

Supplementary Information

Mechanistic study on Cp^{*} iridium-catalyzed N-alkylation of amines with alcohols

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Contents

S1. Cartesian coordinates of all optimized geometries together with thermal corrections to enthalpies (ΔH) and free energies (ΔG) at the B3LYP level of calculations and their electronic energies (E) at the M06 level of calculations

S1.1 Alcohol oxidation

S1.2 Imine formation

S1.3 Imine reduction

S2. Cartesian coordinates of the key states together with thermal corrections to enthalpies (ΔH) and free energies (ΔG) and their electronic energies (E)

S2.1 At the M06/BSIV//B3LYP/BSIII level of calculations

S2.2 At the M06//B3PW91 level of calculations

S2.3 At the M06//PBE1PBE level of calculations

S2.4 At the M06//M06 level of calculations

S3. The energetic span model

S4. Fortran program for TOF and X_i calculations

S1. Cartesian coordinates of all optimized geometries together with thermal corrections to enthalpies (ΔH) and free energies (ΔG) at the B3LYP level of calculations and their electronic energies (E) at the M06 level of calculations

S1.1 Alcohol oxidation

[Cp*IrCl ₂] ₂	$E = -2829.65305968$	$\Delta H = 0.508010$	$\Delta G = 0.351494$
Ir	-1.92792300	0.01750300	0.35377100
C	-3.70827200	-1.20095700	0.09623600
C	-4.04624200	-0.05237500	0.90346400
C	-3.76679600	1.14209100	0.13271400
C	-3.32417200	0.71639800	-1.19517100
C	-3.28391700	-0.71590300	-1.21837900
Cl	-1.14698400	0.14824200	2.66742500
Cl	-0.05736100	-1.63891700	-0.09599700
C	-2.93961300	-1.57614100	-2.39337000
H	-3.84805200	-1.80515400	-2.96620300
H	-2.23174700	-1.08126000	-3.06058300
H	-2.49302900	-2.52163300	-2.08002900
C	-3.89907000	-2.63671700	0.47545800
H	-3.80766700	-2.77966300	1.55418200
H	-4.89679700	-2.97923000	0.17073800
H	-3.16252700	-3.27980600	-0.01136000
C	-4.61674300	-0.08501000	2.28500700
H	-4.30508600	0.78212500	2.86902500
H	-5.71306600	-0.08141700	2.22491600
H	-4.30937500	-0.98072000	2.82736400
C	-4.04993500	2.55074500	0.55523400
H	-3.38752800	3.25946700	0.05307900
H	-5.08397600	2.82304500	0.30532300
H	-3.91801300	2.67746200	1.63201300
C	-3.01428400	1.62644600	-2.34175800
H	-2.26214000	1.19658300	-3.00577600
H	-3.92564600	1.80579200	-2.92730200
H	-2.64152100	2.59326400	-1.99836900
Ir	1.85886200	-0.02665000	-0.51444100
C	4.02820700	-0.04101000	-0.79429700
C	3.61823400	1.18003600	-0.13507900
C	3.02493000	0.81139800	1.15186100
C	3.03011200	-0.61675900	1.25382500
C	3.62696700	-1.15814500	0.03176200
Cl	-0.06804400	1.60846600	-0.28449900
Cl	1.35550800	-0.15386300	-2.89715000
C	3.92463700	-2.60193000	-0.23289100

H	4.90180600	-2.87014100	0.18991300
H	3.17499700	-3.25481200	0.21982200
H	3.95139600	-2.81427500	-1.30384600
C	4.76795000	-0.13336500	-2.09052200
H	4.55050200	0.71607300	-2.73983500
H	5.84765900	-0.14333700	-1.89184500
H	4.51509800	-1.04463600	-2.63523700
C	3.89534500	2.57395100	-0.60648800
H	3.14204700	3.27631700	-0.24260600
H	4.87425900	2.91200700	-0.24145200
H	3.90332900	2.62943200	-1.69724800
C	2.54417400	1.76260400	2.20114600
H	1.69298100	1.35222600	2.74770500
H	3.35301500	1.96506900	2.91569400
H	2.23278800	2.71482300	1.76784100
C	2.56045300	-1.41268000	2.43077400
H	2.31288800	-2.43781000	2.14924000
H	3.35255500	-1.45336300	3.19016800
H	1.67140300	-0.96840800	2.88389800

K_2CO_3 $E = -1463.72987180$ $\Delta H = 0.027387$ $\Delta G = -0.029269$

C	-0.78517700	-0.06603100	0.00367700
O	-1.42843800	1.04695500	0.03911200
O	0.55509200	-0.03707300	-0.01618800
O	-1.37925500	-1.20625200	-0.01446000
K	0.70323100	-2.53802000	-0.04975800
K	0.59755000	2.46601900	0.01011600

KCl $E = -1060.19520366$ $\Delta H = 0.005537$ $\Delta G = -0.030941$

Cl	0.00000000	0.00000000	1.48676900
K	0.00000000	0.00000000	-1.31899100

A $E = -1818.37153336$ $\Delta H = 0.275375$ $\Delta G = 0.168974$

Ir	0.57926200	0.54018500	-0.06519800
C	-0.21885300	-1.11428300	-1.27124000
C	-1.16275000	0.00266000	-1.30178700
C	-0.49401400	1.13041700	-1.88338300
C	0.87730300	0.74391700	-2.19491400
C	1.02044200	-0.66061600	-1.83556300
Cl	-0.38097900	-0.10884500	2.18837700
O	2.46329900	0.68225500	0.91014700
C	2.20509100	1.86012100	1.42936400
O	1.05966400	2.35703100	0.94569700
O	2.85571000	2.43095800	2.31675700

K	0.44087100	2.55794400	3.52663600
C	1.89134900	1.57797900	-2.91735400
H	1.80744900	1.43917800	-4.00344000
H	1.75650900	2.64144500	-2.70483500
H	2.90906900	1.30862900	-2.62384300
C	2.25767700	-1.48097700	-2.03152400
H	2.32704400	-2.28323700	-1.29353700
H	2.25399600	-1.93785100	-3.02948900
H	3.15919500	-0.87026600	-1.94536200
C	-0.53723100	-2.50398900	-0.81083400
H	-1.21054800	-2.49213400	0.04917700
H	-1.02455800	-3.07235300	-1.61404500
H	0.36532700	-3.04496100	-0.51710400
C	-2.59626100	-0.07324200	-0.87315800
H	-3.00811800	0.91863300	-0.67244100
H	-3.20872500	-0.53866900	-1.65650800
H	-2.70369400	-0.66814100	0.03682500
C	-1.09250600	2.47634600	-2.15458400
H	-0.35789000	3.27469500	-2.02411700
H	-1.45941200	2.52440100	-3.18803300
H	-1.93477300	2.68321500	-1.49038900

B	$E = -1818.34452959$	$\Delta H = 0.275203$	$\Delta G = 0.167110$
Ir	0.05420800	-1.28757900	0.54708100
C	-0.11167600	-3.45181600	0.30506100
C	-1.42839800	-2.81957700	0.15864800
C	-1.36246700	-1.92491100	-0.96249400
C	-0.00205900	-1.99848400	-1.50644500
C	0.73939300	-2.97499300	-0.75127100
Cl	2.24500400	-0.54415600	1.32853800
O	-0.90284500	0.11869600	1.53602900
C	-0.30577600	1.09393200	2.32600900
O	0.03123700	2.15835700	1.74435700
O	-0.16849600	0.81822800	3.54694700
K	2.13905600	1.97442200	3.25545800
C	-2.63087300	-3.11879000	0.99772200
H	-3.33964200	-2.28827700	0.99180800
H	-3.14639000	-4.00917900	0.61511100
H	-2.35331400	-3.31181200	2.03681900
C	0.23316500	-4.49563200	1.32016500
H	-0.05013100	-5.48978300	0.94958600
H	1.30400200	-4.50806700	1.53372700
H	-0.29573400	-4.32679800	2.26127300
C	2.15197500	-3.39947300	-1.01329600

H	2.17141500	-4.23706700	-1.72211900
H	2.74138800	-2.58569300	-1.44148700
H	2.65189400	-3.72231200	-0.09774800
C	0.48340500	-1.26121700	-2.71462300
H	0.23940900	-1.82647600	-3.62404100
H	0.01559100	-0.27712900	-2.79559100
H	1.56574000	-1.11824800	-2.68716600
C	-2.48098600	-1.10632700	-1.52745600
H	-2.96153800	-1.64116100	-2.35690000
H	-3.24287700	-0.89514000	-0.77431300
H	-2.11860000	-0.14866800	-1.90958100
PhNH ₂	$E = -287.48283256$	$\Delta H = 0.127788$	$\Delta G = 0.077289$
C	-2.02883300	-1.90782600	-0.15900100
C	-0.63768000	-1.84912300	-0.11692500
C	0.02309400	-0.62617500	0.01944200
C	-0.73531900	0.54318800	0.11214900
C	-2.12700400	0.49697200	0.06997900
C	-2.79645500	-0.73264000	-0.06728900
H	-2.53224800	-2.86548100	-0.26843400
H	-0.06648600	-2.77094000	-0.18984200
H	1.10737000	-0.58524100	0.05296900
H	-0.24032800	1.50462800	0.22139000
H	-2.70621300	1.41462100	0.14088400
N	-4.18744300	-0.77959700	-0.16853900
H	-4.60592600	-1.66459700	0.08728200
H	-4.67422700	-0.00231300	0.25896200
BN-IN1	$E = -2105.85551695$	$\Delta H = 0.406653$	$\Delta G = 0.276922$
Ir	0.04119400	-0.90047500	-0.04718600
C	-0.44890100	-2.91129100	0.63558800
C	-1.66887000	-2.19616900	0.37130400
C	-1.67275300	-1.80854700	-1.02606600
C	-0.47052700	-2.37594800	-1.64344400
C	0.28077800	-3.03856700	-0.62883200
Cl	2.39542200	-0.63386600	0.92272800
C	1.06999300	1.08964400	-3.46828000
C	0.65598100	1.46337500	-4.74775700
C	-0.55835300	2.12842300	-4.93160700
C	-1.35638400	2.42256300	-3.82290700
C	-0.95052200	2.05326800	-2.54008800
C	0.26725600	1.38592600	-2.36071400
H	2.01496200	0.57222000	-3.32375900
H	1.28741200	1.23511400	-5.60179800

H	-0.87661300	2.42068000	-5.92781300
H	-2.29846300	2.94742500	-3.95367700
H	-1.56778500	2.28461900	-1.67663200
N	0.67754300	0.98753900	-1.04853500
H	0.29027200	1.57768600	-0.29875800
H	1.69213200	0.97787100	-0.94905800
O	-0.57083000	0.68077500	1.17576000
C	-0.30912300	0.64735100	2.50993500
O	0.04360400	1.74255300	3.03541300
O	-0.38085300	-0.46328100	3.13395100
K	1.97889000	0.22706800	3.95100000
C	-0.06564000	-3.50800900	1.95472000
H	-0.64980600	-4.41620900	2.15452000
H	0.99236200	-3.78087000	1.97377100
H	-0.25061800	-2.77925500	2.74764300
C	-2.72090500	-1.89436800	1.39206100
H	-3.43765600	-1.15709700	1.02420300
H	-3.27369900	-2.80986000	1.63965800
H	-2.25159200	-1.49821500	2.29792400
C	-2.80376400	-1.15613800	-1.76120300
H	-2.44872000	-0.59468800	-2.62850900
H	-3.51377100	-1.91270500	-2.12160200
H	-3.35247300	-0.46519000	-1.11691000
C	-0.15334800	-2.32492400	-3.10587900
H	0.91235400	-2.47441400	-3.29338700
H	-0.70032100	-3.11568100	-3.63621100
H	-0.44201700	-1.36927500	-3.54905600
C	1.56739000	-3.78593800	-0.79849300
H	2.26549800	-3.55080300	0.00837200
H	1.38393800	-4.86799500	-0.78606500
H	2.05730800	-3.54011900	-1.74358300

BN-TS2 $E = -2105.84034211$ $\Delta H = 0.401039$ $\Delta G = 0.272654$

Ir	-0.03348700	-1.01637400	-0.07734000
C	-0.48536700	-3.08692200	0.54010900
C	-1.70843200	-2.35406400	0.46841600
C	-1.86774200	-1.85824100	-0.89584500
C	-0.74002400	-2.34573000	-1.67149400
C	0.13625900	-3.06969200	-0.78524800
Cl	2.20461500	-0.87877600	1.06701400
C	1.31987100	1.34638200	-3.29850200
C	1.00446900	1.79213400	-4.58213700
C	-0.30559700	2.15251100	-4.90571400
C	-1.29658100	2.06871700	-3.92276800

C	-0.98722000	1.62958600	-2.63607500
C	0.32891900	1.25655000	-2.30465000
H	2.34257800	1.06957500	-3.05225700
H	1.78858900	1.85788800	-5.33207500
H	-0.55038900	2.49999500	-5.90510100
H	-2.31749500	2.36120900	-4.15507000
H	-1.75518200	1.59055600	-1.86960400
N	0.64224500	0.83548000	-0.99520700
H	-0.03413900	1.24564100	0.07431700
H	1.64810300	0.86701400	-0.84013900
O	-0.69711400	0.81403300	0.95631600
C	-0.27851600	1.06161400	2.26834200
O	0.43785700	2.07893600	2.43449900
O	-0.63180900	0.21873700	3.13481700
K	1.87643500	0.45237500	3.89409600
C	-3.07956200	-1.16176600	-1.43490800
H	-2.84770700	-0.60338700	-2.34401100
H	-3.86219500	-1.89177900	-1.68102900
H	-3.49481500	-0.46073300	-0.70666100
C	-0.55365300	-2.16609000	-3.14512500
H	-1.09741200	-2.95162700	-3.68606000
H	-0.93173200	-1.20001800	-3.48593700
H	0.49919300	-2.23305600	-3.42776700
C	1.37750000	-3.81585000	-1.16704200
H	1.13801400	-4.86280000	-1.39581900
H	1.85190300	-3.38019900	-2.04959300
H	2.11034300	-3.80728200	-0.35707000
C	0.04682100	-3.80210100	1.74331600
H	-0.19517500	-4.87170000	1.68750300
H	1.13287000	-3.70696200	1.81527700
H	-0.39002000	-3.40580300	2.66292300
C	-2.64226800	-2.10402000	1.61601800
H	-2.94969800	-3.05240700	2.07134500
H	-2.15695200	-1.48145000	2.37602900
H	-3.54319400	-1.58468300	1.28229400
KHCO ₃	$E = -864.37739807$	$\Delta H = 0.036854$	$\Delta G = -0.012445$
C	-0.74546400	-0.12308100	0.00282800
O	-1.46982200	1.05005400	0.02325100
O	0.51593100	-0.00791400	-0.01423600
O	-1.42032100	-1.18116700	0.00248700
K	0.72682900	-2.56405600	-0.05764300
H	-0.79962500	1.74996400	0.02048700

C	$E = -1241.47011551$	$\Delta H = 0.366863$	$\Delta G = 0.258449$
Ir	0.15566400	-0.90067000	-0.54295500
C	-0.58922300	-2.51197900	0.84089800
C	-1.47866200	-1.38367300	0.85093200
C	-2.03318400	-1.22321500	-0.49122400
C	-1.43478900	-2.22473300	-1.32978300
C	-0.51381400	-3.00414900	-0.50541400
Cl	2.29896300	-0.60925600	0.56683600
C	1.20841900	2.33341400	-3.27342100
C	0.81605800	3.08883100	-4.37359400
C	-0.38672100	2.81514600	-5.03200400
C	-1.18879900	1.76874700	-4.56868300
C	-0.80378000	1.00755600	-3.46746000
C	0.40365000	1.27493000	-2.79394100
H	2.14559000	2.55322200	-2.76678900
H	1.45502300	3.89711200	-4.71948100
H	-0.69132000	3.40498800	-5.89125300
H	-2.12441000	1.54024300	-5.07321400
H	-1.42494600	0.19273900	-3.12069800
N	0.82976400	0.53901200	-1.69339300
H	1.75033000	0.84549500	-1.38499600
C	-1.87654800	-0.57589500	2.04766000
H	-2.11101300	0.45512300	1.77066900
H	-2.76939700	-1.00582800	2.52113300
H	-1.08148300	-0.55092300	2.79608200
C	0.13858400	-3.06831400	2.02647400
H	0.38387300	-2.28934600	2.75120300
H	-0.48534900	-3.81641900	2.53215500
H	1.07268800	-3.55223000	1.73473800
C	0.26901000	-4.19067100	-0.97643400
H	1.17705300	-4.32995100	-0.38558000
H	-0.33272000	-5.10532200	-0.89006700
H	0.56322300	-4.08250900	-2.02345200
C	-3.14306500	-0.27942300	-0.83828700
H	-4.09193400	-0.65632200	-0.43472300
H	-2.97326200	0.71297600	-0.41207900
H	-3.26574500	-0.16426600	-1.91631500
C	-1.78335600	-2.55804500	-2.74866000
H	-0.88976200	-2.69378400	-3.36393100
H	-2.35233400	-3.49619400	-2.78056600
H	-2.39896000	-1.78566700	-3.21298900
D	$E = -758.12854050$	$\Delta H = 0.268064$	$\Delta G = 0.176399$
Ir	0.05272100	0.09641400	0.32009700

C	-0.44364400	1.02439300	-1.62342000
C	-1.35900200	-0.07060400	-1.31427600
C	0.87211600	0.47663000	-1.67801400
C	-0.61074000	-1.30744500	-1.26075400
C	0.77111400	-0.96967500	-1.43650200
C	0.31717400	0.43673400	2.78933500
O	0.47386200	1.38151100	1.83354400
O	-0.00297200	-0.72367900	2.17413700
O	0.44184300	0.60084800	3.97867100
C	-0.83895600	2.44816500	-1.86699600
H	-1.12734500	2.58850900	-2.91660200
H	-1.68917900	2.74045200	-1.24560900
H	-0.01691000	3.13410500	-1.65049000
C	-2.84249700	0.06017300	-1.17937300
H	-3.31540000	-0.03657600	-2.16562300
H	-3.25671500	-0.71469900	-0.53054400
H	-3.12130700	1.03318100	-0.76837800
C	2.13904600	1.21256200	-1.98363500
H	2.98534100	0.79436300	-1.43318100
H	2.36931700	1.14392200	-3.05463800
H	2.05996200	2.27037300	-1.72326800
C	1.92105600	-1.92592400	-1.46445500
H	1.71046800	-2.82384400	-0.87954700
H	2.12409500	-2.23407600	-2.49845800
H	2.83162800	-1.46982200	-1.06816000
C	-1.17630400	-2.67789700	-1.04286900
H	-1.43266000	-3.14620500	-2.00144400
H	-0.46163700	-3.32778800	-0.53245300
H	-2.08362600	-2.64295600	-0.43510200

PhCH₂OH $E = -346.64232406$ $\Delta H = 0.145672$ $\Delta G = 0.088704$

C	0.37606500	1.95975900	0.18626400
H	0.05387100	2.32029900	1.17601600
H	1.45537300	2.17407400	0.10970300
O	-0.33895900	2.61244400	-0.85748600
H	-0.03758000	3.52992200	-0.88573200
C	0.16250900	0.46516500	0.10383000
C	-0.15410100	-0.15487700	-1.10991800
C	0.32679300	-0.32698300	1.24693200
C	-0.30371800	-1.54130100	-1.17725800
H	-0.29250300	0.45795400	-1.99395000
C	0.18588900	-1.71309300	1.17886700
H	0.56407100	0.14497000	2.19789600
C	-0.13093200	-2.32550400	-0.03559100

H	-0.55543700	-2.00945000	-2.12504900
H	0.31578500	-2.31340300	2.07515500
H	-0.24735600	-3.40421600	-0.08967900
B-IN1i	$E = -2165.00235816$	$\Delta H = 0.423662$	$\Delta G = 0.285599$
Ir	-0.09058800	-0.68901000	0.44638200
C	-0.68298600	-2.62954600	1.11269600
C	-1.84385200	-1.95325100	0.56395400
C	-1.57080000	-1.64717600	-0.81988100
C	-0.25894000	-2.21614000	-1.15006100
C	0.27666800	-2.82861300	0.02265000
Cl	2.01807500	-0.26729300	1.72579000
O	-0.94199000	0.99764300	1.34324400
C	-0.85775200	1.16031000	2.70003600
O	-0.51102100	2.30304900	3.10725400
O	-1.09082800	0.15265800	3.43975000
K	1.13788600	0.87367900	4.56138800
O	0.37354600	1.25411700	-0.69279200
C	1.68002400	1.81133200	-0.90314600
H	2.35894700	0.97919900	-1.10744800
H	2.02863300	2.28553000	0.02105300
C	1.70889100	2.79943400	-2.05259800
C	0.54475800	3.35046100	-2.59727400
C	2.95156800	3.19552600	-2.56806400
C	0.62166000	4.27807500	-3.63998700
H	-0.42139400	3.04831400	-2.20685400
C	3.02915300	4.12388100	-3.60538100
H	3.86405600	2.77151800	-2.15361400
C	1.86136600	4.66911500	-4.14642200
H	-0.29173700	4.69676600	-4.05414500
H	4.00005800	4.41931400	-3.99398500
H	1.91934800	5.39109200	-4.95622200
H	-0.09692900	1.68600100	0.07879600
C	1.57010900	-3.57364400	0.13880900
H	1.38933800	-4.65543600	0.09675100
H	2.25755700	-3.31615900	-0.66996700
H	2.07208600	-3.35206100	1.08339800
C	0.36749400	-2.18949500	-2.51038300
H	-0.01592300	-3.02087000	-3.11627100
H	0.13887500	-1.26234700	-3.04183400
H	1.45398200	-2.28758400	-2.45716300
C	-2.50436100	-0.98832200	-1.78856100
H	-3.13494900	-1.73616500	-2.28686700
H	-3.16149900	-0.27572000	-1.28480300

H	-1.95711800	-0.44474500	-2.56270100
C	-3.06489500	-1.59518500	1.35118000
H	-3.63810700	-2.50097000	1.58628300
H	-2.77004200	-1.10369800	2.28405900
H	-3.71529700	-0.91616900	0.79639600
C	-0.57691400	-3.15822300	2.51001600
H	-1.14439000	-4.09283400	2.61208900
H	0.46166700	-3.36681900	2.77737200
H	-0.97306400	-2.42506700	3.21678300
B-TS2i	$E = -2164.99562783$	$\Delta H = 0.418778$	$\Delta G = 0.284270$
Ir	-0.12090600	-0.71996800	0.45708600
C	-0.68101000	-2.72122300	1.08156800
C	-1.85051600	-2.04109900	0.57579900
C	-1.60825200	-1.66867300	-0.80429100
C	-0.28702600	-2.17192800	-1.16563300
C	0.28396400	-2.81378300	-0.01362000
Cl	1.92841700	-0.35368100	1.82439000
O	-1.04996100	1.10224300	1.19985900
C	-0.66689100	1.65509600	2.42796200
O	-0.03565700	2.74303600	2.35720800
O	-0.95997100	1.00267000	3.45900700
K	1.46258200	1.65225800	4.19732700
O	0.30014900	1.12872200	-0.66611400
C	1.58300800	1.73929900	-0.75707100
H	2.34823200	0.96319000	-0.87144100
H	1.80506000	2.27101200	0.17814900
C	1.67057400	2.70610600	-1.92366700
C	0.53036700	3.27775200	-2.49956100
C	2.93047600	3.07221300	-2.41871000
C	0.64768200	4.19479900	-3.54712100
H	-0.44790900	2.99506900	-2.12491400
C	3.05003800	3.99132600	-3.46135400
H	3.82510300	2.63056600	-1.98371100
C	1.90602500	4.55658100	-4.03096600
H	-0.24781000	4.62909100	-3.98435200
H	4.03501500	4.26173000	-3.83313800
H	1.99577000	5.27027200	-4.84539600
H	-0.38330900	1.49772900	0.24336100
C	1.60067900	-3.52347800	0.04684900
H	1.46040900	-4.59496200	-0.14612800
H	2.29957500	-3.13585700	-0.69798000
H	2.06748600	-3.41398500	1.02778200
C	0.34346900	-2.05892300	-2.51825600

