.246305000	3.788672000	0.214910000
C	4.423183000	3.983871000	-0.551198000
H	4.467310000	-1.577417000	2.519058000
H	3.038614000	-3.617363000	2.542415000
H	0.631929000	-3.434653000	1.932261000
H	3.491405000	0.598316000	1.870207000
H	1.082780000	3.285942000	1.250714000
H	-0.042346000	1.295988000	1.669656000
H	-1.315594000	-0.385193000	2.933946000
H	-2.493082000	-1.576843000	-0.443909000
H	-4.821325000	-1.297860000	-1.302391000
H	-6.525589000	-0.159959000	0.100740000
H	-5.912863000	0.689374000	2.348778000

H	-3.600541000	0.384666000	3.199968000
H	4.622611000	5.055521000	-0.530526000
H	5.266302000	3.434859000	-0.122881000
H	4.283818000	3.641890000	-1.580158000
C	-3.208913000	2.460721000	-0.868042000
C	-2.983339000	1.760750000	-2.236064000
C	-1.756466000	0.956168000	-1.955269000
N	-1.142003000	1.390448000	-0.812655000
C	-1.828677000	2.504615000	-0.169785000
N	-1.119479000	-0.045991000	-2.474584000
N	-0.065344000	-0.216484000	-1.594431000
C	-0.057737000	0.632898000	-0.551637000
C	0.815967000	-1.328134000	-1.748220000
C	0.307146000	-2.534434000	-2.219402000
C	1.156323000	-3.632001000	-2.305019000
C	2.487860000	-3.521169000	-1.910482000
C	2.977861000	-2.302220000	-1.448538000
C	2.148920000	-1.186822000	-1.375595000
H	-3.886790000	1.852395000	-0.262726000
H	-3.641789000	3.455791000	-0.975403000
H	-2.791317000	2.479456000	-3.038670000
H	-3.828533000	1.135865000	-2.528395000
H	-1.275986000	3.430230000	-0.353098000
H	-1.903723000	2.341993000	0.907556000
H	-0.735657000	-2.598606000	-2.509229000
H	0.772161000	-4.578623000	-2.670928000
H	3.143275000	-4.384302000	-1.967557000
H	4.014907000	-2.206507000	-1.144530000
H	2.527279000	-0.227484000	-1.029208000

B-1b-Si

C	3.064206000	-2.940133000	-2.031610000
C	1.960419000	-3.761851000	-2.239018000
C	0.677937000	-3.267446000	-2.025030000
C	0.500060000	-1.944708000	-1.606575000
C	1.611028000	-1.100398000	-1.431927000
C	2.885394000	-1.617078000	-1.631212000
C	1.409943000	0.362058000	-1.005649000
N	-0.777333000	-1.403959000	-1.343859000
C	2.629126000	1.215514000	-0.829050000
C	3.466999000	1.019130000	0.261576000
C	-1.614909000	-2.103122000	-0.685393000
O	3.328739000	0.191734000	1.189979000
C	-2.954727000	-1.605649000	-0.339537000
C	-3.387114000	-0.345728000	-0.769503000

C	-4.646770000	0.112878000	-0.409978000
C	-5.484218000	-0.677467000	0.379772000
C	-5.058425000	-1.931186000	0.809564000
C	-3.796609000	-2.393332000	0.449751000
O	4.560526000	1.863957000	0.276068000
C	5.421693000	1.686867000	1.380457000
H	4.066123000	-3.326031000	-2.189183000
H	2.093710000	-4.785593000	-2.574286000
H	-0.193924000	-3.887000000	-2.215202000
H	3.727399000	-0.951262000	-1.469703000
H	2.888486000	1.925589000	-1.601643000
H	0.765274000	0.818995000	-1.769884000
H	-1.359850000	-3.109271000	-0.315648000
H	-2.719097000	0.256404000	-1.378503000
H	-4.979288000	1.090484000	-0.746358000
H	-6.468275000	-0.314641000	0.658762000
H	-5.707794000	-2.547099000	1.422934000
H	-3.458116000	-3.372184000	0.780856000
H	6.223683000	2.417321000	1.259072000
H	4.901918000	1.858512000	2.328182000
H	5.839911000	0.675692000	1.408019000
N	0.594831000	-0.501063000	1.241854000
N	-0.942995000	0.961069000	1.824879000
N	-0.368129000	1.280095000	0.619464000
C	0.576709000	0.390834000	0.244947000
C	-0.330280000	-0.127585000	2.170550000
C	1.293449000	-1.743997000	1.585959000
H	0.834191000	-2.567730000	1.027402000
H	2.346948000	-1.630830000	1.334937000
C	-0.850182000	2.431556000	-0.075760000
C	0.023127000	3.229374000	-0.807284000
C	-2.205585000	2.740025000	0.035537000
C	-0.490771000	4.338722000	-1.474673000
H	1.083888000	2.990052000	-0.818933000
C	-2.696705000	3.855080000	-0.630838000
H	-2.846066000	2.109706000	0.641564000
C	-1.843837000	4.650921000	-1.394610000
H	0.180615000	4.967710000	-2.049593000
H	-3.750162000	4.103614000	-0.551913000
H	-2.233821000	5.518657000	-1.916431000
C	1.010542000	-1.809866000	3.100926000
H	1.008075000	-2.834333000	3.473985000
H	1.796790000	-1.250066000	3.613615000
C	-0.348352000	-1.093118000	3.310575000
H	-0.437129000	-0.598352000	4.277799000