H	0.06861100	-2.92635900	-3.13248300
H	0.01152100	-1.16007200	-3.04161900
H	1.43324300	-2.02719200	-2.45036300
C	-2.58038000	-1.00334900	-1.72886300
H	-3.18406000	-1.75158400	-2.25883900
H	-3.26260000	-0.34814700	-1.18227100
H	-2.06594100	-0.39617900	-2.47739300
C	-3.10420500	-1.76237500	1.34210500
H	-3.82268300	-2.57624200	1.17899100
H	-2.91050100	-1.68757200	2.41334200
H	-3.56956300	-0.82910300	1.02013800
C	-0.53307800	-3.34290200	2.43633000
H	-0.89703500	-4.37884100	2.42441000
H	0.51150100	-3.35781700	2.75426500
H	-1.10223000	-2.79233000	3.18900900

B-IN3i $E = -2165.00647396$ $\Delta H = 0.423243$ $\Delta G = 0.284341$

Ir	-0.18836600	-0.58581400	0.38661100
C	-0.56613000	-2.64940800	1.08188800
C	-1.80275100	-2.06242300	0.67983700
C	-1.69840200	-1.66889500	-0.72672600
C	-0.38426900	-2.06189000	-1.19064300
C	0.33937000	-2.62484800	-0.07062700
Cl	1.64907200	-0.05602900	2.01456100
O	-1.30268100	1.23933600	1.07590900
C	-1.17808200	1.72792900	2.42704700
O	-0.63798800	2.84753800	2.52338800
O	-1.58844500	0.94191700	3.29870200
K	0.73051700	1.64354600	4.44193500
O	0.36861600	1.04629900	-0.78973300
C	1.71078200	1.29714300	-1.09815800
H	2.18245500	0.41085500	-1.56443000
H	2.30682200	1.51297300	-0.19770800
C	1.85909800	2.46324500	-2.06528000
C	0.75035800	3.08408000	-2.64943700
C	3.14095300	2.92814800	-2.39640200
C	0.91740000	4.14403900	-3.54598500
H	-0.24096400	2.72999300	-2.38829000
C	3.31049900	3.98262500	-3.29264500
H	4.01323600	2.45851600	-1.94490100
C	2.19587500	4.59654500	-3.87290300
H	0.04406700	4.61748300	-3.98807800
H	4.31167800	4.32884900	-3.53711600
H	2.32555900	5.42057100	-4.56941500

H	-0.77811000	1.82529000	0.47884700
C	1.70616600	-3.23607900	-0.10753200
H	1.63615600	-4.31271400	-0.31154400
H	2.32655600	-2.78634400	-0.88611600
H	2.22300500	-3.10628500	0.84584600
C	0.11893000	-1.91568400	-2.59239400
H	-0.25856300	-2.74084000	-3.20980200
H	-0.21698800	-0.97812100	-3.04086100
H	1.20970000	-1.93951800	-2.63502500
C	-2.80122900	-1.10569400	-1.56965300
H	-3.43928500	-1.90935400	-1.96003900
H	-3.43454900	-0.42533300	-0.99544500
H	-2.40363600	-0.54993100	-2.42197800
C	-3.00482100	-1.87180400	1.55346700
H	-3.52487200	-2.82788000	1.69353900
H	-2.72126300	-1.47835700	2.53199100
H	-3.71124800	-1.16744900	1.11026200
C	-0.25194600	-3.23332200	2.42441400
H	-0.36564300	-4.32508700	2.40438800
H	0.77361600	-3.00561400	2.72452300
H	-0.92279400	-2.83906300	3.19139100
C-IN1i $E = -1588.12520611$ $\Delta H = 0.515782$ $\Delta G = 0.371001$			
Ir	-0.05439300	-1.36538200	-0.60250900
C	-1.14808900	-3.32928000	-0.51549500
C	-1.81703800	-2.35780100	0.29737500
C	-2.26206200	-1.26494800	-0.56642100
C	-1.82707200	-1.55449700	-1.90430700
C	-1.09813600	-2.82058300	-1.86261700
Cl	2.03660400	-2.19864600	0.31861200
C	1.90278700	2.35497300	-1.68630300
C	1.75189100	3.59823100	-2.29310500
C	0.47962100	4.09283400	-2.59533900
C	-0.64107800	3.32383300	-2.27133900
C	-0.49886900	2.07786300	-1.66438200
C	0.77709800	1.56413300	-1.36812100
H	2.89602200	1.97838500	-1.45307500
H	2.63531800	4.18498500	-2.53031800
H	0.36381200	5.06334800	-3.06843700
H	-1.63811300	3.70026200	-2.48602700
H	-1.37097400	1.49654900	-1.39543500
N	0.95923900	0.31896900	-0.76342800
H	1.93346800	0.18329500	-0.49891700
O	-0.35167400	1.01770400	2.17095800

C	0.59920800	0.95066900	3.22982900
H	1.05018600	-0.04952400	3.29566100
H	0.02057200	1.10183600	4.15022400
C	1.69473800	1.99690700	3.13860700
C	3.00150100	1.69711600	3.54281700
C	1.40829200	3.29039200	2.68108800
C	4.00173300	2.67127900	3.50104500
H	3.23925300	0.69270900	3.88626100
C	2.40730600	4.26286500	2.63234200
H	0.39969700	3.52219100	2.35229800
C	3.70681900	3.95770500	3.04616100
H	5.01178400	2.42165800	3.81497400
H	2.17125000	5.26043900	2.27131800
H	4.48454300	4.71566400	3.00826600
H	0.09638200	0.75593500	1.34741600
C	-0.58329800	-4.63563100	-0.04770200
H	-1.34284800	-5.42365600	-0.12944600
H	0.28017100	-4.93814000	-0.64361700
H	-0.26263000	-4.58554400	0.99477600
C	-2.11505300	-2.46140900	1.76108200
H	-3.13224800	-2.84415400	1.91824300
H	-1.42111400	-3.13954200	2.26223000
H	-2.04202300	-1.48492900	2.24646500
C	-3.15201000	-0.15064000	-0.10652700
H	-4.15058900	-0.54630500	0.11980100
H	-2.76706700	0.32000900	0.80210000
H	-3.27140400	0.62224600	-0.86803200
C	-2.16693400	-0.80861100	-3.15764700
H	-2.98244000	-1.31912600	-3.68633000
H	-2.49174000	0.21228800	-2.95266900
H	-1.31283400	-0.75712500	-3.83811300
C	-0.51508000	-3.51738800	-3.05301900
H	-1.27403700	-4.14662900	-3.53678900
H	-0.15356100	-2.80028600	-3.79437800
H	0.32210600	-4.15929400	-2.77033600
C-TS2i $E = -1588.10469248$ $\Delta H = 0.510355$ $\Delta G = 0.374085$			
Ir	0.07836100	-0.99540300	-0.32293100
C	-1.03994600	-2.88369000	-0.03260700
C	-1.75399800	-1.82159300	0.60379200
C	-2.11376100	-0.83044700	-0.40411200
C	-1.62647300	-1.31383600	-1.67854200
C	-0.92533500	-2.55606300	-1.45424600
Cl	2.33871400	-1.98320600	-0.26383000

C	1.22664300	1.76421500	-3.29115000
C	0.74677100	2.71286700	-4.19433800
C	-0.29296200	3.57313700	-3.83424600
C	-0.84215200	3.47747900	-2.55196400
C	-0.36410000	2.53459600	-1.64272100
C	0.67809800	1.65928000	-2.00042900
H	2.03839900	1.09933400	-3.57776700
H	1.19011600	2.77871500	-5.18451200
H	-0.66459400	4.31218800	-4.53782400
H	-1.64182600	4.15003400	-2.25212700
H	-0.78100800	2.47563800	-0.64175200
N	1.17350300	0.72146100	-1.06993500
H	2.07192900	0.35188300	-1.37476100
O	0.69672100	0.47401600	1.24605200
C	1.62639300	0.17436400	2.28020200
H	2.52870800	-0.29309300	1.86785100
H	1.16340800	-0.57018400	2.94337100
C	2.01126000	1.39949500	3.09104000
C	3.10650900	1.32104800	3.96412700
C	1.30199300	2.60225100	3.01042400
C	3.47984100	2.41645700	4.74168800
H	3.67208900	0.39383200	4.03125300
C	1.67917200	3.70370900	3.78406500
H	0.45781800	2.67283700	2.33281700
C	2.76684500	3.61560400	4.65321600
H	4.33242300	2.33756300	5.41109600
H	1.12114300	4.63307600	3.70390100
H	3.06047500	4.47235900	5.25342900
H	1.12970000	0.91539400	0.24554000
C	-0.53437200	-4.14092200	0.60549900
H	-1.23423000	-4.96675900	0.42322000
H	0.43907400	-4.42764900	0.20122000
H	-0.42492800	-4.02772700	1.68659000
C	-2.10765400	-1.72055300	2.05518700
H	-3.14059600	-2.05404400	2.21776900
H	-1.45448600	-2.33879600	2.67451700
H	-2.03095000	-0.68906800	2.40692000
C	-3.01291700	0.34709500	-0.18169500
H	-4.06465100	0.03101400	-0.20012000
H	-2.82828700	0.81754900	0.78782500
H	-2.88191800	1.10544600	-0.95636600
C	-1.86187500	-0.66439000	-3.00616200
H	-2.83295400	-0.98495900	-3.40543200
H	-1.87384800	0.42478700	-2.93049700

H	-1.09466900	-0.94259300	-3.73152800
C	-0.33647500	-3.44950900	-2.50241700
H	-1.07897700	-4.18630100	-2.83620600
H	-0.01029200	-2.88116900	-3.37665900
H	0.52948000	-3.99212400	-2.11782000
C-IN3i	$E = -1588.11974168$	$\Delta H = 0.515286$	$\Delta G = 0.375930$
Ir	0.22173200	-0.74326900	-0.39885500
C	-0.77077700	-2.60330500	0.16235200
C	-1.55645600	-1.49738800	0.64691900
C	-1.96832500	-0.69810300	-0.48568200
C	-1.48942600	-1.37027600	-1.69255000
C	-0.75050100	-2.52608200	-1.30122600
Cl	2.56218100	-1.54807900	-0.66148400
C	0.70009000	1.73961900	-3.68519600
C	0.05509600	2.57759700	-4.59602800
C	-0.81189900	3.57585500	-4.14646100
C	-1.02850400	3.73316200	-2.77501200
C	-0.38867200	2.89941500	-1.85726500
C	0.47950300	1.89984500	-2.31282800
H	1.38108600	0.96728000	-4.03340100
H	0.23771600	2.45155500	-5.65938400
H	-1.30855000	4.22973800	-4.85697400
H	-1.69341700	4.51293200	-2.41457700
H	-0.55101200	3.02404400	-0.79036800
N	1.13272900	1.03578900	-1.37618000
H	2.00697400	0.66340700	-1.74780000
O	0.86817400	0.52550400	1.13790500
C	1.54827600	-0.01630100	2.23328600
H	2.45070700	-0.56493300	1.92046600
H	0.92130100	-0.75038700	2.77621900
C	1.95922500	1.05298400	3.23582000
C	2.75238800	0.69630600	4.33725700
C	1.55500300	2.38565500	3.10757800
C	3.13088100	1.64554300	5.28527500
H	3.07777000	-0.33659900	4.44852600
C	1.93538200	3.34099900	4.05535600
H	0.94155500	2.66314800	2.25722700
C	2.72260800	2.97618600	5.14768000
H	3.74742300	1.34991200	6.13045400
H	1.61454200	4.37345800	3.93853500
H	3.01882500	3.71848600	5.88400200
H	1.34641300	1.48727400	-0.47627900
C	-0.20223500	-3.72610000	0.97556600

H	-0.93027200	-4.54312600	1.06528100
H	0.70102900	-4.13123100	0.51389900
H	0.06146600	-3.39908400	1.98435000
C	-1.91111000	-1.20936800	2.07261300
H	-2.95913200	-1.47752900	2.25684600
H	-1.29451500	-1.78349200	2.76639200
H	-1.78910800	-0.14909100	2.30763100
C	-2.90735100	0.46863800	-0.44088800
H	-3.94863300	0.12785800	-0.52025600
H	-2.80983000	1.02050800	0.49747800
H	-2.72309400	1.16553600	-1.26227800
C	-1.81023800	-0.94877000	-3.09344700
H	-2.76814000	-1.38773600	-3.40246700
H	-1.90318800	0.13559400	-3.17915500
H	-1.04904400	-1.27970900	-3.80335500
C	-0.12333900	-3.54605400	-2.20094300
H	-0.75766700	-4.43969900	-2.26397700
H	0.01281200	-3.16087400	-3.21413000
H	0.85689700	-3.85260600	-1.82855000
BC-IN4i $E = -1300.61502942$ $\Delta H = 0.384517$ $\Delta G = 0.269398$			
Ir	0.08892500	-0.65329200	-0.69594400
C	-1.10542300	-2.35588000	-0.10059900
C	-1.87223600	-1.15113800	0.14339300
C	-2.02654500	-0.48890000	-1.13039900
C	-1.41585800	-1.31990100	-2.16863800
C	-0.85454500	-2.47133700	-1.53351700
O	0.74226700	0.55844000	0.73110600
C	2.02390700	1.17724200	0.80413000
H	2.22347800	1.78223600	-0.08944400
H	2.81694200	0.41881100	0.86143400
C	2.06559600	2.05479300	2.03681700
C	2.34401300	1.50365200	3.29529700
C	1.79967400	3.42728100	1.95104200
C	2.35675300	2.30244800	4.43933400
H	2.55987900	0.44052100	3.37327500
C	1.81284400	4.23233100	3.09230700
H	1.58711200	3.86785800	0.97954300
C	2.09094500	3.67092000	4.34021400
H	2.58002900	1.86033600	5.40687800
H	1.60931500	5.29658500	3.00715500
H	2.10557700	4.29551500	5.22936000
C	-0.72900500	-3.37697900	0.92595200
H	-1.52799200	-4.12525800	1.01339900

H	0.18973400	-3.90076000	0.65232700
H	-0.58263700	-2.92405600	1.90888900
C	-2.42004800	-0.69166900	1.45885200
H	-3.43478700	-1.08031400	1.61214600
H	-1.80091000	-1.03347800	2.29141100
H	-2.46629500	0.39839800	1.51183400
C	-2.77541800	0.78343500	-1.37475900
H	-3.82510800	0.55803200	-1.60529700
H	-2.75556100	1.43682100	-0.49992300
H	-2.35936900	1.33592900	-2.22044200
C	-1.43372300	-1.02058600	-3.63618700
H	-2.37672300	-1.35973700	-4.08395900
H	-1.34048900	0.05172700	-3.82590000
H	-0.61479500	-1.51984000	-4.15777200
C	-0.16007900	-3.61838800	-2.20121600
H	-0.85803000	-4.45083400	-2.35703300
H	0.24234200	-3.33029100	-3.17424200
H	0.67269900	-3.98677200	-1.59692200
Cl	2.13457800	-0.45200700	-1.91763300

BC-TS5i $E = -1300.58974241$ $\Delta H = 0.379017$ $\Delta G = 0.267204$

Ir	-0.35025700	-0.56877600	0.15836600
C	-0.83160700	-2.71111300	0.34004900
C	-2.02918200	-1.93568700	0.60179700
C	-2.36604400	-1.21691500	-0.61708800
C	-1.36158800	-1.49570000	-1.59389700
C	-0.38860600	-2.41877300	-0.99927000
O	-0.71159200	1.27477200	1.20063400
C	0.07130500	0.70447900	2.09228000
H	0.78274700	-0.40103300	1.41623200
H	-0.41650500	0.10993300	2.88138500
C	1.28939300	1.42122500	2.59783800
C	1.84942700	1.02750000	3.82035900
C	1.84172900	2.49844500	1.89378800
C	2.95623800	1.69993700	4.33636600
H	1.41039900	0.19780300	4.37099600
C	2.94582400	3.17209600	2.41464700
H	1.40158300	2.78596900	0.94608500
C	3.50582800	2.77445000	3.63224800
H	3.38405600	1.39198400	5.28628300
H	3.37365500	4.00783000	1.86817500
H	4.36702500	3.30192600	4.03307800
C	-0.19629500	-3.69277900	1.27857300
H	-0.64172800	-4.68615000	1.13829900

H	0.87758300	-3.77975400	1.09912400
H	-0.34132600	-3.41045100	2.32417000
C	-2.87683000	-1.99279600	1.83784900
H	-3.68502200	-2.72655300	1.72019000
H	-2.29331100	-2.28606500	2.71404500
H	-3.33903900	-1.02534600	2.05172200
C	-3.56933400	-0.34398400	-0.79543300
H	-4.44278000	-0.95569200	-1.05669100
H	-3.80918300	0.20158100	0.12064700
H	-3.42198100	0.38849400	-1.59173100
C	-1.31781700	-1.00436000	-3.00710300
H	-1.68843900	-1.77997100	-3.68977800
H	-1.93378400	-0.11283400	-3.14309200
H	-0.29732800	-0.75063100	-3.30203400
C	0.74798600	-3.06282800	-1.73366700
H	0.39516800	-3.93169100	-2.30484700
H	1.21001200	-2.36382200	-2.43412600
H	1.52561500	-3.40562900	-1.04696000
Cl	1.33987800	0.64667700	-1.13482600
BC-IN6i $E = -1300.59608927$ $\Delta H = 0.381257$ $\Delta G = 0.269110$			
Ir	-0.16026800	-0.39111800	0.12436200
C	-0.64041100	-2.50122600	0.41047700
C	-1.84919900	-1.76085500	0.67256100
C	-2.34412500	-1.21370600	-0.59316400
C	-1.40136400	-1.51352600	-1.59245200
C	-0.28847000	-2.25743300	-0.97700900
O	-0.80310400	1.46583100	1.01275300
C	-0.21198500	0.88907900	2.00711000
H	1.27152100	-0.62230300	0.72410300
H	-0.82282000	0.31218400	2.71826000
C	1.06566500	1.39298700	2.57113700
C	1.48119700	0.93504200	3.83009600
C	1.83660000	2.35217800	1.89580300
C	2.65865500	1.41607500	4.40254700
H	0.87622300	0.20408600	4.36264200
C	3.00915900	2.83307300	2.47186700
H	1.51243000	2.69414500	0.91931300
C	3.42535000	2.36563200	3.72337600
H	2.97440500	1.05639700	5.37788200
H	3.60354000	3.57308500	1.94331100
H	4.34209600	2.74353400	4.16751100
C	0.05281300	-3.44198400	1.35129700
H	-0.39063100	-4.44341300	1.27517300

H	1.11600700	-3.52897400	1.11794300
H	-0.03628100	-3.11595000	2.39030000
C	-2.63438200	-1.76936600	1.95040800
H	-3.41079400	-2.54477000	1.91259600
H	-2.00135900	-1.98199200	2.81467700
H	-3.13939300	-0.81463300	2.12121500
C	-3.62531500	-0.45063300	-0.73197500
H	-4.48756500	-1.11601800	-0.59790200
H	-3.70372700	0.33954400	0.02142800
H	-3.71410700	0.01909300	-1.71342200
C	-1.44611500	-1.14892800	-3.04195100
H	-1.53877900	-2.05214800	-3.65753500
H	-2.28747700	-0.49315300	-3.27380800
H	-0.52698300	-0.63476800	-3.33895900
C	0.81254200	-2.92480500	-1.74771800
H	0.45279300	-3.85189500	-2.21332800
H	1.18964100	-2.27425800	-2.54021200
H	1.65407700	-3.17853700	-1.09895400
Cl	1.09581100	0.98019700	-1.44708100
PhCHO	$E = -345.44140427$	$\Delta H = 0.121308$	$\Delta G = 0.068094$
C	2.21543800	-0.25096000	-0.00000100
C	1.73429800	1.06020400	-0.00000100
C	0.35975400	1.29189300	0.00000000
C	-0.53491700	0.21291700	0.00000100
C	-0.04529500	-1.10279400	0.00000100
C	1.32599500	-1.33218000	0.00000000
H	3.28625500	-0.43341200	-0.00000200
H	2.42868900	1.89495800	-0.00000200
H	-0.02661700	2.30836000	0.00000000
H	-0.75551600	-1.92345900	0.00000200
H	1.70816000	-2.34861100	0.00000000
C	-1.99013300	0.47209800	0.00000300
H	-2.26799500	1.54882200	0.00000200
O	-2.85109900	-0.39027300	0.00000400
BC-IN7i	$E = -955.15271764$	$\Delta H = 0.256810$	$\Delta G = 0.170667$
Ir	0.57372900	0.39990000	0.14446200
C	0.25966900	-1.60480900	-0.57506600
C	-0.11255200	-1.54297700	0.81601900
C	-1.18555000	-0.57402700	0.89782300
C	-1.61341300	-0.22085100	-0.47068800
C	-0.73177800	-0.84066700	-1.36414200
H	1.81833200	0.53081600	1.14502400

C	1.30828800	-2.49174900	-1.17206200
H	0.86608400	-3.44899100	-1.48006500
H	1.76099600	-2.03605100	-2.05674000
H	2.10620500	-2.70476400	-0.45743100
C	0.44549400	-2.36344900	1.93958700
H	-0.12248700	-3.29711800	2.04687200
H	1.49140700	-2.62549200	1.76409100
H	0.39369000	-1.82846400	2.89073000
C	-1.92724800	-0.18516900	2.13850100
H	-2.79443400	-0.84487200	2.27937600
H	-1.29536200	-0.26613600	3.02555300
H	-2.29717300	0.84144700	2.07705700
C	-2.76348500	0.68325400	-0.78902900
H	-3.71755900	0.15739400	-0.65531600
H	-2.77742600	1.55787700	-0.13205000
H	-2.72071900	1.04449100	-1.81884400
C	-0.71958900	-0.75058800	-2.85792400
H	-1.05146700	-1.69752100	-3.30238400
H	-1.37831200	0.04053500	-3.22129700
H	0.28714200	-0.54798300	-3.23598000
Cl	1.05600100	2.59206200	-0.59300600

D-IN1i $E = -1104.77702310$ $\Delta H = 0.416631$ $\Delta G = 0.292388$

Ir	-0.85882500	0.12711800	-0.47328700
C	-1.46385300	1.56055900	-2.02881000
C	-2.57770200	0.73094300	-1.56554400
C	-0.47925800	0.69868400	-2.60017300
C	-2.28121500	-0.64649700	-1.94113300
C	-0.98127100	-0.67588200	-2.53830700
C	-1.22439400	0.19400500	2.07201700
O	-0.66440200	1.19126600	1.34333100
O	-1.46076700	-0.84294400	1.26657900
O	-1.45906400	0.24961600	3.26281400
C	2.51807400	-0.02214200	-0.07234500
H	2.46161700	0.85013200	-0.73387600
O	1.22099300	-0.31786200	0.48229600
H	1.00200100	0.35425500	1.16417200
C	-1.40199000	3.05323300	-1.92782700
H	-1.92595700	3.51131200	-2.77662600
H	-1.87691900	3.41140700	-1.01132300
H	-0.37154700	3.41538700	-1.93434100
C	-3.87135700	1.22985100	-0.99811300
H	-4.57779200	1.46543400	-1.80480500
H	-4.33644800	0.48219400	-0.35149100

H	-3.72334900	2.13630600	-0.40639500
C	0.79497100	1.11969900	-3.26645400
H	1.57667200	0.36461500	-3.15745500
H	0.62625200	1.26232200	-4.34205100
H	1.17215100	2.06409100	-2.86621800
C	-0.30433600	-1.87955900	-3.12063000
H	-0.58974100	-2.79280300	-2.59328800
H	-0.58578200	-2.00001400	-4.17513200
H	0.78353500	-1.79668500	-3.07502700
C	-3.18698200	-1.81658700	-1.71505200
H	-3.92129200	-1.88499200	-2.52779000
H	-2.62903400	-2.75493300	-1.68321500
H	-3.73379200	-1.72095100	-0.77405700
C	3.07130300	-1.21693700	-0.80829700
C	2.80782100	-2.52130800	-0.36974900
C	3.91185400	-1.02561400	-1.91293800
C	3.37438400	-3.61296000	-1.02949500
H	2.15564300	-2.67516200	0.48391700
C	4.48560700	-2.11824100	-2.56670200
H	4.12631500	-0.01654000	-2.25801400
C	4.21575200	-3.41562500	-2.12737200
H	3.16088600	-4.62005500	-0.68227600
H	5.13690300	-1.95487300	-3.42083000
H	4.65772700	-4.26729300	-2.63665000
H	3.17847400	0.23949200	0.76534300

D-TS2i	$E = -1104.76058068$	$\Delta H = 0.411090$	$\Delta G = 0.290755$
Ir	-0.80029700	-0.00567600	-0.52531300
C	-1.35912700	1.48266400	-2.04660500
C	-2.54552900	0.76936400	-1.56851300
C	-0.47549300	0.53349000	-2.65005300
C	-2.38005400	-0.62044200	-1.89699900
C	-1.07929500	-0.78870200	-2.52059100
C	-1.16864400	-0.21724800	2.11015900
O	-0.54966000	0.91567600	1.53086100
O	-1.35919700	-1.11945100	1.18280900
O	-1.45614800	-0.26380400	3.28280800
C	2.37269000	0.11402700	-0.13540400
H	2.29270300	0.96645300	-0.82624500
O	1.11740600	-0.24273500	0.40976900
H	0.48714500	0.52027700	1.23417900
C	-1.15576500	2.96323600	-1.95641200
H	-1.66382500	3.46584800	-2.78944000
H	-1.56468800	3.36516800	-1.02615500

H	-0.09695900	3.22830200	-1.99921000
C	-3.75428600	1.40671300	-0.95369900
H	-4.43898900	1.75830400	-1.73621400
H	-4.30104200	0.70346700	-0.32149600
H	-3.48258200	2.26712000	-0.33701600
C	0.80228000	0.83482100	-3.36971100
H	1.53748200	0.03710200	-3.24584700
H	0.60283500	0.93635600	-4.44454000
H	1.25102500	1.77040300	-3.02830600
C	-0.54021700	-2.05925000	-3.10296100
H	-0.87161400	-2.93108400	-2.53427800
H	-0.88736000	-2.18149300	-4.13750000
H	0.55157900	-2.06408400	-3.11252200
C	-3.36828800	-1.71368000	-1.63696800
H	-4.00246500	-1.85652500	-2.52112900
H	-2.86992900	-2.66229400	-1.42495400
H	-4.01579300	-1.47886600	-0.79006800
C	3.05577700	-1.04664500	-0.83609900
C	2.74300400	-2.37107600	-0.50527100
C	4.04283000	-0.80552800	-1.80206600
C	3.40101500	-3.43152800	-1.13307200
H	1.97968100	-2.55922300	0.24274000
C	4.70475200	-1.86495500	-2.42595700
H	4.29742500	0.21885000	-2.06733600
C	4.38311000	-3.18342900	-2.09468200
H	3.14703800	-4.45423700	-0.86685300
H	5.46698800	-1.66082600	-3.17330700
H	4.89348500	-4.00959400	-2.58193900
H	3.00886100	0.45019400	0.69878700
D-IN3i $E = -1104.78442141$ $\Delta H = 0.416655$ $\Delta G = 0.294307$			
Ir	-0.55276600	0.32089800	0.10381300
C	-1.12511300	1.76096800	-1.42071200
C	-2.33069100	1.11228900	-0.89591300
C	-0.30513100	0.76335700	-2.05514800
C	-2.23309600	-0.28563100	-1.17526900
C	-0.96149500	-0.51188100	-1.85560600
C	-0.91394500	-0.47730700	3.14145100
O	0.38229900	-0.22217900	3.38845900
O	-1.34853800	-0.30145700	1.89271300
O	-1.65885900	-0.85261600	4.02889800
C	2.46316700	0.66634500	0.47496500
H	2.37710400	1.42473700	-0.31511500
O	1.20320300	0.38783600	1.04824800

H	0.83406400	0.04009700	2.54137800
C	-0.86087800	3.23280800	-1.38779500
H	-1.32575100	3.71444500	-2.25792000
H	-1.27863500	3.69360200	-0.48962800
H	0.20899100	3.45166700	-1.41517200
C	-3.47176400	1.81523800	-0.22865400
H	-4.17504900	2.19321500	-0.98168400
H	-4.01928900	1.14741400	0.43920300
H	-3.12634800	2.66719200	0.36237900
C	0.94279600	0.99923100	-2.85013400
H	1.65911900	0.18323700	-2.73260200
H	0.69984900	1.07943700	-3.91748800
H	1.43832700	1.92786900	-2.55663000
C	-0.47706400	-1.83007000	-2.36977500
H	-0.81418400	-2.65595700	-1.73962300
H	-0.87138200	-1.99753800	-3.38073900
H	0.61278300	-1.86541000	-2.42381700
C	-3.24104800	-1.33946100	-0.83772100
H	-3.90036500	-1.52387300	-1.69520900
H	-2.75797100	-2.28424300	-0.57625500
H	-3.86109700	-1.04267800	0.01005000
C	3.17152200	-0.56153100	-0.07407200
C	2.86954600	-1.84701600	0.39125200
C	4.18570300	-0.40852900	-1.02994100
C	3.56737600	-2.95678100	-0.09187200
H	2.08942200	-1.97209300	1.13490000
C	4.88728700	-1.51605500	-1.50904400
H	4.43197000	0.58562800	-1.39768800
C	4.57797000	-2.79589800	-1.04198900
H	3.32322300	-3.94823800	0.28019200
H	5.67136300	-1.38055700	-2.24923300
H	5.12115300	-3.65966500	-1.41500100
H	3.08720300	1.11067600	1.26666200
D-IN4i	$E = -1104.78034610$	$\Delta H = 0.416895$	$\Delta G = 0.293435$
Ir	-0.10878900	-0.64552900	-0.00179800
C	-0.41468900	-0.89022600	-2.12966600
C	-1.62482600	-0.29592600	-1.54426100
C	-0.22226100	-2.18429900	-1.54415700
C	-2.17909300	-1.23553700	-0.61450600
C	-1.29324400	-2.37639100	-0.57069700
C	-1.26235900	1.30971300	1.98922200
O	-1.15667500	1.83668300	3.24221100
O	-0.26963100	0.49671000	1.71799100

O	-2.19553100	1.64356400	1.27788800
C	2.53919200	0.18970300	1.28922000
O	1.84976100	-0.59932700	0.32660700
H	-0.36432400	1.45097700	3.64628200
C	0.41796100	-0.26244400	-3.20278200
H	-0.03034500	-0.45538400	-4.18604600
H	0.48350400	0.82025700	-3.07132000
H	1.43426700	-0.66123100	-3.20919700
C	-2.22469800	1.02069700	-1.92335300
H	-3.03320500	0.87149500	-2.65120800
H	-2.62771300	1.52120100	-1.04147400
H	-1.48232400	1.68107100	-2.37820700
C	0.85010600	-3.17373700	-1.88119700
H	1.12343800	-3.77713500	-1.01192200
H	0.51062600	-3.85662800	-2.67038600
H	1.75544700	-2.67471300	-2.23337900
C	-1.49634700	-3.60708500	0.25546200
H	-2.01426700	-3.38161000	1.19037700
H	-2.10672100	-4.33051900	-0.30117100
H	-0.54637700	-4.08863300	0.49876200
C	-3.46177200	-1.08135600	0.14327800
H	-4.30170100	-1.45197600	-0.45870400
H	-3.44788100	-1.65122200	1.07619100
H	-3.64233200	-0.03606500	0.39454800
C	2.93943400	1.53964600	0.72580000
C	4.02484600	1.64348500	-0.15598300
C	2.21873600	2.69938600	1.04143100
C	4.38003500	2.87292600	-0.71226500
H	4.59756700	0.75174100	-0.40064200
C	2.57279500	3.93291300	0.48962300
H	1.37415500	2.63260600	1.72106100
C	3.65247000	4.02237400	-0.39121200
H	5.22650700	2.93671300	-1.39120300
H	2.00501900	4.82297100	0.74775800
H	3.92938100	4.98151800	-0.82046700
H	3.44577900	-0.37361600	1.55662500
H	1.95038600	0.32931000	2.20126500
D-TS5i	$E = -1104.75648813$	$\Delta H = 0.411090$	$\Delta G = 0.288604$
Ir	-0.21775500	-0.37438500	-0.05435400
C	-0.50359800	-0.33025600	-2.24694200
C	-1.79308700	-0.26105400	-1.58340800
C	0.12477800	-1.57362800	-1.88030500
C	-1.95942300	-1.49585500	-0.84027800

C	-0.79013200	-2.31086700	-1.01879900
C	-2.00715300	0.53133900	2.21549700
O	-2.27857700	0.50667700	3.55555700
O	-0.91048700	-0.11482400	1.93302000
O	-2.77704900	1.12206900	1.46857600
C	1.60655000	0.74811200	0.85421800
O	1.62246300	-0.55552800	1.04425500
H	-1.56199400	0.00402100	3.97290500
C	0.02994200	0.68022300	-3.21588900
H	-0.35081500	0.46707700	-4.22308300
H	-0.28226700	1.69289600	-2.95012200
H	1.12073700	0.66473700	-3.26303100
C	-2.84552100	0.79070100	-1.76280100
H	-3.61379600	0.45123300	-2.47001600
H	-3.31695600	1.02153200	-0.80608800
H	-2.41726700	1.71665700	-2.15516100
C	1.43318900	-2.09386000	-2.39264200
H	1.93546400	-2.71533100	-1.64717000
H	1.26908000	-2.71227400	-3.28474100
H	2.11077800	-1.28353800	-2.66911600
C	-0.57120300	-3.69530600	-0.48881700
H	-1.11476100	-3.85808900	0.44478000
H	-0.91623700	-4.44565200	-1.21260700
H	0.48705200	-3.88563400	-0.29235100
C	-3.17902700	-1.85496200	-0.04951000
H	-3.94638000	-2.26118100	-0.72099500
H	-2.96306400	-2.61386300	0.70614700
H	-3.59164700	-0.97567800	0.44871800
C	2.63061400	1.39174200	-0.04210500
C	3.63506700	0.62101500	-0.63903100
C	2.61621100	2.77954100	-0.23866200
C	4.60248700	1.23082900	-1.43995700
H	3.65514000	-0.44774500	-0.45410400
C	3.57917800	3.38623100	-1.04342200
H	1.84538300	3.38270600	0.23674800
C	4.57349300	2.61163000	-1.64894200
H	5.38415500	0.62886400	-1.89530400
H	3.55771100	4.46161000	-1.19585900
H	5.32661300	3.08455600	-2.27292700
H	1.34502300	1.36193300	1.73090500
H	0.33713700	1.19405800	0.19058600
D-IN6i	$E = -1104.76238750$	$\Delta H = 0.413391$	$\Delta G = 0.291549$
Ir	-0.29030200	-0.06252800	-0.05056000

C	-0.63481400	-0.16527400	-2.21865400
C	-1.90240200	-0.27401400	-1.50794000
C	0.15138700	-1.31088700	-1.86186200
C	-1.91566600	-1.56779300	-0.82664200
C	-0.66861000	-2.19932500	-1.03352000
C	-2.17999800	0.68169700	2.20438000
O	-2.37385900	0.75398900	3.55540300
O	-0.98349400	0.25126100	1.91473000
O	-3.09351500	1.00550800	1.45788300
C	1.63111100	0.69783000	0.85875700
O	1.46129800	-0.55953500	1.11636600
H	-1.54822400	0.46001800	3.97044000
C	-0.27155400	0.88055300	-3.23034400
H	-0.57857100	0.55570700	-4.23305400
H	-0.76873600	1.83006400	-3.02139400
H	0.80508900	1.06369800	-3.25250800
C	-3.10255100	0.60474800	-1.69383400
H	-3.78974900	0.15874800	-2.42511800
H	-3.62342600	0.74395400	-0.74631600
H	-2.81485800	1.59205800	-2.06305700
C	1.48416500	-1.68214200	-2.43693200
H	2.07616700	-2.27288500	-1.73422600
H	1.33824700	-2.29279200	-3.33801500
H	2.06679200	-0.80419000	-2.72051700
C	-0.23509200	-3.54446000	-0.53603000
H	-0.85647000	-3.88810700	0.29402200
H	-0.30593000	-4.29135400	-1.33784400
H	0.80320200	-3.53285800	-0.19326100
C	-3.07736500	-2.07900800	-0.03357500
H	-3.84406000	-2.48172800	-0.70808900
H	-2.78472000	-2.87733500	0.65208000
H	-3.53199500	-1.27156000	0.54509300
C	2.71752800	1.19691400	-0.02448100
C	3.68997600	0.33017300	-0.54468900
C	2.82098800	2.57422500	-0.27518500
C	4.73567300	0.83229100	-1.31913500
H	3.62463500	-0.72888600	-0.31912500
C	3.86110700	3.07302400	-1.05639700
H	2.07829600	3.24975700	0.14291400
C	4.82078700	2.20225400	-1.58227800
H	5.49125800	0.15621800	-1.70991700
H	3.92928200	4.13982200	-1.24973600
H	5.63692100	2.59168500	-2.18424300
H	1.27658200	1.41889800	1.60575500

H	-0.40448200	1.51404700	-0.14597300
D-IN7i	$E = -759.31594568$	$\Delta H = 0.288899$	$\Delta G = 0.191189$
Ir	-0.76574200	0.22453000	-0.22908500
C	-0.76159200	-0.13374800	-2.37120900
C	-2.10465200	-0.23188100	-1.85517900
C	-0.00018700	-1.15571600	-1.69501500
C	-2.20946800	-1.45011100	-1.02791500
C	-0.92969700	-2.00969600	-0.92716900
C	-1.23622200	-0.36306700	2.63269000
O	-1.09419700	0.02803200	3.92451000
O	-0.75921200	0.54277200	1.79222600
O	-1.75486200	-1.43273300	2.37107600
H	-0.66777100	0.89909300	3.91071600
C	-0.26945100	0.81049500	-3.42742300
H	-0.39164400	0.36808700	-4.42465500
H	-0.82192900	1.75297700	-3.40952900
H	0.78890000	1.04575100	-3.29282900
C	-3.27161600	0.61107600	-2.26651600
H	-3.79427700	0.14595900	-3.11326100
H	-3.99267800	0.71772300	-1.45193200
H	-2.95570600	1.61037500	-2.57424700
C	1.44885900	-1.46280000	-1.91209200
H	1.91383100	-1.85895100	-1.00553400
H	1.55968000	-2.21899600	-2.70093600
H	2.00503300	-0.57359100	-2.21693200
C	-0.52959200	-3.23020700	-0.16042800
H	-1.21682700	-3.42215900	0.66410600
H	-0.51479500	-4.10940900	-0.81803500
H	0.47329600	-3.12249100	0.26222500
C	-3.47491900	-1.94610100	-0.40475100
H	-4.09061400	-2.46235900	-1.15315200
H	-3.27244500	-2.63637500	0.41416300
H	-4.07101900	-1.12198300	-0.00263700
H	-0.09387600	1.68331500	-0.28648500
B-IN1o	$E = -2165.03431454$	$\Delta H = 0.423906$	$\Delta G = 0.282712$
Ir	-0.96081500	-1.49292600	0.36798700
C	-2.22597100	-3.26242400	0.60608400
C	-2.93606000	-2.22082000	-0.12916800
C	-2.20151600	-1.98598200	-1.36143900
C	-1.03811600	-2.83334100	-1.37147000
C	-1.06023200	-3.62717400	-0.14573500
Cl	1.52682400	-1.39115500	0.78909000

H	0.25627700	1.74999200	-0.55835100
O	-0.81116700	0.63854000	0.32033700
C	-0.86088700	0.73953900	1.65604500
O	-0.59284900	1.78165900	2.26995300
O	-1.14629600	-0.42087800	2.19707600
K	1.98444300	1.60445700	1.62457600
H	1.77287800	0.80198400	-2.05039300
C	5.27384000	4.00464800	-2.83215400
C	5.14030100	2.66422300	-3.19919500
C	3.95505600	1.97761300	-2.92546600
C	2.88471300	2.62228200	-2.29271600
C	3.02681400	3.96947200	-1.92903000
C	4.21365800	4.65439500	-2.19449400
H	6.19660400	4.53914400	-3.04027600
H	5.96091300	2.14937000	-3.69144600
H	3.86119200	0.93045500	-3.20403900
H	2.20225500	4.47349000	-1.43417700
H	4.30947600	5.69827900	-1.90726700
C	1.59003600	1.88564100	-2.02684200
H	0.87031400	2.10933200	-2.83129500
O	1.05510300	2.29071700	-0.77042600
C	-0.03869000	-2.97241800	-2.47938400
H	0.96239100	-3.16744800	-2.08762300
H	-0.30767600	-3.80416300	-3.14395400
H	0.01304000	-2.06499900	-3.08609600
C	-0.06049200	-4.68380400	0.21062300
H	-0.03852200	-4.87031400	1.28648000
H	-0.31071700	-5.62727000	-0.29180400
H	0.94681400	-4.39403400	-0.09590000
C	-2.66883900	-3.85707700	1.90739800
H	-3.18082200	-3.11976000	2.53006400
H	-3.36549300	-4.68594400	1.72652400
H	-1.82364700	-4.24696700	2.47887000
C	-4.26598600	-1.63670200	0.23852500
H	-5.08209500	-2.25124100	-0.16414400
H	-4.39146400	-1.58487700	1.32272400
H	-4.38417600	-0.62494400	-0.15716200
C	-2.61084200	-1.03584700	-2.44399300
H	-3.28402700	-1.53992700	-3.14934400
H	-3.13864800	-0.16945200	-2.03873500
H	-1.74778000	-0.67197900	-3.00637900
B-TS2o	$E = -2164.97783256$	$\Delta H = 0.414814$	$\Delta G = 0.280148$
Ir	0.38114500	-1.08529100	0.15076100

C	-0.45023000	-3.04814500	0.71156600
C	-1.48851600	-2.26171000	0.09870200
C	-1.07447100	-1.91820500	-1.24748700
C	0.22279200	-2.54867100	-1.47740900
C	0.61535000	-3.22601600	-0.27411000
Cl	2.27079200	-0.88230500	1.76030600
H	0.03950300	1.53922100	0.48945900
O	-0.46121800	0.67842400	1.00810000
C	-0.53528200	0.81731800	2.41561500
O	-0.11441700	1.89822300	2.87570800
O	-0.97730500	-0.18117600	3.03457500
K	1.20375300	0.25414100	4.47935100
H	1.24496500	0.18091700	-0.75767200
C	5.51041900	1.85247300	-1.98510800
C	4.68653300	1.21189000	-2.91448700
C	3.32208900	1.07670600	-2.65734500
C	2.77049600	1.57686500	-1.47077600
C	3.59948000	2.22201500	-0.54514300
C	4.96292900	2.35898700	-0.80268300
H	6.57282100	1.96225300	-2.18515100
H	5.10551300	0.82715300	-3.84047800
H	2.67644000	0.59258900	-3.38739700
H	3.15266700	2.61770100	0.36080500
H	5.60105900	2.86431900	-0.08256200
C	1.29266800	1.44778400	-1.20238600
H	0.72696200	1.24577000	-2.13343200
O	0.74632200	2.25030000	-0.33462700
C	-1.90066600	-1.19394900	-2.26748400
H	-1.27457100	-0.68570200	-3.00499600
H	-2.55027800	-1.89361400	-2.80943400
H	-2.53740700	-0.43936600	-1.79974300
C	0.97178000	-2.55639700	-2.77495100
H	2.05238500	-2.57551500	-2.61665700
H	0.69992200	-3.44585100	-3.35853200
H	0.73477300	-1.68000500	-3.38214800
C	1.84300000	-4.06179600	-0.08363200
H	2.22391600	-3.98099900	0.93649600
H	1.61629100	-5.11781800	-0.27977000
H	2.64367000	-3.75722100	-0.76101200
C	-0.50401700	-3.63865000	2.08540700
H	-1.02992000	-2.96938800	2.76997100
H	-1.03134700	-4.60213900	2.07035500
H	0.49883000	-3.81389400	2.48163200
C	-2.75741200	-1.85308200	0.77963800

H	-3.32906200	-1.14641000	0.17488700
H	-3.38658900	-2.73376500	0.95878300
H	-2.52730000	-1.37798000	1.73836800
B-IN3o	$E = -1819.54706442$	$\Delta H = 0.296330$	$\Delta G = 0.184570$
Ir	0.40085300	-0.90943400	-0.10355200
C	0.16223600	-3.17134900	0.54766400
C	-1.12985600	-2.62986700	0.51589800
C	-1.33553600	-2.00943300	-0.80607800
C	-0.18339500	-2.30403900	-1.62409700
C	0.81126400	-2.90911500	-0.75372700
Cl	2.37673200	-0.29057600	1.31353900
H	-0.24040500	1.72323300	0.30853100
O	-0.63358200	0.94571800	0.73609500
C	-0.54329300	1.20622200	2.15943000
O	-0.05232500	2.31409200	2.44413800
O	-0.92276000	0.26505400	2.87491200
K	1.43632500	0.75481300	4.05914800
H	0.98189700	0.14973200	-1.14251300
C	-0.05896500	-2.10002400	-3.10439000
H	0.97673500	-1.91229700	-3.39630100
H	-0.40290600	-2.99637600	-3.63773000
H	-0.66101800	-1.25475400	-3.44584200
C	2.12520300	-3.49135900	-1.18350600
H	2.85868600	-3.45783500	-0.37399300
H	2.00624200	-4.54132200	-1.48495300
H	2.54425000	-2.94383300	-2.03116900
C	0.84470200	-3.84856200	1.69595900
H	0.28339600	-3.73123900	2.62588600
H	0.96007600	-4.92272300	1.50220100
H	1.84540400	-3.43466900	1.85381500
C	-2.63972400	-1.43342700	-1.26996400
H	-3.33999400	-2.23243300	-1.54938300
H	-3.11178500	-0.83870500	-0.48342200
H	-2.50488700	-0.78854300	-2.14157100
C	-2.14539400	-2.60105900	1.61928700
H	-3.11291700	-2.97434100	1.26355400
H	-1.83666700	-3.22885000	2.45888200
H	-2.28284300	-1.58494800	2.00135600
C-IN1o	$E = -1588.12605459$	$\Delta H = 0.515564$	$\Delta G = 0.374667$
Ir	0.13547900	-2.39827000	-0.97855100
C	-1.00732100	-4.32182500	-0.80313400
C	-1.68213300	-3.29072600	-0.07451800

C	-2.06465000	-2.24222300	-1.01879800
C	-1.59998700	-2.62447200	-2.32480800
C	-0.90421500	-3.89942200	-2.17907100
Cl	2.08435600	-3.12091600	0.28487700
C	2.30146000	0.90971300	-2.68595400
C	2.22421200	2.02078700	-3.52099600
C	0.98534400	2.58061400	-3.84719100
C	-0.17619400	2.01544100	-3.31478000
C	-0.10785300	0.90174000	-2.48004800
C	1.13255700	0.32002500	-2.15916600
H	3.26850000	0.47970200	-2.43602200
H	3.13866900	2.45238300	-3.91919300
H	0.92714400	3.44872200	-4.49695400
H	-1.14543300	2.45251400	-3.54136900
H	-1.00828300	0.48732500	-2.04407400
N	1.23330300	-0.79696200	-1.32411500
H	2.18897200	-0.92611700	-0.99639300
H	0.28565800	0.02356900	0.55450700
H	0.94175000	-0.49790200	2.71663800
C	-0.30639500	-4.68684800	-3.30304200
H	-1.06569800	-5.33885000	-3.75529500
H	0.07975700	-4.03014600	-4.08645600
H	0.51525500	-5.31864400	-2.95876500
C	-0.48542600	-5.60763100	-0.23836800
H	-0.17686600	-5.49321500	0.80261300
H	-1.26386200	-6.38030600	-0.27826000
H	0.37772000	-5.97218300	-0.79913900
C	-1.89659700	-1.95569500	-3.63147800
H	-2.73546200	-2.46109400	-4.12785000
H	-2.16823400	-0.90711000	-3.50394400
H	-1.03918000	-1.99567400	-4.30843900
C	-2.91016300	-1.05912400	-0.65664900
H	-3.92223000	-1.39331300	-0.39444500
H	-2.49879400	-0.52503100	0.20428100
H	-3.00137200	-0.35427600	-1.48532200
C	-2.03829300	-3.31002800	1.38000600
H	-3.03628200	-3.74575200	1.52228100
H	-1.32833300	-3.90562800	1.95829400
H	-2.05128500	-2.30111200	1.79909300
C	4.07892900	3.10088800	2.09433400
C	4.11439100	1.98063600	2.92772000
C	3.00603700	1.13617400	3.01305200
C	1.84386400	1.40557700	2.27853200
C	1.81788900	2.52913900	1.44237000