H -1.195122000 -1.778650000 3.193606000

B-1b-Re

C -1.353784000 -3.697582000 -1.521659000
C -0.056077000 -4.098212000 -1.220231000
C 0.929248000 -3.142383000 -0.992426000
C 0.615685000 -1.782503000 -1.064225000
C -0.707240000 -1.375750000 -1.310061000
C -1.672125000 -2.341349000 -1.564300000
C -1.069137000 0.112610000 -1.348564000
N 1.562736000 -0.774451000 -0.788705000
C -2.444073000 0.484471000 -1.817604000
C -3.453631000 0.551288000 -0.873676000
C 2.767064000 -0.901492000 -1.179927000
O -3.330498000 0.410000000 0.369743000
C 3.797038000 0.093125000 -0.838300000
C 3.498194000 1.183331000 -0.010800000
C 4.484909000 2.106369000 0.303855000
C 5.777174000 1.953554000 -0.202502000
C 6.079725000 0.872190000 -1.024525000
C 5.091817000 -0.055602000 -1.339425000
O -4.699603000 0.861310000 -1.390566000
C -5.735201000 0.899619000 -0.431251000
H -2.123946000 -4.440237000 -1.704365000
H 0.191597000 -5.153028000 -1.153711000
H 1.934722000 -3.443366000 -0.712552000
H -2.679418000 -1.998625000 -1.781217000
H -2.639232000 0.596910000 -2.873900000
H -0.327405000 0.581442000 -2.015626000
H 3.093815000 -1.754602000 -1.792342000
H 2.486415000 1.282574000 0.373402000
H 4.252419000 2.948582000 0.947850000
H 6.546480000 2.677736000 0.046130000
H 7.083074000 0.751139000 -1.419369000
H 5.322827000 -0.903392000 -1.979442000
H -6.644881000 1.156322000 -0.977534000
H -5.860300000 -0.067720000 0.065257000
H -5.541244000 1.647063000 0.344329000
N -0.920247000 2.172822000 0.035777000
N -0.298637000 1.526595000 2.041735000
N -0.425623000 0.465056000 1.175864000
C -0.824587000 0.836834000 -0.047601000
C -0.621510000 2.546634000 1.310000000
C -1.433088000 3.261668000 -0.792025000
H -2.518039000 3.154722000 -0.862048000

H	-1.014322000	3.216945000	-1.797351000
C	-0.269118000	-0.856696000	1.703545000
C	-1.356062000	-1.720607000	1.665721000
C	0.957916000	-1.217261000	2.246773000
C	-1.183144000	-3.010046000	2.161774000
H	-2.295459000	-1.360742000	1.249834000
C	1.107513000	-2.504153000	2.750204000
H	1.774693000	-0.502932000	2.250705000
C	0.041311000	-3.400820000	2.698310000
H	-2.011693000	-3.709503000	2.127944000
H	2.058090000	-2.810027000	3.174524000
H	0.165933000	-4.408027000	3.083144000
C	-0.965131000	4.492276000	0.022218000
H	0.014272000	4.814835000	-0.340289000
H	-1.656768000	5.328168000	-0.083865000
C	-0.837954000	4.014406000	1.493033000
H	-0.026868000	4.500896000	2.035347000
H	-1.765960000	4.170724000	2.051037000

B-11b

C	-1.439234000	1.019547000	-3.802113000
C	-0.435350000	0.293206000	-4.435419000
C	0.583721000	-0.278987000	-3.681830000
C	0.587226000	-0.137780000	-2.290985000
C	-0.448454000	0.563173000	-1.641642000
C	-1.441479000	1.154626000	-2.415109000
C	-0.500139000	0.569965000	-0.118523000
N	1.601056000	-0.693415000	-1.476223000
C	-1.549894000	1.405977000	0.572635000
C	-1.529849000	2.806902000	0.424887000
C	2.814592000	-0.623619000	-1.860262000
O	-0.867031000	3.477285000	-0.381038000
C	3.935732000	-1.080833000	-1.026661000
C	3.720636000	-1.589308000	0.260189000
C	4.799988000	-1.962726000	1.047988000
C	6.101382000	-1.839543000	0.558620000
C	6.321930000	-1.338072000	-0.721282000
C	5.241321000	-0.955764000	-1.509826000
O	-2.404679000	3.445419000	1.276558000
C	-2.487692000	4.845952000	1.094334000
H	-2.233355000	1.473440000	-4.385620000
H	-0.447590000	0.163610000	-5.512830000
H	1.354618000	-0.877247000	-4.158808000
H	-2.227490000	1.707438000	-1.914149000
H	-1.903486000	1.020022000	1.524162000

H	-0.696176000	-0.472589000	0.144061000
H	3.085358000	-0.163204000	-2.823567000
H	2.703204000	-1.680749000	0.626745000
H	4.628627000	-2.349059000	2.047304000
H	6.943379000	-2.133329000	1.177179000
H	7.332877000	-1.242908000	-1.103709000
H	5.406001000	-0.558233000	-2.508427000
H	-3.205237000	5.205661000	1.832864000
H	-1.516499000	5.325002000	1.248621000
H	-2.829848000	5.095669000	0.085828000
N	1.664381000	1.890401000	0.042779000
N	2.504694000	1.201249000	1.961979000
N	1.354463000	0.523302000	1.631418000
C	0.819279000	0.942242000	0.468107000
C	2.664713000	2.014833000	0.965285000
C	1.856951000	2.728042000	-1.145089000
H	2.296821000	2.109429000	-1.936436000
H	0.897617000	3.140584000	-1.453222000
C	0.817239000	-0.444940000	2.533387000
C	0.317593000	-1.648013000	2.043591000
C	0.799866000	-0.146415000	3.893382000
C	-0.258538000	-2.547032000	2.935839000
H	0.351168000	-1.881421000	0.984552000
C	0.254619000	-1.071574000	4.775108000
H	1.206214000	0.797793000	4.237595000
C	-0.286184000	-2.264989000	4.297797000
H	-0.689748000	-3.462819000	2.546576000
H	0.235477000	-0.850395000	5.836961000
H	-0.730743000	-2.971985000	4.990391000
C	2.849454000	3.769745000	-0.586777000
H	3.485272000	4.189407000	-1.366679000
H	2.272144000	4.579315000	-0.132656000
C	3.660323000	3.034164000	0.513511000
H	3.992522000	3.686949000	1.320916000
H	4.536230000	2.522613000	0.099392000
C	-2.921428000	-4.329301000	-0.718269000
C	-1.931313000	-3.220713000	-1.081060000
H	-2.644144000	-4.777215000	0.240694000
H	-3.930020000	-3.913891000	-0.621811000
H	-2.944070000	-5.114603000	-1.480654000
C	-2.334082000	-2.548990000	-2.393903000
C	-0.512416000	-3.773344000	-1.171451000
H	-1.614994000	-1.768342000	-2.659170000
H	-2.372592000	-3.281041000	-3.206820000
H	-3.318074000	-2.079232000	-2.295174000

H	-0.432747000	-4.539428000	-1.948520000
H	0.186750000	-2.961392000	-1.400348000
H	-0.221897000	-4.220864000	-0.214307000
C	-4.489180000	-0.765801000	1.717624000
C	-4.826579000	-0.148989000	0.357445000
H	-4.099590000	-1.780371000	1.584513000
H	-3.724844000	-0.172607000	2.228816000
H	-5.374779000	-0.808876000	2.359677000
C	-5.276711000	1.303399000	0.515098000
C	-5.892035000	-0.977041000	-0.351487000
H	-5.505239000	1.729099000	-0.466788000
H	-6.172656000	1.368136000	1.140729000
H	-4.484067000	1.904869000	0.974275000
H	-6.821052000	-0.997498000	0.225900000
H	-6.095915000	-0.554561000	-1.339114000
H	-5.541859000	-2.006243000	-0.482732000
O	-1.909630000	-2.265827000	-0.024346000
H	-2.626505000	-1.612784000	-0.178553000
O	-3.676819000	-0.193130000	-0.489512000
H	-3.032008000	0.505140000	-0.179442000

B-TSb2

C	1.506484000	-1.357548000	-3.664461000
C	0.471907000	-0.768895000	-4.385348000
C	-0.577413000	-0.155402000	-3.711229000
C	-0.589506000	-0.132996000	-2.313391000
C	0.457517000	-0.725855000	-1.579406000
C	1.500092000	-1.334832000	-2.271845000
C	0.474777000	-0.559365000	-0.067976000
N	-1.610962000	0.498935000	-1.570562000
C	1.607592000	-1.239908000	0.703064000
C	1.562491000	-2.707151000	0.728180000
C	-2.822894000	0.434983000	-1.958826000
O	0.864216000	-3.431749000	0.034227000
C	-3.925361000	0.993464000	-1.161417000
C	-3.673128000	1.680582000	0.032929000
C	-4.729976000	2.140453000	0.804713000
C	-6.045875000	1.926051000	0.391185000
C	-6.303392000	1.250102000	-0.798292000
C	-5.244855000	0.783729000	-1.571858000
O	2.440404000	-3.222504000	1.614787000
C	2.526242000	-4.641917000	1.630489000
H	2.339246000	-1.817257000	-4.185905000
H	0.493079000	-0.763627000	-5.470260000
H	-1.361044000	0.358588000	-4.259945000

H	2.342736000	-1.734480000	-1.720719000
H	1.679390000	-0.843431000	1.720921000
H	0.656661000	0.512766000	0.064237000
H	-3.108320000	-0.094649000	-2.881449000
H	-2.643844000	1.842581000	0.338690000
H	-4.529813000	2.666413000	1.732321000
H	-6.870189000	2.287672000	0.997528000
H	-7.325890000	1.086998000	-1.122844000
H	-5.438583000	0.254084000	-2.501618000
H	3.271883000	-4.886881000	2.385507000
H	1.561268000	-5.086360000	1.887185000
H	2.834807000	-5.020505000	0.653359000
N	-1.718223000	-1.830600000	0.186899000
N	-2.570442000	-0.920817000	2.004527000
N	-1.374221000	-0.344693000	1.656410000
C	-0.841930000	-0.883626000	0.545887000
C	-2.752910000	-1.810282000	1.078199000
C	-1.914196000	-2.779690000	-0.913497000
H	-2.265248000	-2.224076000	-1.789905000
H	-0.973716000	-3.281451000	-1.133143000
C	-0.804429000	0.666209000	2.498508000
C	-0.251847000	1.811859000	1.937169000
C	-0.807419000	0.448935000	3.874126000
C	0.361352000	2.736181000	2.777714000
H	-0.258255000	1.983667000	0.866618000
C	-0.225350000	1.400907000	4.701387000
H	-1.256351000	-0.453680000	4.273120000
C	0.370688000	2.536846000	4.154073000
H	0.840405000	3.601856000	2.333904000
H	-0.219692000	1.244655000	5.774746000
H	0.847762000	3.262403000	4.804485000
C	-3.005938000	-3.689628000	-0.308513000
H	-3.640283000	-4.129052000	-1.078484000
H	-2.519780000	-4.499088000	0.241836000
C	-3.801024000	-2.797891000	0.680827000
H	-4.211367000	-3.345605000	1.529233000
H	-4.619382000	-2.266615000	0.182416000
C	2.990914000	4.088862000	-0.949621000
C	1.966922000	2.988445000	-1.247724000
H	2.749318000	4.570074000	0.003619000
H	3.991682000	3.654134000	-0.864926000
H	3.009507000	4.852042000	-1.735148000
C	2.326104000	2.269186000	-2.551571000
C	0.565468000	3.591100000	-1.346123000
H	1.548024000	1.544177000	-2.810930000