C	2.92807000	3.37032700	1.35002200
H	4.94340000	3.75523900	2.02154500
H	5.00914800	1.75686600	3.50260100
H	3.04423900	0.25728700	3.65298600
H	0.92466400	2.73178100	0.85974900
H	2.89465300	4.23577000	0.69337400
C	0.62404800	0.51230200	2.42093400
H	-0.01573000	0.89286200	3.22792300
O	-0.20537900	0.47304600	1.26560700
C-TS2o	$E = -1588.09427512$	$\Delta H = 0.507288$	$\Delta G = 0.372930$
Ir	0.46598500	-1.47870000	-0.80382100
C	-0.24823500	-3.49060900	-0.19664200
C	-1.16155900	-2.51262300	0.30818300
C	-1.72958900	-1.77826300	-0.81690800
C	-1.17323100	-2.34070800	-2.02488400
C	-0.22826400	-3.37110700	-1.65097900
Cl	2.86254700	-1.92946900	-0.61886500
C	1.00535700	0.46081000	-4.28498500
C	0.37648700	0.97293200	-5.42062800
C	-0.75172300	1.78760100	-5.29803500
C	-1.24140300	2.09488800	-4.02567300
C	-0.61763800	1.58806500	-2.88506000
C	0.50820800	0.76059300	-3.00926800
H	1.88721000	-0.16793300	-4.38149200
H	0.77381300	0.73678700	-6.40399200
H	-1.23664200	2.18829500	-6.18329300
H	-2.10612800	2.74407300	-3.91773700
H	-0.97115100	1.85140100	-1.89311400
N	1.14629500	0.25845600	-1.83239800
H	2.12944700	0.06300700	-2.02485800
H	1.11143900	1.07749900	-0.97701800
H	0.79730900	-0.24420500	0.58261800
C	0.52754100	-4.26830900	-2.58045300
H	-0.02263300	-5.20632300	-2.73285100
H	0.67462800	-3.80249500	-3.55754500
H	1.51117500	-4.51741100	-2.17620800
C	0.51202200	-4.50909300	0.59644300
H	0.65050500	-4.19199800	1.63256000
H	-0.02802800	-5.46469000	0.60591100
H	1.50243100	-4.68390000	0.17066900
C	-1.56688600	-1.97848000	-3.42111800
H	-2.44066400	-2.57186500	-3.72129400
H	-1.83232800	-0.92315200	-3.50676500

H	-0.76456600	-2.18323300	-4.13246600
C	-2.83923700	-0.77411400	-0.73883400
H	-3.81190600	-1.28215100	-0.69600600
H	-2.75583500	-0.14701400	0.15258900
H	-2.84561600	-0.11690100	-1.61127300
C	-1.53957900	-2.31197800	1.74313700
H	-2.41718100	-2.92573000	1.98528000
H	-0.73225100	-2.60485500	2.41737200
H	-1.80049100	-1.27144400	1.95110900
C	3.71746300	0.68600400	4.22644500
C	2.47244700	0.06946400	4.38067600
C	1.52844300	0.14169800	3.35645800
C	1.81764200	0.82283400	2.16659800
C	3.06461800	1.43956700	2.01972900
C	4.00855700	1.37258200	3.04511100
H	4.45339200	0.63578400	5.02438500
H	2.23639400	-0.45936800	5.30043100
H	0.55329800	-0.32470800	3.48418700
H	3.26773400	1.98121500	1.10192100
H	4.97253200	1.85988300	2.92440700
C	0.78568700	0.91416800	1.06085000
H	-0.23737000	0.89645500	1.48914500
O	0.98734700	1.79870400	0.09899300
C-IN3o $E = -1242.66287735$ $\Delta H = 0.388792$ $\Delta G = 0.278423$			
Ir	0.15431900	-0.65776300	-0.20469000
C	-0.30683900	-2.74237800	0.22541000
C	-1.46567900	-1.91860000	0.48086500
C	-1.86018600	-1.32726400	-0.77894300
C	-1.05132600	-1.95126200	-1.83835000
C	-0.10688900	-2.79382200	-1.23241600
Cl	2.63784200	-0.61742500	-0.01582400
C	1.07059800	1.24836700	-3.47859500
C	0.72637100	1.53204100	-4.80022000
C	-0.45186700	2.22336100	-5.09518400
C	-1.28693900	2.63384400	-4.05437900
C	-0.94895100	2.35735000	-2.72787400
C	0.23081700	1.66432800	-2.43966400
H	1.98574200	0.71004500	-3.24933900
H	1.38614600	1.21340900	-5.60217100
H	-0.71375100	2.44359800	-6.12564900
H	-2.20171100	3.17860500	-4.27000100
H	-1.59318100	2.68664900	-1.91650000
N	0.57077400	1.36082500	-1.07502300

H	1.58239600	1.39398400	-0.92667400
H	0.14394500	2.03192700	-0.44211100
H	0.16940500	0.19521800	1.13575200
C	0.95562600	-3.61140900	-1.89968500
H	0.71798600	-4.68137500	-1.83934200
H	1.06277700	-3.35276000	-2.95578900
H	1.92696300	-3.46220100	-1.41817400
C	0.38913700	-3.63366100	1.21154900
H	0.32630900	-3.23164400	2.22562300
H	-0.06016300	-4.63631900	1.21853000
H	1.44858800	-3.74535500	0.96781600
C	-1.24382000	-1.70036600	-3.30309900
H	-2.10325600	-2.27096500	-3.67994300
H	-1.44135700	-0.64518100	-3.51067800
H	-0.36879600	-1.99708200	-3.88609900
C	-3.09456300	-0.50967400	-1.02569900
H	-3.94558900	-1.15532700	-1.28367000
H	-3.37368600	0.06976200	-0.14177100
H	-2.95191400	0.19007300	-1.85400700
C	-2.18557900	-1.78082500	1.79005200
H	-2.96208800	-2.55299700	1.87455300
H	-1.50543300	-1.89683200	2.63683300
H	-2.67210700	-0.80676100	1.88278400

D-TS1o $E = -1104.73758580$ $\Delta H = 0.407026$ $\Delta G = 0.286792$

Ir	-0.00421100	-0.22037200	-0.14633700
C	-1.03479200	-0.02178800	-2.05924700
C	-0.60024600	1.29208900	-1.64528400
C	0.84005300	1.29932300	-1.55255500
C	1.30044300	-0.03332300	-1.91516900
C	0.15849500	-0.83989900	-2.24714000
H	-0.68363300	-1.68207100	0.47893900
O	-0.64512000	0.63933300	1.69684500
C	0.34459500	0.23050700	2.42839300
O	1.23248100	-0.51304500	1.58259700
O	0.58181200	0.39483700	3.59999300
H	1.10445800	-1.59547600	1.83799400
C	-4.19945100	-3.08178200	3.37845600
C	-4.11188400	-3.56472400	2.06951200
C	-2.89864100	-3.50188900	1.38606800
C	-1.76488100	-2.95819700	2.00658600
C	-1.85639400	-2.48040200	3.32167500
C	-3.07089000	-2.54034700	4.00151200
H	-5.14452300	-3.12924800	3.91225800

H	-4.98561700	-3.99435700	1.58766600
H	-2.82315300	-3.88500800	0.37050000
H	-0.97320500	-2.06700600	3.79727500
H	-3.13798800	-2.16621700	5.01905100
C	-0.46140200	-2.91859400	1.27679300
H	-0.45065500	-3.52823500	0.35731400
O	0.64599200	-2.79967500	1.92887200
C	2.73569600	-0.45521900	-1.99629200
H	3.33448900	0.00654000	-1.20725300
H	2.84261500	-1.53863000	-1.90897600
H	3.16276800	-0.15138200	-2.96055300
C	0.18547400	-2.23615800	-2.79220300
H	0.27187100	-2.21545400	-3.88643100
H	1.03258000	-2.80662000	-2.40330100
H	-0.72876000	-2.78178200	-2.54680400
C	-2.43951600	-0.42161600	-2.39984300
H	-2.65198700	-0.21673600	-3.45742600
H	-2.60713200	-1.48752600	-2.22671200
H	-3.16811700	0.12857300	-1.79962300
C	-1.49879100	2.45801500	-1.37050000
H	-1.64361200	3.04332900	-2.28755200
H	-2.48185700	2.13235000	-1.02300600
H	-1.07831700	3.12153900	-0.61178800
C	1.71073500	2.48076400	-1.25189500
H	1.96211400	3.01852700	-2.17603400
H	1.21460700	3.18804100	-0.58289900
H	2.64926700	2.17847900	-0.78070100

D-IN2o $E = -759.30680293$ $\Delta H = 0.288527$ $\Delta G = 0.192836$

Ir	-0.11580100	-0.25507300	-0.11165200
C	-1.20552200	0.28513100	-1.87126900
C	-0.44646600	1.52411700	-1.61850100
C	0.92058000	1.21162100	-1.66091600
C	1.05877000	-0.22679000	-1.95059800
C	-0.25317500	-0.76188500	-2.20112000
H	-0.48565400	-1.72442700	0.39529700
O	-1.07104000	0.39942600	1.72439200
C	-0.16741000	0.13480000	2.58666400
O	1.05532400	-0.13707300	1.83573100
O	-0.15305900	0.07356000	3.79252400
H	1.56804500	-0.82703800	2.28719600
C	-0.58156000	-2.11532700	-2.75638200
H	-1.55140800	-2.46992800	-2.39982800
H	-0.62122500	-2.07238500	-3.85277900

H	0.16947200	-2.85738500	-2.47627900
C	2.36545400	-0.91762000	-2.20894400
H	2.71725400	-0.71136000	-3.22861100
H	3.14182700	-0.57662500	-1.51814800
H	2.27351800	-2.00086400	-2.10046100
C	2.07871300	2.13326300	-1.42949900
H	2.60439000	2.33447400	-2.37168300
H	1.75892900	3.09179100	-1.01501200
H	2.80741100	1.69621200	-0.73947600
C	-1.07466900	2.85349500	-1.33143600
H	-1.41245200	3.32988600	-2.26087500
H	-1.94928000	2.74894900	-0.68329800
H	-0.37604100	3.53520500	-0.84098200
C	-2.69185900	0.22093400	-2.05864700
H	-3.21309000	0.83041600	-1.31549600
H	-2.97209900	0.59283200	-3.05342100
H	-3.05958300	-0.80338200	-1.96606800

S1.2 Imine formation

PhCH=NPh	$E = -556.49404862$	$\Delta H = 0.222211$	$\Delta G = 0.150018$
C	-1.19659800	2.71247500	-0.39671200
C	-0.96197600	4.08361500	-0.45203200
C	0.25741500	4.60878700	-0.01459100
C	1.24059600	3.74865500	0.47837100
C	1.01999600	2.37255700	0.51970700
C	-0.19961900	1.83741700	0.06701900
H	-2.14334600	2.29200800	-0.72165900
H	-1.73668600	4.74647200	-0.82699000
H	0.43341200	5.67996800	-0.04333200
H	2.18218500	4.15078000	0.84204000
H	1.77559700	1.71213300	0.93439200
N	-0.50228200	0.46436800	0.10674800
C	-0.23058800	-4.61925900	0.08628300
C	-1.25540000	-3.74145400	0.45878600
C	-1.06362100	-2.36680700	0.37819900
C	0.16132600	-1.84915500	-0.07942100
C	1.18342400	-2.73692000	-0.45044600
C	0.98887900	-4.11502100	-0.36835100
H	-0.38458600	-5.69251500	0.15154900
H	-2.20363600	-4.13476000	0.81368100
H	-1.84775000	-1.67379200	0.66485600
H	2.13203800	-2.34080900	-0.80440200
H	1.78597300	-4.79327400	-0.65814700

C	0.39831000	-0.40342100	-0.17359500
H	1.40221500	-0.10868600	-0.51195300
H ₂ O	$E = -76.42668152$	$\Delta H = 0.026140$	$\Delta G = -0.003485$
O	-1.07291300	-0.38706400	0.00000000
H	-0.10801300	-0.33572700	0.00000000
H	-1.34662700	0.53964500	0.00000000

S1.3 Imine reduction

BC-IN8i	$E = -1511.66175220$	$\Delta H = 0.481795$	$\Delta G = 0.351563$
Ir	0.96017600	-0.58279600	-0.42958900
C	0.50558000	-2.68153400	0.03057700
C	-0.43765200	-1.84289300	0.74496900
C	-1.23983900	-1.16242100	-0.23589600
C	-0.88948300	-1.68546900	-1.55216700
C	0.17396000	-2.60267200	-1.39426100
Cl	3.27222800	-0.81521400	-1.16092900
H	1.72857000	-0.36539100	0.92582500
C	0.87280600	-3.39046400	-2.45876300
H	0.66195900	-4.46078500	-2.34441700
H	0.55421300	-3.09190900	-3.45973400
H	1.95693200	-3.25470600	-2.39673000
C	1.45560100	-3.67780500	0.62682400
H	1.74655300	-3.39485300	1.64100700
H	0.99475700	-4.67313600	0.67471100
H	2.36792100	-3.75683300	0.03094800
C	-1.58978400	-1.29730900	-2.81768200
H	-2.58737400	-1.75461200	-2.85234300
H	-1.72602300	-0.21404000	-2.88136900
H	-1.04567800	-1.62530800	-3.70573200
C	-2.43057500	-0.29949600	0.04544800
H	-3.33989200	-0.91543100	0.07504900
H	-2.34485500	0.21210700	1.00539400
H	-2.57171300	0.45762700	-0.72873200
C	-0.63034200	-1.78785100	2.23176500
H	-1.40690500	-2.50284300	2.53339400
H	0.28642500	-2.04735600	2.76573000
H	-0.94436900	-0.79536000	2.56216800
C	1.59985300	0.91459500	-3.78828300
C	2.36074200	1.29144000	-4.88919400
C	3.20510000	2.40544700	-4.82242600
C	3.27089900	3.13752800	-3.63744400
C	2.51437200	2.76230400	-2.52605500

C	1.67437900	1.63567900	-2.58314200
H	0.94992800	0.04724200	-3.83959500
H	2.29526800	0.71374800	-5.80741000
H	3.79562500	2.70020100	-5.68490500
H	3.91138500	4.01319600	-3.57218100
H	2.55511000	3.36125000	-1.62188900
N	0.80433300	1.30650800	-1.52053300
C	-1.60233000	3.62102600	2.40190500
C	-0.42249300	3.05922700	2.90151900
C	0.45447700	2.39616300	2.04551700
C	0.16277300	2.27216000	0.67625300
C	-1.01444100	2.85311700	0.18146400
C	-1.89075200	3.52034600	1.03949800
H	-2.28345200	4.14250200	3.06853800
H	-0.18437600	3.14351100	3.95841300
H	1.37198800	1.96229900	2.43617300
H	-1.22314500	2.78592400	-0.88140400
H	-2.79600900	3.97017900	0.64029600
C	1.13750600	1.61127400	-0.23592000
H	2.18469500	1.83967300	-0.01545600

BC-TS9i	$E = -1511.65403222$	$\Delta H = 0.479781$	$\Delta G = 0.349964$
Ir	0.83378600	-0.69602200	-0.57932300
C	0.43792600	-2.78433900	0.04708200
C	-0.48388700	-1.94066000	0.74718500
C	-1.30870200	-1.25792000	-0.23196700
C	-0.94320400	-1.75500900	-1.54442100
C	0.14708600	-2.66404500	-1.38720300
Cl	3.21539800	-0.95850600	-1.10205600
H	1.49090500	0.29185900	0.58283900
C	0.81905400	-3.47094600	-2.45529800
H	0.43624100	-4.49973800	-2.45098500
H	0.64499800	-3.05366400	-3.44958400
H	1.89908000	-3.51278900	-2.29562900
C	1.41856000	-3.74623500	0.64553600
H	1.70924100	-3.44533300	1.65486100
H	0.98426000	-4.75290000	0.70604500
H	2.32867600	-3.80781700	0.04437700
C	-1.62524800	-1.37492200	-2.82317900
H	-2.57638400	-1.91530900	-2.91724500
H	-1.84620800	-0.30490400	-2.85613300
H	-1.01712000	-1.62132300	-3.69597300
C	-2.49141800	-0.38867900	0.06849400
H	-3.39269100	-1.00410600	0.19286200

H	-2.35247600	0.18467500	0.98743500
H	-2.68419200	0.31856700	-0.74132200
C	-0.62431500	-1.82140600	2.23527100
H	-1.37884800	-2.53128100	2.59849700
H	0.31463400	-2.04422300	2.74743000
H	-0.94328300	-0.81976500	2.53304600
C	1.71413800	0.92766000	-3.76064300
C	2.44983300	1.37158500	-4.85392800
C	3.19449900	2.55419700	-4.78136800
C	3.18431600	3.28716100	-3.59494500
C	2.44747400	2.85021700	-2.49289000
C	1.70821800	1.65320700	-2.55472800
H	1.15281000	0.00072300	-3.81245200
H	2.44777000	0.78672300	-5.77020300
H	3.76878600	2.89739600	-5.63684400
H	3.74655200	4.21474400	-3.52220200
H	2.42322300	3.45654900	-1.59214500
N	0.86970500	1.25326300	-1.49848300
C	-1.50530600	3.70309800	2.35156600
C	-0.34409100	3.13456200	2.88505300
C	0.52834600	2.42522400	2.06146000
C	0.24781600	2.26741500	0.69551900
C	-0.91117200	2.84757600	0.16511900
C	-1.78271700	3.56109000	0.99079500
H	-2.18322500	4.26006000	2.99220400
H	-0.11691700	3.24860200	3.94132900
H	1.43278100	1.98694600	2.47838600
H	-1.10980300	2.73946100	-0.89600700
H	-2.67636300	4.01162800	0.56742500
C	1.22111000	1.54988800	-0.19641500
H	2.26498200	1.84555700	-0.02703700

BC-IN10i $E = -1511.68780553$ $\Delta H = 0.485387$ $\Delta G = 0.353789$

Ir	0.63899400	-1.12786900	-0.21440400
C	0.06570200	-3.31286500	-0.22910700
C	-1.10350000	-2.49619200	-0.07044100
C	-1.22662800	-1.65125600	-1.25403100
C	-0.11459200	-1.93104000	-2.12345200
C	0.70939500	-2.93935700	-1.46149200
Cl	1.67894700	-1.29131400	1.99150100
H	2.58150600	0.80939600	1.17974100
C	1.93869000	-3.56749200	-2.04192700
H	1.66723800	-4.43029100	-2.66496400
H	2.48686700	-2.86204700	-2.67108000

H	2.61664900	-3.91856400	-1.26078800
C	0.53965300	-4.36277900	0.72834700
H	0.31166600	-4.09517300	1.76172600
H	0.05165100	-5.32111000	0.50873200
H	1.61913500	-4.51307800	0.65916000
C	0.07597900	-1.43249000	-3.52214300
H	-0.36837600	-2.13982000	-4.23524100
H	-0.39709800	-0.46096400	-3.67506900
H	1.13414400	-1.33080800	-3.77340900
C	-2.40055400	-0.77556200	-1.56352600
H	-3.20449600	-1.38004700	-2.00457800
H	-2.79928500	-0.30423800	-0.66166400
H	-2.14415600	0.01041300	-2.27552100
C	-2.09833300	-2.57359000	1.04715800
H	-2.91527300	-3.26032300	0.78809500
H	-1.63803500	-2.93573200	1.96889500
H	-2.54047600	-1.59608700	1.25771900
C	1.99598400	1.48522800	-2.70037400
C	1.74202200	2.18610600	-3.87992600
C	0.51785100	2.83412300	-4.06528400
C	-0.44707300	2.77820800	-3.05716700
C	-0.19572300	2.07774000	-1.87442200
C	1.02544300	1.41299900	-1.68689800
H	2.94691300	0.98001400	-2.55374600
H	2.50230600	2.22516300	-4.65573100
H	0.32094900	3.38216600	-4.98229500
H	-1.39661400	3.29192700	-3.18339400
H	-0.93566500	2.05159900	-1.08123000
N	1.30490600	0.70268700	-0.47506800
C	0.18069500	4.78597900	2.40723700
C	1.17157700	5.03733100	1.45792900
C	1.81026400	3.97345900	0.81453900
C	1.47202200	2.64756800	1.10988800
C	0.47380300	2.40588800	2.06671500
C	-0.16602400	3.46532000	2.70974700
H	-0.31647700	5.61083100	2.91051600
H	1.44887200	6.05987900	1.21543700
H	2.58129200	4.17523200	0.07459600
H	0.21052300	1.37996200	2.30883300
H	-0.93106900	3.26148600	3.45461300
C	2.18032600	1.48698100	0.42819800
H	3.02232000	1.87980400	-0.15738800

B-IN11i $E = -2376.06722588$ $\Delta H = 0.524702$ $\Delta G = 0.371891$

Ir	0.67404100	-0.69606700	0.05999200
C	1.85376800	-2.15603900	1.31493100
C	0.50059200	-2.64984600	1.05004800
C	0.34859500	-2.82037500	-0.37116700
C	1.56483100	-2.32927000	-1.00302900
C	2.50494400	-1.98280100	0.06527000
H	0.09987100	1.56300600	-1.78467200
C	3.91833800	-1.53913900	-0.14684400
H	4.56965300	-2.41738500	-0.24573600
H	4.01781800	-0.94125000	-1.05433700
H	4.28031800	-0.93817100	0.68918000
C	2.42217100	-1.91164800	2.68218600
H	1.99839700	-1.00802400	3.13435900
H	2.21222700	-2.76328600	3.33917500
H	3.50681400	-1.78539500	2.63846800
C	1.89515600	-2.41588600	-2.46201100
H	2.36853100	-3.37954500	-2.69372800
H	0.99669100	-2.32796600	-3.07797200
H	2.58465500	-1.62303100	-2.76121300
C	-0.79008700	-3.48558800	-1.07535700
H	-0.58067900	-4.55985800	-1.16618100
H	-1.73069600	-3.36739400	-0.53643400
H	-0.92788700	-3.08713600	-2.08242200
C	-0.45386700	-3.07950900	2.11940700
H	-0.14560700	-4.05448400	2.51993600
H	-0.46325900	-2.36808000	2.94893600
H	-1.47056800	-3.18021400	1.73868300
C	-3.04936800	-0.74649800	-1.87700900
C	-4.24788400	-1.46120900	-1.81796400
C	-4.73116500	-1.95726800	-0.60786600
C	-3.99076900	-1.71453100	0.55473900
C	-2.79619200	-1.00195700	0.50306400
C	-2.28124300	-0.49877700	-0.71649000
H	-2.71638100	-0.37753500	-2.83895700
H	-4.80794900	-1.62679900	-2.73544200
H	-5.66910800	-2.50323600	-0.56535000
H	-4.35557100	-2.06885800	1.51613000
H	-2.25213500	-0.80491800	1.42031400
N	-1.08039000	0.24504800	-0.70597500
C	-3.63227100	4.51907400	-2.04241100
C	-3.49855200	3.66475900	-3.13702400
C	-2.63445900	2.56881500	-3.06662200
C	-1.89062100	2.30610700	-1.90950200
C	-2.02575300	3.17815100	-0.81708200