H	2.426587000	2.982115000	-3.376927000
H	3.263084000	1.717887000	-2.428423000
H	0.495870000	4.321496000	-2.158718000
H	-0.167550000	2.795365000	-1.526192000
H	0.306435000	4.096323000	-0.407842000
C	4.597393000	0.970052000	1.514049000
C	4.751696000	0.192519000	0.196750000
H	4.188430000	1.965197000	1.310281000
H	3.894578000	0.450254000	2.175209000
H	5.551178000	1.077599000	2.043260000
C	5.257001000	-1.227669000	0.491739000
C	5.761870000	0.909798000	-0.707342000
H	5.338425000	-1.786733000	-0.446755000
H	6.238652000	-1.220107000	0.979400000
H	4.551580000	-1.755716000	1.142999000
H	6.755218000	0.975327000	-0.248361000
H	5.844729000	0.372767000	-1.657328000
H	5.412851000	1.925309000	-0.922941000
O	1.941888000	2.078214000	-0.165820000
H	2.660552000	1.344657000	-0.299676000
O	3.524768000	0.119672000	-0.473308000
H	2.627692000	-0.751590000	0.172282000

B-2b

C	-1.782988000	4.279328000	-1.414855000
C	-0.484135000	4.597513000	-1.817987000
C	0.508192000	3.632014000	-1.738292000
C	0.220185000	2.343878000	-1.267825000
C	-1.094374000	2.006496000	-0.848244000
C	-2.077490000	3.011097000	-0.939008000
C	-1.424554000	0.651722000	-0.405373000
N	1.188043000	1.325453000	-1.237953000
C	-2.745347000	0.035250000	-0.827560000
C	-3.566989000	-0.237691000	0.407688000
C	2.372034000	1.572231000	-0.840849000
O	-3.535475000	-1.254473000	1.058137000
C	3.353647000	0.500400000	-0.611190000
C	2.959584000	-0.843867000	-0.639339000
C	3.867269000	-1.841805000	-0.312394000
C	5.178260000	-1.511491000	0.034313000
C	5.577886000	-0.177438000	0.060288000
C	4.665567000	0.825088000	-0.253477000
O	-4.305348000	0.835732000	0.764200000
C	-5.021862000	0.684727000	1.986534000
H	-2.567363000	5.027816000	-1.471986000

H	-0.253740000	5.584468000	-2.205365000
H	1.511575000	3.845356000	-2.096569000
H	-3.084262000	2.778671000	-0.601704000
H	-3.274717000	0.735833000	-1.475542000
H	-2.635123000	-0.911401000	-1.365393000
H	2.692344000	2.588576000	-0.558641000
H	1.931891000	-1.084791000	-0.896245000
H	3.547380000	-2.878720000	-0.316284000
H	5.885198000	-2.294326000	0.290465000
H	6.596567000	0.081163000	0.330929000
H	4.967535000	1.869256000	-0.220937000
H	-5.548171000	1.624834000	2.144780000
H	-5.729115000	-0.144694000	1.916782000
H	-4.332831000	0.485709000	2.810678000
N	0.360352000	0.465809000	1.292933000
N	0.518519000	-1.725676000	1.593613000
N	-0.407200000	-1.415832000	0.591217000
C	-0.548354000	-0.052584000	0.393830000
C	0.945642000	-0.570747000	1.966961000
C	0.560625000	1.763450000	1.906141000
H	1.148452000	2.419020000	1.255543000
H	-0.405607000	2.245067000	2.084792000
C	-0.767310000	-2.444711000	-0.311371000
C	-1.212986000	-3.663147000	0.194942000
C	-0.626520000	-2.247433000	-1.685245000
C	-1.518843000	-4.693300000	-0.685742000
H	-1.315795000	-3.779198000	1.267758000
C	-0.953546000	-3.281946000	-2.556902000
H	-0.271721000	-1.285314000	-2.048503000
C	-1.395625000	-4.505835000	-2.061436000
H	-1.869541000	-5.643561000	-0.296417000
H	-0.850180000	-3.131387000	-3.626706000
H	-1.646262000	-5.310726000	-2.744549000
C	1.305842000	1.387360000	3.215755000
H	2.071315000	2.120883000	3.472158000
H	0.587481000	1.348814000	4.038536000
C	1.893381000	-0.030045000	2.986376000
H	2.897706000	0.014069000	2.548717000
H	1.932413000	-0.634855000	3.891896000

B-TSb3

C	4.015555000	2.389623000	-0.583612000
C	4.765516000	1.392571000	-1.210078000
C	4.176501000	0.210211000	-1.644233000
C	2.800968000	0.001429000	-1.455474000

C	2.031072000	1.039247000	-0.840708000
C	2.642690000	2.201602000	-0.391212000
C	0.603600000	0.627458000	-0.591635000
N	2.140484000	-1.177612000	-1.662790000
C	-0.501412000	1.468266000	-1.181197000
C	-0.830691000	2.727525000	-0.410310000
C	0.839362000	-0.891415000	-1.845446000
O	-0.295783000	3.105131000	0.606289000
C	-0.175084000	-1.962843000	-1.652750000
C	0.016822000	-2.959191000	-0.689556000
C	-0.927377000	-3.966089000	-0.520584000
C	-2.069698000	-3.998323000	-1.323535000
C	-2.266577000	-3.012327000	-2.287711000
C	-1.327228000	-1.995107000	-2.442341000
O	-1.833144000	3.398568000	-0.998373000
C	-2.229912000	4.594324000	-0.331711000
H	4.492157000	3.305272000	-0.249500000
H	5.831157000	1.541837000	-1.363193000
H	4.761989000	-0.567879000	-2.123008000
H	2.051655000	2.952803000	0.124926000
H	-0.192019000	1.783789000	-2.184390000
H	-1.438844000	0.912424000	-1.313971000
H	0.562220000	-0.217851000	-2.678398000
H	0.935052000	-2.937198000	-0.107942000
H	-0.772419000	-4.735245000	0.229662000
H	-2.800263000	-4.791182000	-1.197757000
H	-3.149155000	-3.036223000	-2.919485000
H	-1.473128000	-1.226467000	-3.197462000
H	-2.556777000	4.370971000	0.687195000
H	-1.398600000	5.300918000	-0.284837000
H	-3.051644000	5.004725000	-0.916107000
N	1.391960000	-0.582443000	1.430333000
N	-0.495230000	-1.127252000	2.452241000
N	-0.725463000	-0.324608000	1.355657000
C	0.415900000	0.019465000	0.689618000
C	0.789109000	-1.259525000	2.456616000
C	2.863922000	-0.720885000	1.457380000
H	3.156952000	-1.435145000	0.684878000
H	3.348737000	0.236100000	1.266199000
C	-2.080792000	0.030226000	1.062392000
C	-2.866182000	-0.873713000	0.356815000
C	-2.592915000	1.239952000	1.521388000
C	-4.180685000	-0.531314000	0.055845000
H	-2.440930000	-1.822624000	0.048466000
C	-3.908764000	1.572462000	1.211475000

H	-1.955708000	1.908939000	2.089406000
C	-4.697681000	0.693272000	0.472879000
H	-4.796501000	-1.223950000	-0.508642000
H	-4.320083000	2.516023000	1.555452000
H	-5.721542000	0.959215000	0.230611000
C	3.091927000	-1.238112000	2.893743000
H	3.977305000	-1.871778000	2.953309000
H	3.235475000	-0.387640000	3.565452000
C	1.796216000	-1.983673000	3.287465000
H	1.828499000	-3.035423000	2.983524000
H	1.570592000	-1.941300000	4.353066000

B-3b

C	4.092531000	2.051663000	-0.792234000
C	4.813017000	0.928005000	-1.228167000
C	4.193349000	-0.264232000	-1.563054000
C	2.780987000	-0.375554000	-1.467653000
C	2.060513000	0.795200000	-1.056026000
C	2.698866000	1.971417000	-0.698369000
C	0.616410000	0.357729000	-0.851710000
N	2.046360000	-1.482398000	-1.637466000
C	-0.460702000	1.280958000	-1.409999000
C	-0.667301000	2.560629000	-0.639809000
C	0.702505000	-1.001642000	-1.737964000
O	-0.111979000	2.866613000	0.391586000
C	-0.358575000	-2.036307000	-1.460486000
C	-0.196364000	-2.968616000	-0.430981000
C	-1.172662000	-3.929614000	-0.184789000
C	-2.319442000	-3.985507000	-0.979564000
C	-2.480461000	-3.075315000	-2.021037000
C	-1.505582000	-2.106867000	-2.254031000
O	-1.581724000	3.336103000	-1.235157000
C	-1.865367000	4.563450000	-0.565397000
H	4.607410000	2.972876000	-0.543949000
H	5.895977000	0.995975000	-1.306084000
H	4.766628000	-1.126832000	-1.887285000
H	2.129723000	2.817479000	-0.324898000
H	-0.163301000	1.552059000	-2.427557000
H	-1.435495000	0.782958000	-1.493732000
H	0.496276000	-0.595510000	-2.752217000
H	0.730327000	-2.945610000	0.137427000
H	-1.034946000	-4.650439000	0.615383000
H	-3.073202000	-4.744710000	-0.795909000
H	-3.359912000	-3.122967000	-2.656136000
H	-1.622978000	-1.404810000	-3.076223000

H	-2.293319000	4.365872000	0.421009000
H	-0.954067000	5.152183000	-0.444002000
H	-2.583127000	5.087085000	-1.194037000
N	1.386331000	-0.434697000	1.433435000
N	-0.481025000	-0.588236000	2.597388000
N	-0.706325000	-0.100219000	1.338111000
C	0.420074000	-0.000013000	0.599970000
C	0.798964000	-0.790348000	2.613844000
C	2.848979000	-0.676442000	1.440186000
H	3.038714000	-1.557056000	0.822378000
H	3.378877000	0.179298000	1.023658000
C	-2.067156000	0.245866000	1.020518000
C	-2.871838000	-0.697756000	0.397585000
C	-2.561888000	1.480075000	1.430974000
C	-4.192372000	-0.363518000	0.109432000
H	-2.469738000	-1.672870000	0.152621000
C	-3.884607000	1.798329000	1.141589000
H	-1.907055000	2.174022000	1.945902000
C	-4.694219000	0.883631000	0.469991000
H	-4.824623000	-1.088529000	-0.392319000
H	-4.284986000	2.759203000	1.448182000
H	-5.723684000	1.139631000	0.241483000
C	3.120873000	-0.878769000	2.946353000
H	3.933531000	-1.587018000	3.108526000
H	3.411502000	0.076902000	3.389443000
C	1.790274000	-1.351537000	3.577086000
H	1.706035000	-2.442825000	3.585758000
H	1.634854000	-0.988739000	4.593308000