C	-2.89217300	4.26998800	-0.88282700
H	-4.30712600	5.36964400	-2.09017400
H	-4.06866600	3.84628200	-4.04468400
H	-2.53674100	1.90754800	-3.92505100
H	-1.44650500	3.01029700	0.08796700
H	-2.98598500	4.93213800	-0.02560100
C	-0.90345200	1.14628400	-1.85974000
H	-0.93478400	0.60924200	-2.82171600
Cl	2.09611800	1.31551000	-0.46937800
O	-0.28075100	0.60733500	1.84411200
C	0.43181200	1.67570700	2.45198200
O	0.01555900	2.82340600	2.17029100
O	1.40613600	1.32951800	3.14976500
K	2.55483800	3.36692600	1.83011300
H	-0.89963600	0.98959600	1.18178000
B-TS12i	$E = -2376.05825812$	$\Delta H = 0.519875$	$\Delta G = 0.366031$
Ir	2.03911900	-1.43749400	-4.77752300
C	3.04481000	-2.96477800	-3.50292600
C	1.71124900	-3.41533000	-3.90094900
C	1.69931600	-3.53966500	-5.33997300
C	2.97643900	-3.08002600	-5.84314900
C	3.81634900	-2.77331900	-4.68494900
H	1.37389200	1.08491400	-6.42836200
C	5.25577300	-2.36865200	-4.74654300
H	5.88757800	-3.26263300	-4.83035800
H	5.45420600	-1.73068500	-5.60925500
H	5.55616300	-1.82114500	-3.85108900
C	3.49528700	-2.74787500	-2.08722200
H	3.18240100	-1.76141400	-1.72606600
H	3.07251100	-3.51393700	-1.42930700
H	4.58434400	-2.80547000	-2.01128100
C	3.44123500	-3.13016300	-7.26711800
H	3.92328500	-4.09292000	-7.48392100
H	2.60662700	-3.01066000	-7.96230400
H	4.16486700	-2.33915600	-7.47719600
C	0.59780100	-4.12845300	-6.16092300
H	0.76281900	-5.20965300	-6.26083000
H	-0.37957300	-3.97905700	-5.70115300
H	0.56907100	-3.70322300	-7.16625500
C	0.64862200	-3.87096800	-2.95017500
H	0.84702100	-4.90364000	-2.63300200
H	0.62439600	-3.24656600	-2.05370700
H	-0.34118200	-3.84504500	-3.40771800

C	-1.63821500	-1.43079000	-6.71926700
C	-2.82931500	-2.16058800	-6.71401400
C	-3.40205900	-2.58422900	-5.51504900
C	-2.76580100	-2.25856100	-4.31297900
C	-1.57987100	-1.52711900	-4.31177900
C	-0.98476800	-1.10092700	-5.51738600
H	-1.22373400	-1.11412900	-7.66907000
H	-3.31240200	-2.39318400	-7.65979500
H	-4.33303400	-3.14366900	-5.51393000
H	-3.20419200	-2.56128300	-3.36524100
H	-1.10705500	-1.26283000	-3.37158200
N	0.22063000	-0.33747100	-5.45946600
C	-2.52744600	3.83193500	-6.69890700
C	-2.32051000	3.02660900	-7.81905000
C	-1.39496400	1.98098800	-7.76582100
C	-0.65771800	1.72868500	-6.60240100
C	-0.86600800	2.54992400	-5.48189200
C	-1.79649400	3.58865000	-5.53222900
H	-3.25096300	4.64225300	-6.73330200
H	-2.88250400	3.20531100	-8.73223500
H	-1.24082700	1.35625000	-8.64297700
H	-0.28645300	2.38613600	-4.57493900
H	-1.94819700	4.21449800	-4.65623500
C	0.39400200	0.62990000	-6.56742500
H	0.43163300	0.12372600	-7.54118300
Cl	3.51780400	0.47810100	-5.49185000
O	1.10571200	-0.11381500	-3.24716500
C	1.80843200	0.94101600	-2.65710800
O	1.38961200	2.09755400	-2.92191300
O	2.80005800	0.62426600	-1.95526500
K	3.92521400	2.63669100	-3.25128800
H	0.48467400	0.11902500	-4.18049600
B-IN13i	$E = -2376.07697256$	$\Delta H = 0.525726$	$\Delta G = 0.373697$
Ir	2.05380300	-1.44631400	-4.92299800
C	2.71727300	-3.01372000	-3.55580000
C	1.58717400	-3.49944000	-4.31829400
C	1.98699200	-3.53159000	-5.72699300
C	3.31963100	-3.03447500	-5.82506100
C	3.77568200	-2.68379300	-4.47777800
H	1.11490900	0.83630600	-6.92235200
C	5.13525900	-2.19040000	-4.08929000
H	5.74589800	-3.01321900	-3.69387000
H	5.66165800	-1.76440100	-4.94626300

H	5.03939400	-1.41726000	-3.32259200
C	2.79946900	-2.83960100	-2.07206100
H	3.18969200	-1.84309600	-1.84076300
H	1.82028300	-2.94469400	-1.60020500
H	3.46670400	-3.59877000	-1.64382700
C	4.15298100	-2.94310100	-7.06543500
H	4.83578200	-3.80070200	-7.12556700
H	3.53583700	-2.94103100	-7.96707900
H	4.75254900	-2.03036200	-7.07151300
C	1.17117600	-4.10568700	-6.84501000
H	1.39664000	-5.17430200	-6.96055600
H	0.10077400	-4.01643600	-6.65047100
H	1.38759100	-3.61619500	-7.79780600
C	0.32269500	-4.07438800	-3.75871100
H	0.42862900	-5.15867700	-3.61802800
H	0.08064700	-3.63462900	-2.78920800
H	-0.52719200	-3.90523400	-4.42299500
C	-1.72344900	-1.86871900	-6.30772500
C	-2.90005800	-2.56942100	-6.03261600
C	-3.48309100	-2.50805300	-4.76537800
C	-2.87752400	-1.73561600	-3.77139600
C	-1.70571800	-1.02834400	-4.03925300
C	-1.12015900	-1.09097900	-5.31137800
H	-1.28106900	-1.92896900	-7.29646600
H	-3.36207600	-3.16305500	-6.81679600
H	-4.40061900	-3.05049400	-4.55712900
H	-3.32260700	-1.67240000	-2.78233300
H	-1.23252500	-0.42831600	-3.26819100
N	0.09996000	-0.36085500	-5.55809300
C	-2.54509900	3.91867100	-6.51706800
C	-2.72187500	2.97864600	-7.53256100
C	-1.88069200	1.86582400	-7.60808800
C	-0.84999000	1.68038900	-6.67926200
C	-0.67612800	2.63433700	-5.66200400
C	-1.52201300	3.74060900	-5.58121200
H	-3.20012100	4.78313200	-6.45229400
H	-3.51584000	3.10585100	-8.26348800
H	-2.02549400	1.13404200	-8.39914300
H	0.11572300	2.51376500	-4.92399100
H	-1.37945100	4.46775100	-4.78639300
C	0.08877200	0.49363700	-6.78500600
H	-0.16567400	-0.12545800	-7.64731800
Cl	3.34847800	0.41285700	-6.06968500
O	1.49754200	-0.07726300	-3.43077800

C	2.41534200	0.77846600	-2.90573300
O	2.06841700	1.99562800	-2.83717400
O	3.55315200	0.32973400	-2.55115800
K	4.43783900	2.38619900	-3.85825100
H	0.28672000	0.23709800	-4.73657800
PhCH ₂ NHPh	$E = -557.70894229$	$\Delta H = 0.246961$	$\Delta G = 0.171954$
H	-0.13863400	-0.86120900	0.90123900
H	0.29898100	-0.51646300	-1.67085200
C	-2.66576600	-0.64681800	1.12061500
C	-4.05024600	-0.58900100	1.01588300
C	-4.65965800	0.02802300	-0.08194000
C	-3.85109000	0.57999800	-1.07431300
C	-2.45887000	0.52307000	-0.98665600
C	-1.84104900	-0.08606200	0.12214200
H	-2.20287000	-1.12259900	1.98224000
H	-4.65999400	-1.03071000	1.79973000
H	-5.74140700	0.07244500	-0.16062400
H	-4.30345500	1.05798000	-1.93940200
H	-1.85873600	0.95159500	-1.78162900
N	-0.45957300	-0.12465100	0.28578300
C	4.58330100	-0.06976500	0.46874800
C	3.65542400	0.66299100	1.21340200
C	2.32406600	0.73059300	0.80440200
C	1.89855600	0.06318900	-0.35354700
C	2.83422700	-0.67297200	-1.08898200
C	4.16942100	-0.73708400	-0.68422800
H	5.62062200	-0.12086700	0.78698300
H	3.97020400	1.18525700	2.11256500
H	1.60270600	1.29915300	1.38438500
H	2.51495500	-1.20034800	-1.98441500
H	4.88276400	-1.31296200	-1.26707400
C	0.45703400	0.15561400	-0.81162100
H	0.25821700	1.17367000	-1.17219000
C-IN11i	$E = -1799.18335798$	$\Delta H = 0.616914$	$\Delta G = 0.462871$
Ir	0.48944900	-0.64324800	-0.48332200
C	0.04309300	-2.61759300	-1.54342100
C	-0.92432100	-1.58892800	-1.91513500
C	-0.19908400	-0.52188400	-2.56737800
C	1.20453500	-0.84741200	-2.53202100
C	1.33755100	-2.17056800	-1.91438100
Cl	2.70968400	-0.34082600	0.64269400
H	1.91879500	1.85404800	-0.45547300

C	2.62471100	-2.92353800	-1.78317700
H	2.87630200	-3.40445400	-2.73749400
H	3.44703700	-2.25859700	-1.51139300
H	2.56162700	-3.70302300	-1.02053200
C	-0.32003000	-3.94802400	-0.96106600
H	-1.10952400	-3.86066900	-0.21103400
H	-0.69275700	-4.61002800	-1.75400700
H	0.53638900	-4.43837600	-0.49443000
C	2.32491600	-0.08694000	-3.17404600
H	2.55461100	-0.50627000	-4.16249400
H	2.07127300	0.96642300	-3.31222500
H	3.23444400	-0.13622400	-2.57044100
C	-0.81558100	0.67003700	-3.23193500
H	-1.08833000	0.41500500	-4.26427300
H	-1.71949000	0.99813800	-2.71561100
H	-0.12429400	1.51425300	-3.26958700
C	-2.41098700	-1.77603500	-1.90209500
H	-2.71922900	-2.36657900	-2.77569300
H	-2.74244700	-2.31641900	-1.01110500
H	-2.94207100	-0.82394500	-1.93876400
C	-1.70827300	3.18184000	-0.02449300
C	-3.03877800	3.59081100	0.04887700
C	-4.08068300	2.67679500	0.21691800
C	-3.74883800	1.32226500	0.30559400
C	-2.42480700	0.89742300	0.23352800
C	-1.34089300	1.80766500	0.07570700
H	-0.94767700	3.94331200	-0.13333600
H	-3.25862400	4.65358800	-0.02777400
H	-5.11364100	3.00638600	0.27333500
H	-4.53285700	0.57672900	0.42473900
H	-2.20998500	-0.16258100	0.27344100
N	-0.02593300	1.36914300	0.05784800
C	2.03535300	5.25949300	2.83846400
C	2.20684900	5.56448200	1.48632700
C	1.83957900	4.63877300	0.50869300
C	1.30200000	3.39135000	0.85798800
C	1.13436600	3.09829400	2.21590400
C	1.49706400	4.02241200	3.19786400
H	2.31591500	5.97910500	3.60274500
H	2.62016300	6.52577200	1.19167700
H	1.96921100	4.88794300	-0.54300900
H	0.71433900	2.13848000	2.49821600
H	1.35759200	3.77479200	4.24713700
C	0.98612800	2.38035100	-0.24369900

H	0.72784200	2.94597200	-1.15680000
N	-0.06851500	-0.91572500	1.68673200
C	-0.62246200	-2.11730400	2.24798800
H	-0.64634100	-0.10033900	1.88397300
C	0.22154900	-3.19439300	2.54342100
C	-1.99550900	-2.21609300	2.49643400
C	-0.31123900	-4.36360100	3.08562900
H	1.28774100	-3.10741400	2.35357000
C	-2.52015700	-3.39305700	3.03444200
H	-2.64386300	-1.36990600	2.28774300
C	-1.68294700	-4.47045600	3.33017200
H	0.35056500	-5.19186300	3.32219800
H	-3.58595700	-3.45908300	3.23356300
H	-2.09354200	-5.38117700	3.75557100
H	0.86018000	-0.72857800	2.07159400
C-TS12i $E = -1799.15853239$ $\Delta H = 0.611243$ $\Delta G = 0.457438$			
Ir	0.72334700	-0.71471600	-0.84517500
C	-0.22338000	-2.54576900	-1.70531200
C	-1.02165900	-1.38101500	-2.03917800
C	-0.20143300	-0.52213300	-2.88309100
C	1.09368800	-1.11220500	-2.99780200
C	1.08757600	-2.37498300	-2.26188300
Cl	3.15132800	-0.38960000	-0.35361900
H	2.21775500	1.72447700	0.45399800
C	2.21339600	-3.36244700	-2.23148100
H	2.20931200	-3.97745700	-3.14120200
H	3.17941600	-2.85709100	-2.16889800
H	2.13519700	-4.03366000	-1.37291400
C	-0.71323900	-3.75573500	-0.97593000
H	-1.43999700	-3.49904500	-0.20398000
H	-1.20113600	-4.43694100	-1.68555100
H	0.10424600	-4.30022600	-0.49889200
C	2.23705900	-0.60403100	-3.82073900
H	2.25524700	-1.11205600	-4.79394200
H	2.15583300	0.46987600	-4.00398900
H	3.19225300	-0.78644400	-3.32436300
C	-0.68411200	0.69163200	-3.61294200
H	-1.08309700	0.39369500	-4.59199300
H	-1.48235800	1.19976800	-3.07047100
H	0.12181400	1.40795400	-3.78940700
C	-2.49253700	-1.21534500	-1.80456100
H	-3.06084800	-1.56102100	-2.67884500
H	-2.83004400	-1.79763800	-0.94370700

H	-2.75579300	-0.17023100	-1.62751100
C	-1.40601700	2.65073000	-0.89992100
C	-2.69894800	3.15587000	-1.04664000
C	-3.72434300	2.74532300	-0.19142800
C	-3.43211400	1.83539300	0.82651700
C	-2.13710300	1.33860700	0.98153900
C	-1.10086800	1.71879400	0.10993700
H	-0.62508900	2.98349900	-1.57533800
H	-2.90389100	3.87675700	-1.83425400
H	-4.72906600	3.14175200	-0.30564300
H	-4.20914300	1.52589200	1.52078200
H	-1.91253800	0.67036600	1.80573200
N	0.21371600	1.18760000	0.30075900
C	0.81828400	4.99297300	3.67837000
C	0.76995200	5.46495700	2.36657500
C	0.89975800	4.57510500	1.29693900
C	1.08478500	3.20483700	1.51692000
C	1.13384500	2.74381800	2.84161600
C	1.00125400	3.62690000	3.91248000
H	0.71627500	5.68196500	4.51237700
H	0.62796500	6.52493400	2.17299500
H	0.86024300	4.95041400	0.27718300
H	1.28046200	1.68359900	3.03301300
H	1.04526100	3.25081200	4.93126300
C	1.26095900	2.23872400	0.35672500
H	1.31194400	2.80361000	-0.58296100
N	0.67286300	-1.00234400	1.33321700
C	-0.01477800	-1.98394000	2.08640700
H	0.32688300	0.16873200	1.21754000
C	0.69982700	-2.84974600	2.93401700
C	-1.41462000	-2.10372500	2.03625200
C	0.03475200	-3.79561700	3.71312700
H	1.78338100	-2.76930700	2.98231200
C	-2.07409800	-3.04821900	2.82331100
H	-1.98067000	-1.45185200	1.38053800
C	-1.35712900	-3.90124200	3.66570200
H	0.60977300	-4.45105500	4.36179000
H	-3.15779100	-3.11701000	2.77509400
H	-1.87455500	-4.63606300	4.27516500
H	1.66394100	-1.01952200	1.57246400
C-IN13i	$E = -1799.18025814$	$\Delta H = 0.617057$	$\Delta G = 0.461239$
Ir	0.75218400	-0.80420800	-0.74552900
C	-0.21206500	-2.53660200	-1.71848300

C	-0.95606700	-1.34301600	-2.04923100
C	-0.07326100	-0.47902200	-2.83448800
C	1.20302300	-1.09681500	-2.91788000
C	1.14195000	-2.36610200	-2.19110500
Cl	3.14026700	-0.37978800	-0.17543200
H	2.23689900	1.88839700	0.25918700
C	2.23661800	-3.38720400	-2.13559600
H	2.22865000	-4.00677900	-3.04231200
H	3.21637000	-2.91147100	-2.05892400
H	2.12022300	-4.04928200	-1.27431400
C	-0.75389400	-3.78575100	-1.10042600
H	-1.60862200	-3.59101700	-0.45310200
H	-1.07792500	-4.46739600	-1.89828700
H	0.00185300	-4.30367500	-0.50618300
C	2.39423300	-0.60193900	-3.67888900
H	2.45678000	-1.11140900	-4.64953400
H	2.33646100	0.47255100	-3.86835200
H	3.32111900	-0.79527300	-3.13472400
C	-0.49169200	0.77751200	-3.53407300
H	-0.80529300	0.54196400	-4.55992400
H	-1.33623600	1.25518000	-3.03552800
H	0.32566100	1.50047800	-3.59945600
C	-2.42827900	-1.13078600	-1.86692100
H	-2.97246400	-1.41965700	-2.77642800
H	-2.82065100	-1.73163800	-1.04406600
H	-2.66102200	-0.08381000	-1.65893000
C	-1.58446400	2.56190400	-0.67756100
C	-2.92720200	2.94390700	-0.71314700
C	-3.82444600	2.47819400	0.24972800
C	-3.35992300	1.63300600	1.25947600
C	-2.01806100	1.25437500	1.30577200
C	-1.11931300	1.70338800	0.32818600
H	-0.90170300	2.93848000	-1.43056600
H	-3.26888500	3.61364400	-1.49769400
H	-4.86734600	2.77929600	0.22036700
H	-4.03954500	1.27404400	2.02730200
H	-1.66386400	0.60792300	2.10213500
N	0.25571700	1.27696500	0.37402400
C	0.98748400	5.33075300	3.39829700
C	0.63936300	5.67254800	2.09113000
C	0.72786600	4.72155000	1.07184200
C	1.16669600	3.41922200	1.34148000
C	1.52500100	3.09070000	2.65796600
C	1.43219300	4.03588000	3.67913700

H	0.91708100	6.06831800	4.19293500
H	0.29699600	6.67821000	1.86259700
H	0.45379800	4.99510700	0.05616500
H	1.88334100	2.08839300	2.88306100
H	1.71369500	3.76450300	4.69287100
C	1.26218200	2.37710300	0.24506600
H	1.14418700	2.83959500	-0.73684800
N	0.67188700	-1.30175600	1.30428400
C	-0.11275500	-2.23726800	1.96344900
H	0.41115100	0.76505900	1.24961300
C	0.46037500	-3.15084100	2.88326500
C	-1.52036700	-2.27318400	1.81928400
C	-0.32834100	-4.02905000	3.62226000
H	1.54080200	-3.15083400	3.01524100
C	-2.30058500	-3.16032400	2.55828000
H	-1.98991300	-1.57806600	1.13150200
C	-1.71798300	-4.04786000	3.46836400
H	0.15031300	-4.71005300	4.32236300
H	-3.38052800	-3.15264600	2.42610600
H	-2.33106800	-4.73491100	4.04396700
H	1.64272100	-1.41281200	1.58704800
Ph-IN11i	$E = -1858.32666210$	$\Delta H = 0.633547$	$\Delta G = 0.471256$
Ir	0.35604600	-1.15253000	-0.41619000
C	-0.23951400	-3.21498000	0.22541100
C	-1.38373000	-2.53275600	-0.38535700
C	-1.04292600	-2.22456700	-1.74513300
C	0.33671300	-2.63334000	-1.96284600
C	0.79157100	-3.31260800	-0.74827900
Cl	2.73755800	-0.67502200	-0.02539000
H	1.98836900	1.11159900	-1.45047800
C	2.10932400	-4.00376600	-0.59105800
H	2.03822900	-5.02448300	-0.98916700
H	2.90200000	-3.48315500	-1.13072500
H	2.41061500	-4.07071800	0.45608700
C	-0.22112900	-3.78039000	1.61264000
H	-0.78517800	-3.15374900	2.30783400
H	-0.67837200	-4.77858800	1.62152300
H	0.79724400	-3.87672600	1.99557000
C	1.06768100	-2.60873000	-3.27058300
H	0.86767500	-3.52754300	-3.83830500
H	0.75704100	-1.76115900	-3.88672600
H	2.14721600	-2.53528700	-3.12128300
C	-1.96167000	-1.67677300	-2.79023400

H	-2.45418600	-2.50989900	-3.30945500
H	-2.73721400	-1.04010700	-2.36311700
H	-1.42127900	-1.09398300	-3.53909800
C	-2.73188300	-2.40072700	0.25316200
H	-3.26708900	-3.35728000	0.18224200
H	-2.65465100	-2.14745000	1.31367900
H	-3.33991800	-1.63906700	-0.23572300
C	-1.68060000	1.97365200	-2.43701700
C	-3.00524200	2.33427500	-2.69751200
C	-4.02608700	2.02702100	-1.79986100
C	-3.69328400	1.35351300	-0.61888100
C	-2.37615100	0.99265200	-0.35112400
C	-1.32642000	1.28308100	-1.25602900
H	-0.92261700	2.25225400	-3.15810200
H	-3.23237700	2.86844100	-3.61704400
H	-5.05258100	2.31706800	-2.00390800
H	-4.46596200	1.11886200	0.10978400
H	-2.13664200	0.48769900	0.57833100
N	-0.00046100	0.92284500	-0.91720300
C	1.61098800	5.84491800	-1.41931700
C	1.95328500	5.16235000	-2.58871400
C	1.73189600	3.78831400	-2.68719500
C	1.17249700	3.06550700	-1.62307600
C	0.83211300	3.76197200	-0.45698500
C	1.04760600	5.13814400	-0.35549400
H	1.77779500	6.91564000	-1.34028800
H	2.38845800	5.70020700	-3.42710500
H	1.99754900	3.26550300	-3.60392000
H	0.38568400	3.22435400	0.37352200
H	0.77325200	5.65892600	0.55831700
C	1.03584800	1.55115200	-1.74794100
H	0.91102900	1.30137200	-2.81456400
O	0.05018400	0.13287300	1.56972400
C	1.00052800	0.28658300	2.64231400
H	1.71095500	1.07817400	2.37925600
H	1.57437200	-0.63924800	2.72285100
C	0.32148000	0.59998400	3.95825400
C	-0.77180100	1.47355800	4.03088700
C	0.82880800	0.05465100	5.14459700
C	-1.34442600	1.79165900	5.26291300
H	-1.17933500	1.90108400	3.11943500
C	0.26243500	0.37796900	6.37920800
H	1.67494700	-0.62754900	5.10066000
C	-0.82742800	1.24779500	6.44155400