B-4b

C	-1.798904000	2.434969000	-3.637357000
C	-1.221911000	3.633545000	-3.218968000
C	-0.529294000	3.720958000	-2.011617000
C	-0.426606000	2.580215000	-1.220212000
C	-1.003909000	1.375386000	-1.642976000
C	-1.674905000	1.284223000	-2.854307000
C	-0.556692000	0.290302000	-0.668582000
N	0.223666000	2.471237000	0.018602000
C	0.717583000	-0.359771000	-1.246878000
C	0.422353000	-1.418231000	-2.272123000
C	-0.156786000	1.185030000	0.598877000
O	-0.674173000	-1.668727000	-2.731172000
C	-1.279025000	1.344474000	1.617871000
C	-1.977764000	2.547374000	1.745330000
C	-3.025660000	2.669974000	2.657723000

C	-3.382487000	1.596586000	3.470099000
C	-2.676194000	0.398801000	3.369932000
C	-1.631642000	0.279974000	2.458101000
O	1.527057000	-2.080050000	-2.620004000
C	1.337898000	-3.124014000	-3.574832000
H	-2.325941000	2.388982000	-4.584450000
H	-1.312382000	4.517107000	-3.843374000
H	-0.079429000	4.652083000	-1.683295000
H	-2.061058000	0.327552000	-3.195859000
H	1.297711000	0.440347000	-1.715085000
H	1.391661000	-0.747092000	-0.479297000
H	0.718671000	0.725801000	1.081803000
H	-1.676557000	3.389930000	1.131416000
H	-3.553362000	3.615109000	2.744066000
H	-4.189427000	1.697861000	4.189206000
H	-2.924490000	-0.439368000	4.013603000
H	-1.078406000	-0.655215000	2.408002000
H	0.639357000	-3.866475000	-3.182476000
H	0.943889000	-2.719841000	-4.509555000
H	2.320810000	-3.564662000	-3.729138000
N	-2.965979000	-0.345191000	-0.309929000
N	-2.866001000	-2.426586000	0.394498000
N	-1.624255000	-1.936791000	0.090678000
C	-1.661446000	-0.666013000	-0.345126000
C	-3.655772000	-1.427521000	0.151400000
C	-3.839511000	0.813838000	-0.565612000
H	-3.365706000	1.732989000	-0.226521000
H	-4.026682000	0.876968000	-1.640098000
O	2.531752000	-0.238617000	1.464745000
H	2.782342000	0.704806000	0.638481000
O	2.813409000	1.577712000	-0.100859000
H	1.257363000	2.506212000	-0.057108000
C	3.979100000	1.707311000	-0.869860000
C	5.158742000	1.028195000	-0.165654000
C	3.776292000	1.061788000	-2.249776000
C	4.262981000	3.201371000	-1.045898000
H	5.363628000	1.525385000	0.788301000
H	4.909567000	-0.016807000	0.044062000
H	6.067304000	1.065190000	-0.776150000
H	2.939782000	1.547633000	-2.767273000
H	4.666790000	1.159309000	-2.880563000
H	3.546008000	-0.003898000	-2.140032000
H	5.160115000	3.380900000	-1.648466000
H	3.411141000	3.682872000	-1.539234000
H	4.395982000	3.666592000	-0.064648000

C	2.895550000	0.056155000	2.782886000
C	1.879290000	-0.582156000	3.742278000
C	4.285669000	-0.523758000	3.090074000
C	2.907957000	1.574725000	3.024737000
H	0.885799000	-0.149881000	3.573357000
H	1.822483000	-1.663584000	3.568412000
H	2.144061000	-0.418297000	4.792884000
H	5.035895000	-0.074860000	2.433989000
H	4.584633000	-0.349495000	4.130282000
H	4.281906000	-1.604319000	2.908277000
H	3.192097000	1.817430000	4.054790000
H	3.602700000	2.064380000	2.337151000
H	1.911663000	1.992294000	2.834000000
C	-0.503687000	-2.828232000	0.217963000
C	0.614513000	-2.450968000	0.944396000
C	-0.589064000	-4.064026000	-0.421177000
C	1.707440000	-3.314111000	0.985114000
H	0.724201000	-1.478533000	1.418633000
C	0.492147000	-4.931180000	-0.335780000
H	-1.482369000	-4.318280000	-0.980920000
C	1.644250000	-4.552693000	0.357702000
H	2.601414000	-2.964366000	1.491032000
H	0.442119000	-5.897395000	-0.827180000
H	2.494999000	-5.225092000	0.396150000
C	-5.087991000	0.423696000	0.252497000
H	-5.995741000	0.855100000	-0.169840000
H	-4.961511000	0.796630000	1.272522000
C	-5.113021000	-1.125315000	0.269903000
H	-5.544853000	-1.541266000	1.180132000
H	-5.651520000	-1.537366000	-0.589522000