H	-2.19320600	2.46908500	5.30341000
H	0.66898500	-0.05429500	7.28953700
H	-1.27315100	1.49802500	7.40023800
H	0.12231100	0.86407100	0.89621300
Ph-TS12i	$E = -1858.32326776$	$\Delta H = 0.629138$	$\Delta G = 0.470171$
Ir	0.96499800	-0.61847900	-0.93845000
C	0.44290500	-2.62958000	-1.71379400
C	-0.74868300	-1.78028600	-1.71533800
C	-0.49838300	-0.67838700	-2.60512000
C	0.86334400	-0.78733300	-3.09305500
C	1.41129600	-2.04044700	-2.58101800
Cl	3.37163700	-0.27077400	-0.54682900
H	2.48065500	1.84642900	0.21931900
C	2.74421600	-2.61064400	-2.95146300
H	2.65802700	-3.14974200	-3.90396800
H	3.49519300	-1.82778500	-3.06899000
H	3.11153900	-3.31225000	-2.19999100
C	0.57048400	-3.93051000	-0.98276700
H	0.03582900	-3.90670400	-0.03016900
H	0.14425500	-4.74549400	-1.58235500
H	1.61432700	-4.17710400	-0.77701000
C	1.50711900	0.08672000	-4.12628700
H	1.29810800	-0.28928700	-5.13671300
H	1.13477800	1.11241500	-4.06786200
H	2.59123900	0.11858600	-3.99775400
C	-1.49261300	0.34911600	-3.04042200
H	-1.97604000	0.00596200	-3.96504700
H	-2.27201900	0.51143500	-2.29530600
H	-1.01970000	1.30988400	-3.25290600
C	-2.05334200	-2.13104200	-1.06968300
H	-2.61929100	-2.81440400	-1.71696800
H	-1.90444200	-2.63389800	-0.11069500
H	-2.66831000	-1.24674000	-0.89691800
C	-1.20337300	2.91262000	-0.65824300
C	-2.53649000	3.31976500	-0.74967900
C	-3.55651400	2.56484300	-0.17151700
C	-3.22087100	1.39060100	0.51043000
C	-1.89284100	0.98030100	0.60529900
C	-0.85255400	1.72835000	0.01675500
H	-0.43710500	3.53028300	-1.11123600
H	-2.77269800	4.24103900	-1.27618700
H	-4.59078800	2.88954800	-0.23724500
H	-3.99726800	0.79595100	0.98551400

H	-1.64233300	0.07319300	1.14531700
N	0.49226700	1.27060800	0.15576000
C	1.25579800	5.37162700	3.21127100
C	1.55576600	5.72481900	1.89490800
C	1.61210200	4.74383000	0.90264300
C	1.37680700	3.39558000	1.20381000
C	1.08327000	3.05324700	2.53158900
C	1.01942100	4.03109800	3.52485200
H	1.20523200	6.13263400	3.98519400
H	1.74012300	6.76447600	1.63696400
H	1.84305700	5.02902900	-0.12163900
H	0.89503000	2.01605000	2.79276800
H	0.78630100	3.74378900	4.54676800
C	1.51296900	2.33890400	0.11647900
H	1.53636200	2.83212800	-0.86454200
O	0.72135700	-0.83944300	1.29081100
C	1.74134600	-1.30864000	2.16542600
H	2.58480100	-0.60818200	2.18736700
H	2.13255900	-2.24847000	1.75661700
C	1.23991000	-1.54843500	3.57944200
C	-0.09240200	-1.34807200	3.95323300
C	2.15275300	-1.98985700	4.54994100
C	-0.50505500	-1.58347500	5.26869700
H	-0.80487900	-1.00450800	3.21131600
C	1.74238500	-2.22786600	5.86027800
H	3.19392700	-2.14582200	4.27423900
C	0.40802500	-2.02439100	6.22591300
H	-1.54407300	-1.41962800	5.54299300
H	2.46346700	-2.56950600	6.59817400
H	0.08720500	-2.20690700	7.24783700
H	0.63948300	0.28043500	1.11722800
Ph-IN13i	$E = -1858.34214143$	$\Delta H = 0.634855$	$\Delta G = 0.474478$
Ir	0.97740000	-0.48536400	-0.83979700
C	0.08585200	-2.36056500	-1.57088800
C	-0.75347200	-1.25652200	-1.97040200
C	0.03081600	-0.41451300	-2.87294600
C	1.33926100	-0.96711900	-2.98345600
C	1.39519400	-2.16944100	-2.14773300
Cl	3.33087500	0.16899300	-0.38784100
H	2.21122000	2.36225500	-0.33558100
C	2.56156600	-3.10560600	-2.05851200
H	2.54545000	-3.82668400	-2.88642000
H	3.50619400	-2.55934400	-2.10269900

H	2.55189600	-3.66955800	-1.12266200
C	-0.35473200	-3.51885200	-0.73176500
H	-1.01783000	-3.19941700	0.07497100
H	-0.90457500	-4.23734400	-1.35331100
H	0.49231800	-4.04554600	-0.28845900
C	2.45913800	-0.46877100	-3.84376800
H	2.52899500	-1.06550300	-4.76255600
H	2.31035200	0.57439800	-4.13246600
H	3.41599000	-0.53533200	-3.32125600
C	-0.49687000	0.77246200	-3.61934800
H	-0.90645700	0.45526400	-4.58750600
H	-1.30136000	1.26581800	-3.06985700
H	0.28578100	1.50909900	-3.81747100
C	-2.22052700	-1.12129300	-1.69834700
H	-2.80405200	-1.58783900	-2.50369400
H	-2.49885900	-1.60849000	-0.76116400
H	-2.52335600	-0.07417000	-1.63049300
C	-1.75057800	2.49752200	-0.56591200
C	-3.12664300	2.67056000	-0.39540400
C	-3.79351800	2.05767800	0.66586400
C	-3.06796000	1.26805200	1.56118300
C	-1.69394400	1.09374100	1.40204400
C	-1.02458000	1.70480400	0.33239200
H	-1.25365100	2.98903300	-1.39426600
H	-3.67403300	3.29520600	-1.09600700
H	-4.86192900	2.20000100	0.79840700
H	-3.57012900	0.79147400	2.39851300
H	-1.12819600	0.47630100	2.09115400
N	0.39920400	1.49270700	0.18408400
C	1.18021300	5.68853900	2.98480900
C	0.50701500	5.93931500	1.78862100
C	0.50688400	4.98219300	0.77121300
C	1.18114700	3.76551300	0.93286100
C	1.86388500	3.52857100	2.13630800
C	1.85948600	4.47927700	3.15638500
H	1.17953700	6.43141000	3.77768200
H	-0.02041300	6.87861200	1.64611800
H	-0.02122100	5.18452800	-0.15690300
H	2.40791800	2.59625500	2.27058200
H	2.39368800	4.28012300	4.08126800
C	1.19516100	2.71509300	-0.15907600
H	0.81926200	3.12144000	-1.09908000
O	0.81236100	-0.86367900	1.21213900
C	1.66541900	-1.80789600	1.80450900

H	2.72175500	-1.51017300	1.73435900
H	1.58763300	-2.78770500	1.29455300
C	1.30976900	-2.01708300	3.26818400
C	-0.02824700	-2.10249000	3.67987000
C	2.31436500	-2.16731800	4.23270800
C	-0.35227600	-2.33409700	5.01712300
H	-0.81361200	-1.97815200	2.94056100
C	1.99450900	-2.40524500	5.57183400
H	3.35731500	-2.09315000	3.93246700
C	0.65896400	-2.48855900	5.96947900
H	-1.39536900	-2.39512900	5.31800300
H	2.78898300	-2.51608400	6.30547700
H	0.40743200	-2.66793200	7.01137800
H	0.74898800	1.09496900	1.06446600

D-IN8i $E = -1315.82152890$ $\Delta H = 0.514659$ $\Delta G = 0.377217$

Ir	-0.58805100	-0.19070000	-0.19888500
C	-0.13329900	-0.15609400	-2.41114900
C	-1.54563700	-0.02271200	-2.15429400
C	0.25656100	-1.53888000	-2.13085400
C	-1.97808700	-1.25573800	-1.52144700
C	-0.85428000	-2.19453700	-1.56960000
C	-0.34521200	-2.00140000	2.17459100
O	-0.66875600	-2.28531200	3.47232600
O	-1.02301300	-0.98558600	1.71900400
O	0.48123300	-2.70175500	1.60459100
H	-1.32135200	-1.62226800	3.74493000
C	0.72566400	0.83153200	-3.14549600
H	0.75276800	0.58689700	-4.21558900
H	0.34078100	1.84996800	-3.05248000
H	1.75549100	0.82191000	-2.77949200
C	-2.42486600	1.11617000	-2.58231900
H	-2.76381700	0.96015000	-3.61481900
H	-3.31095700	1.20132600	-1.94942000
H	-1.89627400	2.07186800	-2.54694700
C	1.60159700	-2.11600600	-2.43448000
H	1.76747900	-3.06043600	-1.91262400
H	1.69696700	-2.30669700	-3.51202200
H	2.40838100	-1.43509000	-2.15237500
C	-0.94602300	-3.62038800	-1.12457800
H	-1.35123500	-3.69560400	-0.11304600
H	-1.60926100	-4.18061800	-1.79639800
H	0.02867900	-4.10912100	-1.12189200
C	-3.39120500	-1.64082200	-1.19018900

H	-3.86213100	-2.15532700	-2.03845600
H	-3.42897600	-2.31604100	-0.33145700
H	-3.99993300	-0.76605800	-0.94983500
H	-1.74501800	0.72751100	0.30738800
C	3.02706300	-0.94851900	0.49377000
C	4.33450700	-1.20996700	0.09435600
C	5.12539300	-0.20416000	-0.47376600
C	4.59033900	1.07476600	-0.62779300
C	3.27933600	1.35063700	-0.23166100
C	2.47342800	0.33648700	0.32426000
H	2.40438800	-1.71930900	0.93841100
H	4.74320900	-2.20736000	0.23384400
H	6.14768500	-0.41222400	-0.77596700
H	5.19839300	1.87396100	-1.04400100
H	2.90245100	2.36509500	-0.31240200
N	1.18486600	0.58727900	0.84478000
C	-1.56070700	4.20115700	3.24658200
C	-1.00348500	2.99247100	3.67663500
C	-0.35238000	2.15446200	2.77419800
C	-0.25362600	2.51412600	1.42046900
C	-0.80241300	3.73454100	0.99881000
C	-1.45613300	4.57096400	1.90408500
H	-2.06465500	4.85281800	3.95485200
H	-1.07174500	2.70591800	4.72272700
H	0.08027800	1.21373900	3.09555900
H	-0.71167700	4.03106100	-0.04410600
H	-1.87524500	5.51369900	1.56316500
C	0.46631600	1.66103800	0.43448300
H	0.77549000	2.20208900	-0.46708700
D-TS9i $E = -1315.81289899$ $\Delta H = 0.512097$ $\Delta G = 0.374607$			
Ir	-1.17510000	-0.29108900	-0.00648500
C	-0.47460600	-0.77990000	-2.09835000
C	-1.77809100	-0.16485800	-2.14558500
C	-0.58620400	-2.02450400	-1.36785200
C	-2.71157000	-1.02703100	-1.44254200
C	-1.96125600	-2.15931900	-0.95701600
C	-0.94876700	-1.79810800	2.55082900
O	-1.25650300	-1.92096500	3.87866400
O	-1.65920000	-0.86917400	1.97398600
O	-0.10454400	-2.54262800	2.06814600
H	-1.91554700	-1.23591900	4.06993600
C	0.75136900	-0.30194800	-2.81334900
H	0.84856200	-0.82776800	-3.77242300

H	0.70673800	0.76852200	-3.02580200
H	1.65736500	-0.49370500	-2.23497800
C	-2.14064500	1.07206400	-2.91282500
H	-2.41521000	0.81282200	-3.94360700
H	-2.99363800	1.58808800	-2.46502800
H	-1.30687000	1.77705900	-2.96158700
C	0.49215700	-3.04180100	-1.15956700
H	0.41537300	-3.48639100	-0.16566900
H	0.41967700	-3.84051300	-1.91039400
H	1.48363400	-2.59265300	-1.25041400
C	-2.52163100	-3.32601400	-0.20341600
H	-3.44935000	-3.06726200	0.31165400
H	-2.74337000	-4.14426700	-0.90076700
H	-1.80847100	-3.69203000	0.53734400
C	-4.19955700	-0.84988600	-1.36621200
H	-4.69243500	-1.34081100	-2.21597200
H	-4.60862200	-1.28370900	-0.45073200
H	-4.48088900	0.20612500	-1.38455800
H	-1.87321600	1.11286500	0.49441600
C	2.49976100	-0.36447400	0.44534100
C	3.79404100	-0.32792500	-0.06076500
C	4.33083200	0.86563900	-0.56239800
C	3.55272400	2.02210600	-0.53414700
C	2.24994100	1.99821300	-0.02733600
C	1.69731500	0.79697800	0.45823400
H	2.07491000	-1.27724800	0.85194100
H	4.39497300	-1.23380000	-0.05487600
H	5.34485800	0.89361600	-0.95013400
H	3.96184800	2.96160700	-0.89741100
H	1.68452000	2.92367100	0.02306900
N	0.42930100	0.69493100	1.05272400
C	-2.15923700	3.56436300	4.43697500
C	-1.30139900	2.46974300	4.56891700
C	-0.76876400	1.84979300	3.43789500
C	-1.09031400	2.32545100	2.16042800
C	-1.94221300	3.43252600	2.03373600
C	-2.47719800	4.04706900	3.16455700
H	-2.57287500	4.04350100	5.31992100
H	-1.04268800	2.09862000	5.55684700
H	-0.10243100	0.99938800	3.52671300
H	-2.18628400	3.81346500	1.04390200
H	-3.13568900	4.90406600	3.05421400
C	-0.50243200	1.70406600	0.92465200
H	-0.38154200	2.42711800	0.10874400

D-IN10i	$E = -1315.85194177$	$\Delta H = 0.517941$	$\Delta G = 0.376455$
Ir	-0.71227800	-0.41868100	-0.55932200
C	0.75240300	-1.47585900	-1.81912300
C	-0.20402700	-0.81669500	-2.65914200
C	0.02820000	-2.45347900	-1.00353300
C	-1.52208300	-1.38233100	-2.36653200
C	-1.35363900	-2.41787100	-1.38583100
C	-2.29497100	-1.17061400	1.87996900
O	-3.43510700	-1.04831800	2.62238200
O	-2.24882200	-0.30822700	0.90142500
O	-1.47356600	-2.02401600	2.19225300
H	-3.95048200	-0.32904700	2.22650400
C	2.24116600	-1.32903800	-1.87742100
H	2.65903800	-2.06244400	-2.57992000
H	2.53920100	-0.33416300	-2.21249300
H	2.70287900	-1.50667300	-0.90321900
C	0.08709800	0.16951000	-3.74724700
H	0.19094500	-0.35416800	-4.70690400
H	-0.71963300	0.89879700	-3.85616000
H	1.01348200	0.71604800	-3.56338400
C	0.63365800	-3.40322100	-0.01764300
H	-0.00749000	-3.50272600	0.86028200
H	0.76992800	-4.39357200	-0.47209600
H	1.61169400	-3.05424500	0.32207900
C	-2.43600000	-3.28615900	-0.81863500
H	-3.41412400	-2.80304700	-0.88064400
H	-2.49742200	-4.22924600	-1.37652000
H	-2.24219000	-3.52158000	0.22937700
C	-2.79234200	-1.03216500	-3.07983500
H	-2.89874300	-1.63477000	-3.99182300
H	-3.66803300	-1.21892500	-2.45365100
H	-2.81004700	0.02055400	-3.37317000
H	-1.62277700	1.63658300	1.46620200
C	2.35782200	1.69093000	-0.13139500
C	3.42115400	2.37109300	-0.72952500
C	3.17991400	3.35429600	-1.69161900
C	1.86369600	3.65834900	-2.04957000
C	0.79841100	2.98163400	-1.45323800
C	1.03465500	1.98361900	-0.49343500
H	2.53817000	0.93260100	0.62340600
H	4.44063200	2.13360900	-0.43734900
H	4.00876600	3.88158500	-2.15528100
H	1.66455500	4.42356700	-2.79531000

H	-0.22677100	3.21278800	-1.72992900
N	-0.06445500	1.30033600	0.11927900
C	1.76547400	2.20253700	4.82842400
C	1.23767800	0.98953700	4.37542500
C	0.46509800	0.94709700	3.21468900
C	0.20849400	2.11915500	2.48577600
C	0.74379900	3.32776800	2.94683800
C	1.51510500	3.37288400	4.11149200
H	2.36459500	2.23379800	5.73449000
H	1.42138200	0.07419100	4.93190500
H	0.05672500	-0.00102200	2.87466900
H	0.55452400	4.24229800	2.38933200
H	1.92101200	4.32097900	4.45445700
C	-0.65501100	2.07820500	1.23338800
H	-0.82643800	3.10684800	0.88854700
D-IN11i	$E = -1315.84490291$	$\Delta H = 0.517713$	$\Delta G = 0.378868$
Ir	0.37427800	-0.14665700	-0.88749400
C	2.10580400	0.69515800	-2.03832600
C	1.17104200	1.76596400	-1.68708000
C	1.42395700	-0.22853100	-2.89391400
C	-0.08396700	1.47857400	-2.31173200
C	0.06093000	0.21197900	-3.03185100
C	1.61176500	-2.88096300	-0.28337500
O	1.73701400	-4.08802100	-0.36121000
O	0.50693000	-2.22016100	-0.53247600
O	2.69157900	-2.12271400	0.11736600
C	3.56282400	0.68233500	-1.68510300
H	4.12563300	1.30725100	-2.39119200
H	3.73967600	1.08404300	-0.68344100
H	3.98522200	-0.32345400	-1.72545300
C	1.54290700	3.02305600	-0.96336100
H	1.96723100	3.74546600	-1.67336400
H	0.67955400	3.48948800	-0.48666500
H	2.29722800	2.83861000	-0.19422600
C	1.99669100	-1.47456300	-3.50135500
H	1.28166200	-2.30016600	-3.46604000
H	2.25777700	-1.30042500	-4.55246300
H	2.90066800	-1.79838400	-2.98216400
C	-0.98927400	-0.43412000	-3.88195300
H	-1.99135700	-0.26161700	-3.48165700
H	-0.96087200	-0.02499700	-4.90066500
H	-0.83660000	-1.51360400	-3.95101700
C	-1.29136000	2.36315300	-2.33815300

H	-1.23922300	3.04293500	-3.19887300
H	-2.21339500	1.78401600	-2.43184500
H	-1.36676500	2.97110800	-1.43489100
H	-0.74247500	-2.07200500	1.14974200
C	-0.49701600	2.22524600	1.76113400
C	-1.09109400	3.42463000	2.16054600
C	-2.45927800	3.63176300	1.97257900
C	-3.23246500	2.62745300	1.38385000
C	-2.64335500	1.42716500	0.98518300
C	-1.26569000	1.21628200	1.16391600
H	0.56249800	2.05023800	1.91698500
H	-0.48311400	4.19372600	2.62939200
H	-2.92025800	4.56386200	2.28619400
H	-4.29789700	2.77840900	1.23213800
H	-3.24339100	0.64796000	0.52344300
N	-0.66473700	-0.01967700	0.76293200
C	0.59702500	-0.93214100	5.63624300
C	1.39775800	-1.32864500	4.56145300
C	0.86247000	-1.39572900	3.27494100
C	-0.48114000	-1.06746600	3.03956400
C	-1.27411800	-0.67369000	4.12494500
C	-0.74152800	-0.60593900	5.41479400
H	1.01315700	-0.88403900	6.63879800
H	2.43799400	-1.59630600	4.72648300
H	1.49072600	-1.71721500	2.44905200
H	-2.31826600	-0.42080100	3.95896500
H	-1.37328800	-0.30044800	6.24459400
C	-1.06243300	-1.15356200	1.63753500
H	-2.15779400	-1.16866100	1.70747100
H	2.40455200	-1.19216300	0.12098500
D-TS12i $E = -1315.82473844$ $\Delta H = 0.513617$ $\Delta G = 0.377894$			
Ir	0.61724300	-0.19166700	-1.08229300
C	1.43007300	1.47928100	-2.29577100
C	0.04377800	1.72165100	-2.04124900
C	1.55002500	0.23429800	-3.06174700
C	-0.70804700	0.59257100	-2.57280100
C	0.23904100	-0.28964700	-3.25371600
C	1.50877300	-2.50773900	-0.00066000
O	1.99943500	-3.57268400	0.28808100
O	0.41177900	-2.26305700	-0.66490400
O	2.13021100	-1.28183500	0.35845000
C	2.57254300	2.39132100	-1.97197200
H	2.80117000	3.02454500	-2.83931100

H	2.34187100	3.04481600	-1.12926700
H	3.47732900	1.82849500	-1.72846800
C	-0.55014700	2.93732500	-1.40303200
H	-0.84063300	3.65591800	-2.18050100
H	-1.44428500	2.69382500	-0.82521200
H	0.15466800	3.43114800	-0.73224100
C	2.83319000	-0.32369700	-3.59711200
H	2.74456600	-1.38721500	-3.82896100
H	3.11929000	0.19843700	-4.51930500
H	3.65148700	-0.20385300	-2.88212400
C	-0.12608700	-1.53396400	-4.00135100
H	-0.98893400	-2.03210700	-3.55342700
H	-0.38453500	-1.28425900	-5.03828300
H	0.69789700	-2.25022700	-4.02126400
C	-2.20080000	0.48226200	-2.63376800
H	-2.57884000	0.95594500	-3.54961200
H	-2.52749900	-0.56040200	-2.63897100
H	-2.67452400	0.97905700	-1.78366700
H	-1.16684100	-1.57381800	0.83101200
C	1.59903600	1.90280200	1.53611600
C	1.84998000	3.16704400	2.06125800
C	0.81970600	3.91545900	2.64156200
C	-0.46065200	3.36709000	2.68962900
C	-0.72066800	2.09962100	2.16140100
C	0.30341300	1.33943900	1.56388000
H	2.41543600	1.32876400	1.10795800
H	2.86160400	3.56393500	2.03222300
H	1.01782600	4.89779300	3.06000800
H	-1.27410300	3.92399300	3.14780200
H	-1.72613500	1.70413400	2.23107100
N	0.11249200	0.04248000	1.01736000
C	-1.38315200	-1.82910300	5.59701200
C	-0.20957300	-2.06164800	4.87551900
C	-0.11536900	-1.67069000	3.53979400
C	-1.18985300	-1.03551000	2.90057800
C	-2.36145700	-0.80988700	3.63437300
C	-2.46204100	-1.20444600	4.97038100
H	-1.45522000	-2.13350500	6.63754100
H	0.63452100	-2.55298600	5.35180700
H	0.80130200	-1.86771800	2.99134600
H	-3.20627500	-0.32095300	3.15363300
H	-3.38023600	-1.01791000	5.52118100
C	-1.12304500	-0.65888000	1.42526600
H	-2.01975900	-0.07705600	1.16643900

H	1.40342200	-0.78397800	0.96819600
D-IN13i	$E = -1315.85749604$	$\Delta H = 0.518942$	$\Delta G = 0.381609$
Ir	0.28371200	-0.26424400	-1.18858200
C	0.90729800	1.68246800	-2.12467000
C	-0.53633800	1.51137400	-2.27400400
C	1.54973700	0.58765800	-2.78666600
C	-0.76629400	0.31947000	-3.03378800
C	0.52301700	-0.29033900	-3.33001200
C	0.48315200	-2.67572800	-0.29721700
O	0.57639200	-3.81678400	0.12583200
O	-0.64178100	-2.09360600	-0.72717400
O	1.49164400	-1.79438600	-0.37741200
C	1.58230900	2.87455700	-1.51930900
H	1.66248800	3.68196600	-2.25951400
H	1.02555900	3.26262900	-0.66419800
H	2.59182800	2.63526800	-1.17856200
C	-1.57569400	2.50286800	-1.84444400
H	-1.75727700	3.23487300	-2.64264100
H	-2.52972300	2.01984600	-1.61781700
H	-1.25825100	3.05859000	-0.95928100
C	3.02611100	0.37884400	-2.92674900
H	3.28468800	-0.68241600	-2.91808800
H	3.37622500	0.80068000	-3.87785100
H	3.58009800	0.86499300	-2.12055800
C	0.75541400	-1.49721800	-4.18882000
H	-0.07480200	-2.20406200	-4.11899300
H	0.86232100	-1.20937100	-5.24306400
H	1.66458100	-2.02717700	-3.89405700
C	-2.09410500	-0.21174100	-3.47832100
H	-2.31395600	0.13277600	-4.49716200
H	-2.10692100	-1.30415900	-3.48595000
H	-2.90356600	0.12787200	-2.82788000
H	-1.60752500	-1.21922900	1.01990100
C	1.92551300	1.32328000	2.01036400
C	2.46404000	2.50747100	2.51370700
C	1.67148100	3.65076000	2.63428600
C	0.33365100	3.59877500	2.23960400
C	-0.21047000	2.41942200	1.72584500
C	0.58392400	1.27194700	1.61187700
H	2.54474700	0.43353200	1.93347600
H	3.50469200	2.52895900	2.82407400
H	2.08940300	4.56865000	3.03645900
H	-0.29655900	4.47902900	2.33120700