B-TSb4

C	-1.609966000	-0.328349000	-4.415158000
C	-1.151667000	0.944915000	-4.750693000
C	-0.575848000	1.781543000	-3.794647000
C	-0.473659000	1.323907000	-2.483476000
C	-0.920584000	0.038201000	-2.149078000
C	-1.476998000	-0.799289000	-3.105312000
C	-0.497976000	-0.219309000	-0.700905000
N	0.043960000	2.006020000	-1.373531000
C	0.878632000	-0.910971000	-0.748786000
C	0.826330000	-2.367946000	-1.111371000
C	-0.315546000	1.268639000	-0.150606000
O	-0.175062000	-3.007896000	-1.354046000
C	-1.532255000	1.870348000	0.477184000

C	-2.144559000	3.024434000	-0.050168000
C	-3.265541000	3.596055000	0.545854000
C	-3.819096000	3.049635000	1.701321000
C	-3.208287000	1.930632000	2.266887000
C	-2.084592000	1.364292000	1.674823000
O	2.050601000	-2.912748000	-1.104261000
C	2.092764000	-4.314485000	-1.366657000
H	-2.050399000	-0.964346000	-5.175942000
H	-1.249640000	1.296307000	-5.773455000
H	-0.225317000	2.775035000	-4.054571000
H	-1.770850000	-1.812230000	-2.843294000
H	1.485895000	-0.370376000	-1.483275000
H	1.431770000	-0.797303000	0.185658000
H	0.858857000	1.319241000	0.787576000
H	-1.719015000	3.461569000	-0.946414000
H	-3.710424000	4.481447000	0.100041000
H	-4.688983000	3.500649000	2.167775000
H	-3.594260000	1.506195000	3.190075000
H	-1.612024000	0.520380000	2.173479000
H	1.549386000	-4.855642000	-0.587702000
H	1.642233000	-4.536023000	-2.336017000
H	3.146394000	-4.586875000	-1.358472000
N	-2.865281000	-0.861154000	-0.155076000
N	-2.660075000	-2.232809000	1.554167000
N	-1.440507000	-1.816822000	1.085548000
C	-1.542298000	-0.978552000	0.039858000
C	-3.502808000	-1.618891000	0.782211000
C	-3.789163000	-0.067319000	-0.981429000
H	-3.410881000	0.948934000	-1.092304000
H	-3.873310000	-0.536643000	-1.964257000
O	1.840468000	1.298295000	1.381422000
H	2.695107000	1.365978000	-0.075884000
O	2.977420000	1.399874000	-1.027367000
H	1.041297000	2.202699000	-1.455159000
C	4.272759000	0.831311000	-1.169541000
C	5.319048000	1.941524000	-1.044440000
C	4.493571000	-0.243031000	-0.101248000
C	4.326285000	0.210661000	-2.563293000
H	5.123753000	2.717851000	-1.789637000
H	5.267247000	2.401696000	-0.052793000
H	6.333093000	1.556573000	-1.193755000
H	3.778867000	-1.062672000	-0.230207000
H	5.505684000	-0.654289000	-0.169601000
H	4.352556000	0.179639000	0.899220000
H	5.324265000	-0.181919000	-2.781846000

H	3.607043000	-0.611602000	-2.637370000
H	4.072583000	0.962927000	-3.315793000
C	2.003441000	2.498544000	2.118178000
C	0.986607000	2.538399000	3.261939000
C	3.421518000	2.491427000	2.686901000
C	1.812310000	3.707938000	1.193806000
H	-0.033846000	2.536330000	2.865315000
H	1.113528000	1.658208000	3.902925000
H	1.112741000	3.434795000	3.878521000
H	4.152774000	2.468347000	1.872557000
H	3.613428000	3.379108000	3.298511000
H	3.570527000	1.600540000	3.306070000
H	1.992889000	4.648314000	1.724988000
H	2.508704000	3.640673000	0.350647000
H	0.791600000	3.727804000	0.795030000
C	-0.260068000	-2.287493000	1.751648000
C	0.617008000	-1.375347000	2.321973000
C	-0.033243000	-3.660074000	1.796281000
C	1.782388000	-1.852552000	2.915853000
H	0.456542000	-0.303683000	2.244493000
C	1.119894000	-4.123182000	2.418276000
H	-0.743345000	-4.334144000	1.329462000
C	2.030463000	-3.220453000	2.970275000
H	2.492594000	-1.136294000	3.314900000
H	1.315379000	-5.189606000	2.460548000
H	2.938885000	-3.588827000	3.435563000
C	-5.084405000	-0.153863000	-0.142790000
H	-5.972641000	-0.118079000	-0.773928000
H	-5.106076000	0.695146000	0.544739000
C	-4.984212000	-1.472918000	0.666231000
H	-5.468149000	-1.419033000	1.641539000
H	-5.402056000	-2.323935000	0.118881000

B-5b

C	0.930850000	4.255176000	1.103039000
C	2.063374000	4.576138000	0.349843000
C	2.565239000	3.693927000	-0.598448000
C	1.904090000	2.478261000	-0.795780000
C	0.713721000	2.187212000	-0.109052000
C	0.252055000	3.059008000	0.874784000
C	0.163486000	0.830532000	-0.586867000
N	2.323858000	1.410003000	-1.559517000
C	-1.179568000	0.928600000	-1.346232000
C	-2.356698000	1.589726000	-0.676399000
C	1.306525000	0.362875000	-1.504881000

O	-2.426601000	1.968612000	0.470855000
C	1.751868000	-0.976421000	-1.570756000
C	3.129822000	-1.336136000	-1.687947000
C	3.539464000	-2.661562000	-1.662582000
C	2.628583000	-3.712952000	-1.532624000
C	1.270006000	-3.389908000	-1.475545000
C	0.842483000	-2.074080000	-1.510380000
O	-3.378733000	1.712312000	-1.536761000
C	-4.556225000	2.307620000	-0.994550000
H	0.568672000	4.943412000	1.859101000
H	2.574469000	5.518621000	0.522769000
H	3.471992000	3.919648000	-1.151011000
H	-0.638919000	2.820015000	1.440985000
H	-0.962728000	1.487203000	-2.260538000
H	-1.504036000	-0.061782000	-1.686698000
H	3.869431000	-0.546319000	-1.779011000
H	4.602170000	-2.880661000	-1.743776000
H	2.960795000	-4.744699000	-1.518423000
H	0.529517000	-4.187649000	-1.433152000
H	-0.220828000	-1.859639000	-1.553163000
H	-4.937974000	1.703239000	-0.167883000
H	-4.342316000	3.313461000	-0.627286000
H	-5.276600000	2.339892000	-1.809848000
N	1.242834000	-0.322990000	1.345325000
N	-0.176909000	-1.834135000	2.070764000
N	-0.727926000	-1.041749000	1.086470000
C	0.135415000	-0.117263000	0.613377000
C	1.027207000	-1.366401000	2.188100000
C	2.623434000	0.176910000	1.374978000
H	2.984465000	0.356176000	0.360900000
H	2.642946000	1.109453000	1.947287000
H	2.656388000	1.645793000	-2.489124000
C	-2.072711000	-1.385857000	0.702087000
C	-2.265989000	-2.526620000	-0.072032000
C	-3.144377000	-0.674498000	1.227678000
C	-3.562597000	-2.909575000	-0.396641000
H	-1.405167000	-3.103381000	-0.390284000
C	-4.437950000	-1.067994000	0.895351000
H	-2.959751000	0.176966000	1.869721000
C	-4.646802000	-2.173113000	0.074795000
H	-3.724212000	-3.790158000	-1.008807000
H	-5.283269000	-0.518343000	1.296604000
H	-5.657518000	-2.474402000	-0.180284000
C	3.337078000	-1.002417000	2.071377000
H	4.207791000	-0.675576000	2.640547000

H	3.661009000	-1.700551000	1.293403000
C	2.266015000	-1.688897000	2.957772000
H	2.414356000	-2.763589000	3.061455000
H	2.212223000	-1.246165000	3.957687000

B-TSb5

C	1.511397000	4.282464000	0.891036000
C	2.760898000	4.335501000	0.265933000
C	3.191761000	3.298514000	-0.549873000
C	2.339630000	2.209799000	-0.745640000
C	1.051177000	2.176791000	-0.184822000
C	0.655111000	3.206245000	0.671426000
C	0.345530000	0.905883000	-0.636495000
N	2.627767000	1.030582000	-1.401775000
C	-0.997174000	1.098006000	-1.358749000
C	-2.098085000	1.854227000	-0.661535000
C	1.406485000	0.232361000	-1.437410000
O	-2.115410000	2.233792000	0.487255000
C	1.563395000	-1.172724000	-1.577461000
C	2.849743000	-1.781392000	-1.661727000
C	3.002538000	-3.158775000	-1.730745000
C	1.901711000	-4.016861000	-1.723883000
C	0.630247000	-3.444090000	-1.666367000
C	0.460747000	-2.070363000	-1.599991000
O	-3.122626000	2.064251000	-1.502609000
C	-4.226877000	2.774275000	-0.945816000
H	1.202306000	5.087528000	1.549233000
H	3.413532000	5.186444000	0.437267000
H	4.176819000	3.312282000	-1.006374000
H	-0.311700000	3.172264000	1.155153000
H	-0.771520000	1.631466000	-2.286780000
H	-1.419175000	0.137865000	-1.674851000
H	3.730434000	-1.146734000	-1.651141000
H	4.006685000	-3.572621000	-1.788725000
H	2.028972000	-5.091786000	-1.784641000
H	-0.249283000	-4.084959000	-1.696462000
H	-0.545472000	-1.666484000	-1.612868000
H	-4.652096000	2.217360000	-0.107515000
H	-3.909480000	3.757306000	-0.591818000
H	-4.955147000	2.870974000	-1.748949000
N	1.157989000	-0.475566000	1.455691000
N	-0.397866000	-1.912775000	2.046668000
N	-0.861837000	-0.981196000	1.138186000
C	0.077655000	-0.090346000	0.751778000
C	0.841189000	-1.567049000	2.204653000

C	2.581718000	-0.121540000	1.525377000
H	2.973489000	0.080653000	0.527825000
H	2.695099000	0.765251000	2.156104000
H	3.096467000	1.133053000	-2.296361000
C	-2.235581000	-1.138676000	0.744984000
C	-2.572280000	-2.245192000	-0.031079000
C	-3.209754000	-0.285649000	1.250417000
C	-3.904423000	-2.456547000	-0.367312000
H	-1.789500000	-2.926733000	-0.345054000
C	-4.540520000	-0.506713000	0.904348000
H	-2.922033000	0.541306000	1.886893000
C	-4.887035000	-1.581295000	0.089751000
H	-4.174187000	-3.310626000	-0.978895000
H	-5.309352000	0.153485000	1.292726000
H	-5.926417000	-1.749132000	-0.172867000
C	3.175726000	-1.406239000	2.145592000
H	4.057423000	-1.196431000	2.752071000
H	3.459588000	-2.073563000	1.326551000
C	2.031107000	-2.062276000	2.957885000
H	2.082246000	-3.150739000	2.975042000
H	1.998000000	-1.699138000	3.990221000