H	-1.25062800	2.39968200	1.41978700
N	0.05497800	0.03603700	1.07659300
C	-0.90111500	-1.76091800	5.74698600
C	-0.51455600	-2.58802700	4.68913400
C	-0.64287500	-2.14790200	3.37152600
C	-1.15186800	-0.86859300	3.09469300
C	-1.53785000	-0.04799700	4.16259700
C	-1.41557500	-0.49089300	5.48121300
H	-0.80590900	-2.10671100	6.77257400
H	-0.12161500	-3.58102200	4.88852400
H	-0.35361900	-2.80351600	2.55225100
H	-1.93945500	0.94159600	3.96159900
H	-1.72269200	0.15536900	6.29894000
C	-1.26681800	-0.40479500	1.65848200
H	-1.97166200	0.42157800	1.56335500
H	0.73489400	-0.69897900	1.28778100
B-IN4o	$E = -2376.05504506$	$\Delta H = 0.521065$	$\Delta G = 0.360078$
Ir	0.16967200	-1.11348400	0.64782200
C	0.09629500	-2.96640400	2.14902600
C	-1.08655900	-3.02326600	1.40229300
C	-0.72786800	-2.97588500	-0.02700700
C	0.71395000	-3.03091900	-0.12993100
C	1.23822400	-2.88641000	1.21556400
Cl	1.10271700	0.56158800	2.28232700
H	-1.06762300	1.11769200	-0.43425100
O	-1.40915900	0.39388500	0.13133400
C	-2.31753400	0.98161800	1.13807600
O	-2.27690500	2.23320800	1.14288100
O	-2.95241500	0.15459400	1.77921900
K	-0.18722300	3.26882300	2.12251100
H	0.96821100	-0.32199500	-0.47597300
C	1.50969900	-3.27702900	-1.37715900
H	2.50113900	-2.82217800	-1.31533600
H	1.64361200	-4.35601300	-1.53361000
H	1.00933100	-2.86898200	-2.25846000
C	2.67656600	-2.98730000	1.63134200
H	2.87533100	-2.37101300	2.51193900
H	2.94377300	-4.02401900	1.87907500
H	3.34554300	-2.65030600	0.83552800
C	0.24147600	-2.92184300	3.63862200
H	-0.72652700	-2.84121800	4.13772100
H	0.74268500	-3.82553800	4.00833900
H	0.84431300	-2.06097900	3.94544300

C	-1.71087800	-3.16239100	-1.14410900
H	-1.98421700	-4.22149300	-1.25038800
H	-2.63031000	-2.60075100	-0.95746900
H	-1.29943700	-2.82609800	-2.09831300
C	-2.49602500	-3.07794700	1.90884300
H	-3.04369100	-3.90206500	1.43583100
H	-2.52403300	-3.23779500	2.98957800
H	-3.01979000	-2.13966400	1.70090300
C	-0.52390900	4.59314800	-0.81193100
C	0.01110000	5.67190900	-0.10574700
C	1.35616100	5.66462300	0.29071600
C	2.16391300	4.57065200	-0.03664400
C	1.64196800	3.49584800	-0.76376700
C	0.29463800	3.50425400	-1.16381700
H	-1.56927200	4.57878300	-1.10201800
H	-0.62382800	6.51935300	0.13803700
H	1.76866200	6.50377400	0.84314200
H	3.20529900	4.54925500	0.27200900
H	2.26050900	2.63478100	-0.99588900
N	-0.28892800	2.41600000	-1.84930200
C	-1.31421400	-1.03128000	-5.49689500
C	-1.97617000	-0.73489300	-4.29916300
C	-1.49302400	0.26217700	-3.45718900
C	-0.33632100	0.98105400	-3.81069500
C	0.31754000	0.68085400	-5.01744300
C	-0.16504000	-0.32356200	-5.85452200
H	-1.69765100	-1.80982900	-6.15035200
H	-2.87277400	-1.28265900	-4.02475400
H	-1.99931600	0.48782500	-2.52528900
H	1.20676900	1.24071100	-5.29555200
H	0.35005300	-0.54924200	-6.78356400
C	0.19785700	2.06741900	-2.98451100
H	1.04862500	2.61138900	-3.41728700
B-TS5o	$E = -2376.03604254$	$\Delta H = 0.516931$	$\Delta G = 0.366356$
Ir	0.40308500	-1.04001400	0.32530900
C	0.18168000	-2.73237900	1.71567100
C	-0.88948500	-2.77861000	0.74009000
C	-0.31071900	-2.91624200	-0.57254500
C	1.14063700	-2.96947100	-0.41301000
C	1.43709800	-2.86012800	0.98909200
Cl	2.01056400	0.52239500	1.37515400
H	-0.96290500	1.23008500	-0.11637200
O	-1.11515000	0.47076200	0.54361300

C	-1.52283700	0.97807700	1.88278100
O	-1.46759800	2.22002200	1.95812100
O	-1.85118700	0.09295600	2.66608800
K	0.83316300	3.30027400	2.04052000
H	0.64379400	0.05634200	-1.14685900
C	2.12546400	-3.22364600	-1.51299900
H	3.10922500	-2.81227700	-1.27586400
H	2.24331800	-4.30372600	-1.67249900
H	1.79167500	-2.78441700	-2.45598600
C	2.79621400	-2.94278700	1.61031000
H	2.85340300	-2.35476000	2.52804400
H	3.02512400	-3.98686400	1.86033700
H	3.57162500	-2.58062000	0.93219000
C	-0.00143900	-2.66238400	3.19850800
H	-0.79756300	-1.95760200	3.44949500
H	-0.26636500	-3.65041500	3.59903100
H	0.91284800	-2.33325500	3.69780300
C	-1.05648300	-3.13641100	-1.85123100
H	-1.21758200	-4.21143300	-2.00949500
H	-2.03392000	-2.65124100	-1.83417900
H	-0.50764700	-2.75038400	-2.71197600
C	-2.34633300	-2.71121200	1.07198600
H	-2.95061900	-2.51495700	0.18387000
H	-2.67233100	-3.66774800	1.50053200
H	-2.53127500	-1.91442300	1.79714600
C	-0.53030700	4.24495200	-0.62542000
C	-0.04279700	5.47290800	-0.18978800
C	1.33792700	5.72897300	-0.16285000
C	2.20967800	4.72398300	-0.60151400
C	1.73032700	3.48823000	-1.04168500
C	0.33616000	3.20270500	-1.06355100
H	-1.59726900	4.04706400	-0.63551600
H	-0.74404000	6.24017900	0.12962500
H	1.71922800	6.69074900	0.16698700
H	3.28281900	4.90189600	-0.60086400
H	2.44809400	2.73796900	-1.35412000
N	-0.26938600	2.02921600	-1.46177200
C	-1.33079600	-1.05453200	-5.35850100
C	-2.13361200	-0.32809200	-4.47414300
C	-1.56534500	0.33406000	-3.38536800
C	-0.18390200	0.27058100	-3.15874200
C	0.61582100	-0.45702100	-4.05173800
C	0.04845600	-1.11351500	-5.14671300
H	-1.77503000	-1.55889500	-6.21217700

H	-3.20575500	-0.26591500	-4.64096800
H	-2.17732700	0.92828300	-2.71540700
H	1.69255700	-0.49178200	-3.89937000
H	0.68415500	-1.65983400	-5.83851100
C	0.46471900	1.00436000	-2.00703500
H	1.52617600	1.18657100	-2.22221100
C-IN4o	$E = -1799.16544188$	$\Delta H = 0.614109$	$\Delta G = 0.453390$
Ir	0.54899000	-1.12246500	-0.53993000
C	-0.35744600	-2.90352800	0.29940900
C	-1.35820000	-2.22381000	-0.49361200
C	-0.98151600	-2.36873000	-1.90822300
C	0.26635100	-3.00820700	-1.96910900
C	0.70684600	-3.29576100	-0.59375900
Cl	2.83067400	-0.43648100	-1.25839400
C	-0.02823300	1.47703400	-3.29998300
C	-0.79015600	1.87995100	-4.39610000
C	-2.12000900	2.27792600	-4.23021300
C	-2.68460400	2.27283900	-2.95368200
C	-1.92820600	1.87461100	-1.84866400
C	-0.59914300	1.47629000	-2.02213700
H	1.00410900	1.16340100	-3.42474500
H	-0.33926700	1.88561900	-5.38441100
H	-2.70796300	2.59236300	-5.08729000
H	-3.71486300	2.58643900	-2.81071600
H	-2.36254700	1.88234200	-0.85252900
N	0.18084200	1.04953000	-0.89055500
H	1.14940700	1.36571200	-0.97739400
H	-0.19107600	1.44376500	-0.02803800
H	0.97301300	-0.55704800	0.88181400
C	1.44494600	4.18522900	0.71374400
C	2.66857900	4.77876500	0.41017400
C	3.71671300	4.73751700	1.33267600
C	3.52666900	4.10415100	2.56392500
C	2.30931600	3.49940300	2.86921200
C	1.25536600	3.51580200	1.93568400
H	0.61461400	4.23169200	0.01539700
H	2.80041900	5.28277200	-0.54304300
H	4.66782200	5.20811100	1.10175400
H	4.32937800	4.08824000	3.29608400
H	2.16818300	3.04144300	3.84315600
N	-0.01477600	2.94666500	2.15824400
C	-3.98800000	0.34626900	4.00076100
C	-3.91141000	1.44111500	3.13086400

C	-2.67505700	1.98127800	2.79222200
C	-1.49149900	1.42682000	3.31409500
C	-1.57855900	0.33182900	4.18999000
C	-2.81993500	-0.20555300	4.53125300
H	-4.95567800	-0.06921000	4.26732900
H	-4.82079000	1.87598300	2.72566900
H	-2.60135400	2.84052700	2.13324200
H	-0.66761600	-0.09422400	4.60314700
H	-2.87592800	-1.05006100	5.21202900
C	-0.17034400	1.97532400	2.98479400
H	0.67744500	1.49556400	3.49106400
C	-0.45360500	-3.22637300	1.76166100
H	-0.95727600	-4.19244700	1.90189200
H	0.53468600	-3.29446600	2.22248600
H	-1.02470400	-2.46936000	2.30384700
C	1.91518300	-4.11218100	-0.24050100
H	2.20639800	-3.96092200	0.80173000
H	1.72185000	-5.18419400	-0.38429600
H	2.77171800	-3.84114400	-0.86282000
C	-2.70759100	-1.76864400	-0.01899100
H	-3.44709200	-2.57686300	-0.10950900
H	-2.68313700	-1.45793800	1.02803500
H	-3.07507700	-0.92461600	-0.60941500
C	-1.83036600	-1.90895700	-3.05458600
H	-2.66649000	-2.60290900	-3.21462500
H	-2.26195900	-0.92123200	-2.86956100
H	-1.26312300	-1.85461100	-3.98625400
C	1.06741900	-3.34674700	-3.18866600
H	2.11261700	-3.04584800	-3.06885200
H	1.05549700	-4.42879200	-3.37383200
H	0.67851900	-2.85182800	-4.08178700
C-TS5o	$E = -1799.14337940$	$\Delta H = 0.608984$	$\Delta G = 0.456194$
Ir	0.44862500	-0.95454200	-0.70822800
C	-0.41046300	-2.84479700	0.12488900
C	-1.44582700	-2.09974600	-0.58716700
C	-1.05018000	-2.00821600	-1.96815700
C	0.24698700	-2.63990700	-2.11334400
C	0.62352000	-3.16607200	-0.80873200
Cl	2.84054500	-0.55441500	-0.35389500
C	0.28907200	1.50921800	-3.85067500
C	-0.46870700	1.95554800	-4.93416400
C	-1.77869300	2.40257900	-4.74381100
C	-2.32386700	2.40541200	-3.45771700

C	-1.57373100	1.95758900	-2.36934500
C	-0.26385600	1.50151500	-2.56341900
H	1.31278300	1.17324800	-3.99659600
H	-0.02931700	1.96052900	-5.92775500
H	-2.36478300	2.75396700	-5.58773500
H	-3.33601900	2.76605700	-3.29662600
H	-1.98953300	1.97520000	-1.36661800
N	0.51014500	1.05494000	-1.44094500
H	1.50386300	1.19878400	-1.63114800
H	0.30377600	1.69543700	-0.53760000
H	0.30962200	0.13706400	0.85269400
C	1.51957400	4.14319300	-0.01714900
C	2.53023800	5.09485700	0.06164900
C	3.39716900	5.12824700	1.15931000
C	3.21917300	4.19241800	2.18107800
C	2.20879400	3.23529000	2.11345700
C	1.33419600	3.17172500	0.99990100
H	0.83766900	4.14030000	-0.86361000
H	2.64081400	5.82166100	-0.73983900
H	4.18451600	5.87373000	1.22171300
H	3.86975600	4.21168800	3.05251700
H	2.08141600	2.54927500	2.94459400
N	0.27807500	2.28228100	0.85855100
C	-3.41640200	0.35007900	3.81860300
C	-3.39677400	1.32903000	2.82197500
C	-2.22517700	1.58475100	2.10680600
C	-1.05726200	0.85752700	2.37020600
C	-1.08241200	-0.11714600	3.37892800
C	-2.25154200	-0.36934200	4.09977300
H	-4.32589100	0.15980900	4.38177300
H	-4.29309500	1.90671800	2.61113900
H	-2.18773600	2.37121900	1.36023800
H	-0.17376300	-0.66878000	3.60980800
H	-2.25021700	-1.11855700	4.88721100
C	0.22854800	1.12794100	1.61860500
H	1.10123900	0.90705700	2.24865100
C	-0.48683200	-3.29476300	1.55139100
H	-1.00058400	-4.26375100	1.61077300
H	0.50649900	-3.41846500	1.98935300
H	-1.04506100	-2.58705400	2.16737100
C	1.85742000	-3.96394700	-0.52075700
H	2.15137100	-3.88400900	0.52777000
H	1.67754100	-5.02394300	-0.74197300
H	2.70072800	-3.62975100	-1.12788700

C	-2.76393800	-1.68419100	-0.00974000
H	-3.47667800	-2.51893100	-0.05272700
H	-2.66856600	-1.38206400	1.03515600
H	-3.20057900	-0.84805600	-0.56010400
C	-1.88026300	-1.47702700	-3.09324500
H	-2.41670800	-2.30724200	-3.57157400
H	-2.62212400	-0.75506800	-2.74946500
H	-1.26914400	-0.99171000	-3.85706600
C	0.97939900	-2.86947700	-3.39911300
H	2.06036000	-2.90284900	-3.24360800
H	0.67637600	-3.82539000	-3.84759000
H	0.76725500	-2.08056600	-4.12487800
Ph-IN1o	$E = -1301.80736200$	$\Delta H = 0.406417$	$\Delta G = 0.289621$
Ir	0.17649900	-0.92707600	-0.03879700
C	0.29982800	-3.24646900	0.47231100
C	-1.06100200	-2.94648100	0.32616900
C	-1.25488000	-2.29166000	-0.98110000
C	0.00648800	-2.31132500	-1.67857100
C	1.00702500	-2.77811600	-0.73521200
Cl	1.79996100	0.02540200	1.57395000
H	-0.21494000	1.23353700	1.29841000
O	-0.99638600	0.78571400	0.91751700
H	0.62481900	0.27194300	-0.97850100
C	0.23146300	-1.99224000	-3.12644000
H	1.23203800	-1.58961700	-3.29838900
H	0.12629800	-2.90338000	-3.73045100
H	-0.49185800	-1.26095700	-3.49482400
C	2.44712000	-3.06543400	-1.04303500
H	3.07153900	-2.96166800	-0.15217000
H	2.56687400	-4.09040900	-1.42009700
H	2.83606400	-2.38020200	-1.79994100
C	0.97974400	-3.88608700	1.64261300
H	0.33059200	-3.92594000	2.52066500
H	1.27879200	-4.91417700	1.40085500
H	1.88464300	-3.33748900	1.92007500
C	-2.58882000	-1.95728500	-1.58085100
H	-3.06632300	-2.85473200	-1.99749000
H	-3.27280900	-1.53887900	-0.83700000
H	-2.48919300	-1.22549100	-2.38598900
C	-2.16426200	-3.23244800	1.29987500
H	-2.68968000	-4.15677500	1.02568400
H	-1.78879800	-3.35454300	2.31875700
H	-2.91097300	-2.43344600	1.30984800

C	-1.92328300	0.51860000	2.00703600
H	-1.43886800	-0.12971200	2.74480600
C	-2.40226600	1.79989500	2.63835200
C	-1.84233300	2.25326800	3.84008400
C	-3.39100000	2.57322300	2.01289400
C	-2.26363500	3.45725200	4.40826800
H	-1.07507800	1.66004800	4.33191300
C	-3.81167000	3.77596700	2.57799100
H	-3.83026700	2.22825400	1.08003700
C	-3.24817300	4.21988200	3.77780400
H	-1.82402500	3.79838100	5.34121200
H	-4.57981900	4.36580100	2.08586800
H	-3.57779300	5.15627000	4.21911400
H	-2.74878900	-0.02701200	1.54533600
Ph-IN2o	$E = -1858.31676198$	$\Delta H = 0.631381$	$\Delta G = 0.465076$
Ir	0.42537700	-1.59576100	0.36199100
C	-0.05438900	-3.87845700	0.77446700
C	-1.27101600	-3.27353000	0.42808600
C	-1.09903300	-2.59449500	-0.86871700
C	0.22653800	-2.88586800	-1.35132500
C	0.92997900	-3.57596800	-0.28219500
Cl	1.93919800	-1.21228300	2.25803100
H	-0.19769300	1.07860600	0.78586000
O	-0.69084700	0.26413500	1.06336800
H	1.31127500	-0.52364200	-0.40155500
C	0.75775200	-2.61030700	-2.72657000
H	1.83854500	-2.45171400	-2.71233800
H	0.55135300	-3.46152300	-3.38943700
H	0.29689800	-1.72235600	-3.16533100
C	2.29708300	-4.18838200	-0.36737800
H	2.77877200	-4.21788800	0.61310000
H	2.24318000	-5.21807000	-0.74737200
H	2.94702800	-3.61756600	-1.03514000
C	0.26960900	-4.65179400	2.01486400
H	-0.55852300	-4.64496700	2.72763200
H	0.49318900	-5.69815800	1.77153000
H	1.14760400	-4.23300000	2.51703700
C	-2.21234400	-1.97203100	-1.65716200
H	-2.79912600	-2.74018700	-2.18010200
H	-2.90029700	-1.42047800	-1.01053400
H	-1.82921500	-1.27437000	-2.40505900
C	-2.55156800	-3.28677600	1.20799600
H	-3.24676900	-4.03406100	0.80265700

H	-2.38495700	-3.52577300	2.26105400
H	-3.06086900	-2.31956100	1.15987100
C	-1.07991900	0.38255900	2.44797700
H	-0.20533100	0.58966400	3.07010200
C	-2.15975200	1.42280700	2.65661900
C	-2.11508000	2.26327500	3.77649200
C	-3.24212800	1.53559500	1.77235000
C	-3.12903100	3.19583900	4.00992700
H	-1.28023100	2.18646500	4.46868300
C	-4.25075100	2.47233500	1.99876300
H	-3.28679600	0.89062500	0.89976100
C	-4.19822500	3.30519900	3.11956400
H	-3.07847200	3.84053500	4.88305700
H	-5.08056900	2.55097300	1.30149200
H	-4.98424700	4.03413500	3.29556900
H	-1.44710300	-0.60977700	2.72641800
C	1.22845500	3.57731200	2.38326200
C	2.09293200	3.98771500	3.39627900
C	3.46689700	3.75654600	3.28758200
C	3.97122700	3.11107200	2.15699000
C	3.11562500	2.71083500	1.13052300
C	1.73720600	2.95267600	1.23468300
H	0.15913300	3.74873900	2.45797100
H	1.69146800	4.48436700	4.27529300
H	4.13728500	4.06406900	4.08481100
H	5.03476300	2.90507300	2.07638800
H	3.50404100	2.17614800	0.26957900
N	0.81553900	2.56169300	0.22857700
C	-1.37317200	1.98751400	-4.37809300
C	-1.90495600	1.85741300	-3.08982400
C	-1.11482600	2.11713400	-1.97391500
C	0.22362900	2.51827200	-2.13451600
C	0.74262000	2.66470700	-3.43208700
C	-0.04702000	2.39053500	-4.54756900
H	-1.99441200	1.78348000	-5.24559600
H	-2.94123100	1.55911200	-2.95888200
H	-1.52644500	2.02588500	-0.97513500
H	1.77280800	2.98694600	-3.56078900
H	0.36795500	2.49834900	-5.54531900
C	1.09174100	2.83526400	-0.99580800
H	2.02004800	3.36392500	-1.24765000
Ph-TS3o	$E = -1858.28985238$	$\Delta H = 0.624420$	$\Delta G = 0.463446$
Ir	0.30195100	-1.32031600	0.27430800

C	-0.04266700	-3.47606700	0.69064200
C	-1.29476100	-2.88088800	0.32303800
C	-1.17448800	-2.33981600	-1.02127600
C	0.16051200	-2.64446100	-1.49118900
C	0.88241000	-3.29881800	-0.42708600
Cl	2.06806400	-0.95999300	1.92020200
H	-0.21320600	1.28926900	0.85607900
O	-0.75734500	0.35723300	1.16543000
H	1.02490800	0.11813800	-0.52599500
C	0.67567500	-2.40798400	-2.87566700
H	1.75845500	-2.26501500	-2.88518800
H	0.45081500	-3.28193600	-3.50177600
H	0.21230100	-1.53646400	-3.34035000
C	2.26562400	-3.87092100	-0.50565900
H	2.76635300	-3.82846500	0.46398000
H	2.23171500	-4.92070600	-0.82546500
H	2.88495300	-3.32265000	-1.21944700
C	0.26707900	-4.19827800	1.96343600
H	-0.36351100	-3.85562700	2.78728500
H	0.09994200	-5.27615500	1.83712200
H	1.30767100	-4.05003700	2.25885800
C	-2.30129500	-1.76889200	-1.82817900
H	-2.93109000	-2.57255100	-2.23266600
H	-2.93998800	-1.12371100	-1.21925900
H	-1.93718500	-1.17677000	-2.66988800
C	-2.54390800	-2.86275800	1.14829100
H	-3.17742200	-3.72024600	0.88534100
H	-2.32784900	-2.93069300	2.21680000
H	-3.12968500	-1.95736700	0.97352300
C	-1.02778800	0.36171400	2.57133700
H	-0.12500400	0.61490600	3.13644200
C	-2.16615000	1.29397300	2.93913800
C	-2.24364300	1.79710600	4.24572700
C	-3.17755900	1.62321200	2.02828500
C	-3.31539000	2.60013600	4.63768800
H	-1.45716600	1.55890000	4.95836300
C	-4.24636500	2.43365700	2.41754800
H	-3.11526300	1.24997600	1.01124900
C	-4.32143000	2.92165900	3.72344600
H	-3.35946900	2.98235800	5.65395300
H	-5.02114200	2.68556200	1.69815400
H	-5.15298700	3.55249100	4.02498400
H	-1.29878000	-0.66334100	2.84979900
C	1.05924700	3.32786600	2.34207400

C	1.85246200	4.00612400	3.26174300
C	3.22194900	4.17056500	3.03550500
C	3.77656900	3.64973400	1.86389200
C	2.99017900	2.97021600	0.93623000
C	1.60867900	2.77557600	1.16223300
H	-0.00786100	3.22432000	2.51485600
H	1.39531800	4.41530600	4.15928500
H	3.84205600	4.70206800	3.75136400
H	4.83711700	3.77897100	1.66205700
H	3.45883700	2.60051600	0.03040000
N	0.72419000	2.15457600	0.27824400
C	-0.93841000	1.91564200	-4.52754200
C	-1.51877500	2.36071100	-3.33623500
C	-0.84917200	2.20118400	-2.12308800
C	0.40800600	1.58174000	-2.08240100
C	0.98820200	1.14605200	-3.28248200
C	0.32190400	1.31346200	-4.49797200
H	-1.45669600	2.05247500	-5.47254300
H	-2.48952800	2.84880200	-3.35427400
H	-1.27618300	2.57966700	-1.20090200
H	1.97446000	0.68803400	-3.26452400
H	0.79041900	0.98273600	-5.42096700
C	1.17063100	1.43881300	-0.79243500
H	2.25091900	1.38426900	-0.96302000
D-IN3o	$E = -1315.81710595$	$\Delta H = 0.513669$	$\Delta G = 0.370282$
Ir	-0.37318700	-0.88121900	-1.16153900
C	1.06060800	-2.29821900	-1.92233400
C	-0.14500200	-2.32173500	-2.73366400
C	-0.19088500	-1.06547700	-3.50354100
C	0.87160800	-0.25102000	-3.08299300
C	1.62164700	-0.97908800	-2.04441300
H	-0.54752400	-1.61789900	0.23957900
O	-2.39854300	-0.19334900	-0.81528900
C	-2.15979600	0.77931900	-0.00726900
O	-0.76156600	0.98066100	0.02101600
O	-2.90511300	1.46999300	0.66243800
H	-0.42843400	1.34611200	0.90995100
C	2.90647500	-0.50032500	-1.43573800
H	3.13242800	-1.03183400	-0.50822900
H	3.74496100	-0.66066800	-2.12698200
H	2.86785800	0.56847600	-1.20761000
C	1.21254700	1.13090300	-3.55237500
H	2.09933500	1.11383100	-4.19932500

H	0.39520100	1.58072900	-4.12098700
H	1.43673400	1.79449100	-2.71128900
C	-1.24243200	-0.74821700	-4.52199600
H	-1.05678900	-1.30234400	-5.45131300
H	-2.23797000	-1.03192400	-4.16811100
H	-1.26538500	0.31615800	-4.76612400
C	-1.00264900	-3.52099700	-3.01118500
H	-0.62728300	-4.07313300	-3.88372700
H	-1.01611600	-4.20608900	-2.16011700
H	-2.03611500	-3.23157200	-3.22018600
C	1.64386200	-3.45236100	-1.16238300
H	0.86615900	-4.13940600	-0.82091200
H	2.33500700	-4.01705600	-1.80221700
H	2.19782000	-3.11466200	-0.28342000
C	2.09222100	3.80815400	2.05019500
C	2.49099000	5.07082700	1.61227000
C	1.59038500	5.90492300	0.94555200
C	0.28644700	5.46390100	0.70372500
C	-0.11853800	4.19929100	1.12593900
C	0.77734700	3.37171800	1.82126400
H	2.80520300	3.15105900	2.53932500
H	3.51231900	5.39887400	1.78478900
H	1.90666200	6.88675100	0.60557000
H	-0.41720800	6.10397900	0.17934100
H	-1.12695700	3.84009900	0.94301200
N	0.29980500	2.09764900	2.22042100
C	-0.59575800	-2.20599800	4.83661900
C	-1.36087700	-1.56458100	3.85682200
C	-0.96509700	-0.32837000	3.35461500
C	0.20951300	0.28210000	3.83249200
C	0.95532400	-0.35557100	4.83967300
C	0.56118700	-1.59849200	5.33058600
H	-0.90981800	-3.17137400	5.22325200
H	-2.27302000	-2.02437100	3.48863900
H	-1.58176600	0.18368200	2.62416700
H	1.85198700	0.12296000	5.22594800
H	1.14973000	-2.08927800	6.10016800
C	0.67133500	1.58026400	3.33746700
H	1.36493800	2.12031500	3.99270500
D-TS4o	$E = -1315.79977216$	$\Delta H = 0.512115$	$\Delta G = 0.370688$
Ir	-0.23353100	-0.66300400	-0.71415000
C	1.07845600	-2.14944800	-1.66039200
C	-0.15618800	-2.12973500	-2.42169000

C	-0.33057500	-0.82537800	-2.98923300
C	0.80296900	-0.01019200	-2.57085300
C	1.68125800	-0.83236500	-1.78468900
H	0.49899000	-0.38151000	0.74772700
O	-1.92262900	-1.33685000	0.36419400
C	-2.46329400	-0.13754000	0.49125900
O	-1.65072600	0.78830800	-0.06625400
O	-3.52352900	0.12961600	1.04313300
H	-0.99055800	1.68951600	1.46484900
C	3.04041900	-0.44156500	-1.28315900
H	3.30766100	-0.99219500	-0.37771000
H	3.80421000	-0.66146700	-2.04101500
H	3.09488700	0.62607700	-1.05624300
C	1.07292500	1.39036000	-3.03378600
H	1.53707500	1.38212800	-4.02938500
H	0.15121800	1.97376900	-3.10521500
H	1.74798000	1.91629000	-2.35524800
C	-1.43060700	-0.37799200	-3.90276300
H	-1.12152400	-0.45535100	-4.95432500
H	-2.33122000	-0.98358600	-3.77684700
H	-1.70467400	0.66424000	-3.71694600
C	-1.07597100	-3.29952200	-2.59519100
H	-0.74445600	-3.92379700	-3.43542200
H	-1.09496900	-3.92794900	-1.70143300
H	-2.10108600	-2.98149400	-2.79775700
C	1.70856000	-3.36175400	-1.03892300
H	0.95306100	-4.03871600	-0.63120600
H	2.29809400	-3.92469900	-1.77581900
H	2.37791200	-3.08766500	-0.21940600
C	1.92035700	3.31362800	1.60367100
C	2.52749500	4.40810300	0.98935900
C	1.85945000	5.12477100	-0.00645600
C	0.57123200	4.73991700	-0.38667000
C	-0.04401200	3.64156500	0.20994100
C	0.63575600	2.91855500	1.20181500
H	2.42943400	2.79714700	2.41129300
H	3.52021700	4.71317800	1.30730500
H	2.33403700	5.98284300	-0.47275000
H	0.04063700	5.29362300	-1.15572200
H	-1.03508000	3.32117200	-0.09453000
N	-0.02904300	1.83078000	1.81116500
C	-1.00360200	-2.10762900	4.99942300
C	-1.85789700	-1.15182600	4.44288300
C	-1.37305900	-0.21675300	3.53374900

C	-0.01551300	-0.23551100	3.16520600
C	0.83859900	-1.20286900	3.73157900
C	0.34844500	-2.13084400	4.64279400
H	-1.39038700	-2.83387300	5.70837100
H	-2.90951300	-1.13764700	4.71127900
H	-2.06031900	0.50015500	3.09858800
H	1.88803000	-1.21831500	3.44866000
H	1.01588700	-2.86973500	5.07591300
C	0.58109700	0.72662500	2.24614400
H	1.66600600	0.73437100	2.19855200

S2. Cartesian coordinates of the key states together with thermal corrections to enthalpies (ΔH) and free energies (ΔG) and their electronic energies (E)

S2.1 At the M06/BSIV//B3LYP/BSIII level of calculations

A	$E = -1818.36251979$	$\Delta H = 0.275433$	$\Delta G = 0.169355$
Ir	0.57362000	0.53558000	-0.08384700
C	-0.21754200	-1.11303500	-1.26955900
C	-1.16170900	0.00256900	-1.30062800
C	-0.49386600	1.13033000	-1.88213700
C	0.87698700	0.74484800	-2.19523100
C	1.02077800	-0.65855400	-1.83466100
Cl	-0.38420100	-0.10096000	2.16817500
O	2.44420400	0.66028600	0.89208800
C	2.19592500	1.84088300	1.41126300
O	1.05387900	2.34207000	0.92281900
O	2.84894100	2.40840200	2.29817400
K	0.43715000	2.56817900	3.50533500
C	1.89225600	1.58138200	-2.91395500
H	1.81030500	1.44610100	-4.00059400
H	1.75702600	2.64422900	-2.69831600
H	2.90958800	1.31136200	-2.61956100
C	2.26104300	-1.47662900	-2.02420800
H	2.32808900	-2.27877200	-1.28583400
H	2.26385900	-1.93326400	-3.02222200
H	3.16076000	-0.86400300	-1.93259000
C	-0.53289800	-2.50268700	-0.80534100
H	-1.21203700	-2.49023400	0.05004500
H	-1.01194500	-3.07706200	-1.60922200
H	0.37003000	-3.03826300	-0.50276200
C	-2.59464800	-0.07110400	-0.86823400
H	-3.00148300	0.92089100	-0.65776800

H	-3.21162200	-0.52712100	-1.65355000
H	-2.70217800	-0.67270500	0.03725800
C	-1.09180400	2.47818500	-2.14770200
H	-0.35594800	3.27537000	-2.01677300
H	-1.46175600	2.53006400	-3.17983800
H	-1.93185800	2.68410700	-1.48032900
BN-TS2	$E = -2105.83203932$	$\Delta H = 0.401080$	$\Delta G = 0.272822$
Ir	-0.04078100	-1.02763300	-0.08259900
C	-0.48534800	-3.08062800	0.54072600
C	-1.70727300	-2.34679300	0.46388900
C	-1.86286700	-1.85415900	-0.90093900
C	-0.73244300	-2.34299700	-1.67149600
C	0.13974300	-3.06639400	-0.78194200
Cl	2.19363500	-0.88438700	1.05822200
C	1.30854300	1.33479000	-3.30095400
C	0.99194600	1.78788600	-4.58176600
C	-0.31705100	2.15678900	-4.89997000
C	-1.30548600	2.07454100	-3.91443200
C	-0.99471200	1.62816200	-2.63049600
C	0.31991900	1.24564100	-2.30491300
H	2.33038700	1.05106000	-3.05904100
H	1.77424500	1.85245300	-5.33370600
H	-0.56287100	2.50974000	-5.89718900
H	-2.32541600	2.37384200	-4.14229800
H	-1.76058400	1.59078100	-1.86189600
N	0.63511900	0.81562400	-0.99784100
H	-0.03605800	1.22973300	0.07489400
H	1.64131000	0.84921800	-0.84466100
O	-0.69342000	0.79357900	0.95723100
C	-0.27253900	1.04481800	2.26927100
O	0.43842200	2.06618700	2.43158800
O	-0.61905500	0.20086000	3.13679200
K	1.88953800	0.44872000	3.89035500
C	-3.07244500	-1.15692500	-1.44495400
H	-2.83723900	-0.59978100	-2.35391300
H	-3.85510700	-1.88637700	-1.69248700
H	-3.48925600	-0.45455900	-0.71885600
C	-0.54027000	-2.16511700	-3.14503500
H	-1.07949300	-2.95343000	-3.68644300
H	-0.91986400	-1.20102800	-3.48949000
H	0.51385600	-2.22970100	-3.42355000
C	1.38430500	-3.81043100	-1.15861500
H	1.14768100	-4.85781800	-1.38813900

H	1.86146400	-3.37408200	-2.03937600
H	2.11396500	-3.80012600	-0.34580900
C	0.04339900	-3.79072400	1.74893100
H	-0.20443200	-4.85931500	1.70042900
H	1.12988100	-3.70075200	1.82051100
H	-0.39161900	-3.38586300	2.66572000
C	-2.64325100	-2.09389100	1.60935800
H	-2.98051300	-3.04294700	2.04206300
H	-2.14808500	-1.50010400	2.38537500
H	-3.52677400	-1.54304200	1.27983500

C	$E = -1241.46127723$	$\Delta H = 0.366944$	$\Delta G = 0.258935$
Ir	0.14722500	-0.91729100	-0.54798100
C	-0.59005200	-2.50912300	0.83951700
C	-1.47349800	-1.37703900	0.84318200
C	-2.02439600	-1.21886600	-0.50013000
C	-1.43015100	-2.22790100	-1.33263800
C	-0.51443600	-3.00707100	-0.50341000
Cl	2.28449900	-0.62060400	0.55760000
C	1.19448800	2.32696800	-3.25496500
C	0.80410600	3.09334700	-4.34831500
C	-0.39463000	2.82236600	-5.01502700
C	-1.19423000	1.76755900	-4.56721800
C	-0.81099800	0.99551900	-3.47269600
C	0.39186200	1.26039600	-2.79085800
H	2.12857000	2.54492000	-2.74180200
H	1.44135900	3.90802400	-4.68214600
H	-0.69789000	3.42059400	-5.86894600
H	-2.12651200	1.54059400	-5.07854900
H	-1.43077900	0.17435900	-3.13915100
N	0.81777300	0.51466600	-1.69485900
H	1.73850700	0.82173700	-1.38667800
C	-1.86545200	-0.55874900	2.03523500
H	-2.09574200	0.47138200	1.75135600
H	-2.75926200	-0.98130900	2.51333200
H	-1.06864200	-0.53230800	2.78180500
C	0.13632700	-3.06102200	2.02844400
H	0.37994800	-2.27947100	2.75096500
H	-0.48826100	-3.80754600	2.53561800
H	1.07110600	-3.54575900	1.74013700
C	0.26865000	-4.19594200	-0.96943200
H	1.17332900	-4.33650200	-0.37368700
H	-0.33521200	-5.10935900	-0.88548700
H	0.56867500	-4.08931300	-2.01502300

C	-3.12897600	-0.27014500	-0.85260200
H	-4.07806900	-0.63355500	-0.43752800
H	-2.94792700	0.72663100	-0.44133800
H	-3.25834900	-0.16881800	-1.93119200
C	-1.77529800	-2.56620600	-2.75168500
H	-0.88033600	-2.69955200	-3.36561700
H	-2.34011000	-3.50686200	-2.78193200
H	-2.39390000	-1.79799600	-3.21890500

C-TS2i $E = -1588.09658231$ $\Delta H = 0.510371$ $\Delta G = 0.373473$

Ir	0.06927400	-0.99952300	-0.32965100
C	-1.03332200	-2.87448900	-0.02748600
C	-1.74337300	-1.80969800	0.60816500
C	-2.10638300	-0.82188300	-0.40047300
C	-1.62385200	-1.30970000	-1.67467900
C	-0.92436900	-2.55215800	-1.44991200
Cl	2.32274300	-1.98758800	-0.26915900
C	1.22227800	1.75847800	-3.29897000
C	0.74715200	2.71485400	-4.19658400
C	-0.28716400	3.57922300	-3.83086900
C	-0.83544800	3.47995600	-2.54853200
C	-0.36190400	2.52940100	-1.64487500
C	0.67432800	1.64970600	-2.00845800
H	2.02984300	1.09043900	-3.59007700
H	1.18990900	2.78339500	-5.18683700
H	-0.65517600	4.32420400	-4.53008300
H	-1.63078300	4.15559700	-2.24412800
H	-0.77797200	2.46774400	-0.64378000
N	1.16570400	0.70340300	-1.08328200
H	2.06304700	0.33346000	-1.39114000
O	0.69916000	0.46065100	1.23231500
C	1.62469900	0.16259300	2.27136200
H	2.52991300	-0.30266700	1.86332300
H	1.15957700	-0.58313400	2.93148900
C	2.00236300	1.38837800	3.08426700
C	3.09984500	1.31530300	3.95496800
C	1.28356300	2.58587800	3.00929900
C	3.46637100	2.41089300	4.73554300
H	3.67263900	0.39223900	4.01773800
C	1.65399300	3.68755600	3.78582200
H	0.43748800	2.65254000	2.33367200
C	2.74404800	3.60479600	4.65255200
H	4.32084400	2.33621400	5.40300500
H	1.08877300	4.61291700	3.70997200

H	3.03232100	4.46176800	5.25503800
H	1.13243000	0.90195600	0.23441200
C	-0.52364900	-4.12799900	0.61567000
H	-1.23326000	-4.95070400	0.45877600
H	0.43911500	-4.42676700	0.19524500
H	-0.39026200	-4.00187300	1.69272800
C	-2.08974100	-1.70388200	2.06135500
H	-3.12247400	-2.03530000	2.22935900
H	-1.43536600	-2.32219000	2.67939200
H	-2.01000500	-0.67171500	2.41019600
C	-3.00185600	0.35872200	-0.17704400
H	-4.05427000	0.04461900	-0.18682300
H	-2.80976400	0.83309000	0.78915100
H	-2.87492800	1.11343700	-0.95588600
C	-1.85980500	-0.66181100	-3.00341900
H	-2.83098000	-0.98301400	-3.40185300
H	-1.87152600	0.42738200	-2.92907900
H	-1.09288800	-0.94089200	-3.72879700
C	-0.33627700	-3.44696700	-2.49795800
H	-1.07826300	-4.18525700	-2.82938900
H	-0.01230900	-2.87944900	-3.37363000
H	0.53130100	-3.98749300	-2.11404600

BC-IN4i $E = -1300.60596231$ $\Delta H = 0.384569$ $\Delta G = 0.268683$

Ir	0.07515000	-0.65401300	-0.70194500
C	-1.10218700	-2.34183900	-0.09008000
C	-1.86855600	-1.13641100	0.14661400
C	-2.02410600	-0.48376300	-1.13156700
C	-1.41417000	-1.32066300	-2.16398500
C	-0.85210000	-2.46716800	-1.52143800
O	0.73615900	0.55538100	0.70373300
C	2.01539700	1.18105500	0.77920600
H	2.20678900	1.79666900	-0.10876000
H	2.81242600	0.42649000	0.82467800
C	2.05621900	2.04488600	2.02138500
C	2.34506200	1.48133000	3.27199700
C	1.77790100	3.41587500	1.95294500
C	2.35543700	2.26651700	4.42542500
H	2.57087300	0.41934900	3.33651200
C	1.78866300	4.20734000	3.10372200
H	1.55739900	3.86614800	0.98767300
C	2.07670200	3.63354700	4.34373200
H	2.58649100	1.81487300	5.38671400
H	1.57513400	5.27063100	3.03211900

H	2.08911900	4.24750900	5.24029100
C	-0.71700600	-3.35225200	0.94457400
H	-1.51155400	-4.10387000	1.04233200
H	0.20340000	-3.87379100	0.67206100
H	-0.56881800	-2.88985900	1.92284600
C	-2.41084000	-0.66491500	1.46056700
H	-3.42436700	-1.05303300	1.62271100
H	-1.78721800	-0.99774300	2.29346400
H	-2.45813300	0.42557600	1.50322900
C	-2.76916300	0.79006500	-1.38310800
H	-3.82049100	0.56706500	-1.60822400
H	-2.74370000	1.45033200	-0.51352600
H	-2.35406500	1.33441600	-2.23455200
C	-1.42761200	-1.02808400	-3.63341800
H	-2.37095900	-1.36467000	-4.08225500
H	-1.32832600	0.04294700	-3.82773700
H	-0.60970800	-1.53333600	-4.15081400
C	-0.15197400	-3.61583200	-2.18141900
H	-0.84671000	-4.45112000	-2.33613600
H	0.25350200	-3.33113500	-3.15420900
H	0.67982500	-3.97898800	-1.57253000
Cl	2.11114700	-0.45362200	-1.92655900

BC-TS5i $E = -1300.58135667$ $\Delta H = 0.379159$ $\Delta G = 0.268177$

Ir	-0.34854000	-0.57857100	0.15385600
C	-0.82269600	-2.70456500	0.34434200
C	-2.01831500	-1.92896100	0.60943700
C	-2.36096000	-1.21441500	-0.61008300
C	-1.36270100	-1.49540900	-1.59041700
C	-0.38519000	-2.41383500	-0.99710900
O	-0.71106900	1.26885700	1.16733700
C	0.05722300	0.70802500	2.07292000
H	0.79090000	-0.42140700	1.39029000
H	-0.43786700	0.11311900	2.85670800
C	1.27534600	1.41731200	2.58423700
C	1.82287200	1.02180300	3.81199900
C	1.84004800	2.49035900	1.88338300
C	2.93004300	1.68732600	4.33579800
H	1.37388600	0.19573300	4.36001600
C	2.94432700	3.15733000	2.41228200
H	1.40966300	2.77966500	0.93176700
C	3.49218700	2.75730000	3.63464400
H	3.34837900	1.37760200	5.28934400
H	3.38194600	3.98968900	1.86844100

H	4.35378500	3.27942500	4.04156700
C	-0.18091900	-3.68254600	1.28300900
H	-0.62472700	-4.67734000	1.14802500
H	0.89229100	-3.76751800	1.09866100
H	-0.32114700	-3.39704200	2.32842000
C	-2.86083000	-1.98265400	1.84966800
H	-3.67125300	-2.71459600	1.73638100
H	-2.27419500	-2.27669600	2.72356000
H	-3.32010800	-1.01407000	2.06495300
C	-3.56224200	-0.33698100	-0.78288400
H	-4.43886700	-0.94532100	-1.04113300
H	-3.79673400	0.20860500	0.13454300
H	-3.41571400	0.39579200	-1.57910400
C	-1.32269600	-1.00351600	-3.00401400
H	-1.69153000	-1.77993600	-3.68665100
H	-1.94188600	-0.11399500	-3.13904200
H	-0.30350000	-0.74602300	-3.30037100
C	0.75063300	-3.05716500	-1.73430400
H	0.39833200	-3.92837900	-2.30212500
H	1.20866600	-2.35852000	-2.43775500
H	1.53157600	-3.39595400	-1.04929700
Cl	1.33745600	0.63324500	-1.13662200

BC-IN7i $E = -955.14503468$ $\Delta H = 0.257011$ $\Delta G = 0.171726$

Ir	0.55065500	0.38216100	0.13155300
C	0.25514500	-1.61283100	-0.57310600
C	-0.11751200	-1.54989400	0.81702100
C	-1.19024700	-0.58102400	0.89900700
C	-1.61279300	-0.22068400	-0.46678800
C	-0.72772000	-0.83924000	-1.36056800
H	1.82058100	0.53527100	1.10723600
C	1.30818500	-2.49596600	-1.16887600
H	0.86989800	-3.45361500	-1.48084600
H	1.76306600	-2.03664800	-2.05057700
H	2.10423400	-2.70839400	-0.45192600
C	0.44608400	-2.36399100	1.94275800
H	-0.11651800	-3.30039600	2.05406800
H	1.49331900	-2.62060800	1.76702800
H	0.39265200	-1.82610800	2.89222700
C	-1.92654200	-0.18743400	2.14175500
H	-2.78937000	-0.85076900	2.29163700
H	-1.28914700	-0.25961300	3.02566700
H	-2.30195600	0.83689300	2.07606500
C	-2.75808700	0.68903200	-0.78786400

H	-3.71423700	0.16266400	-0.67243200
H	-2.77888000	1.55589800	-0.12099700
H	-2.70210300	1.06256600	-1.81268600
C	-0.71093100	-0.74116000	-2.85415200
H	-1.06154100	-1.67880100	-3.30386800
H	-1.35260200	0.06530100	-3.21426200
H	0.30037200	-0.55717100	-3.22927100
Cl	1.00447800	2.57066200	-0.61473300

BC-TS9i $E = -1511.64648208$ $\Delta H = 0.479926$ $\Delta G = 0.351259$

Ir	0.83101400	-0.69468300	-0.56729700
C	0.44423400	-2.77605000	0.03859600
C	-0.47143300	-1.93666000	0.75105800
C	-1.29939200	-1.24298800	-0.21681400
C	-0.94149400	-1.72869500	-1.53502000
C	0.14649900	-2.64197200	-1.39249800
Cl	3.20833200	-0.95216500	-1.08250800
H	1.49179300	0.27051400	0.60047500
C	0.81463100	-3.43598000	-2.47319800
H	0.42999900	-4.46399500	-2.48274000
H	0.63970500	-3.00412800	-3.46118500
H	1.89495400	-3.48190500	-2.31659600
C	1.42910800	-3.74255000	0.62323100
H	1.72281100	-3.45153600	1.63460000
H	0.99701900	-4.75058400	0.67467200
H	2.33722600	-3.79551600	0.01829400
C	-1.62560900	-1.32922500	-2.80705700
H	-2.58294900	-1.85837900	-2.90105100
H	-1.83479500	-0.25650700	-2.82867000
H	-1.02474400	-1.57381600	-3.68535200
C	-2.47804800	-0.37280900	0.09737200
H	-3.38122600	-0.98647000	0.21639200
H	-2.33456200	0.18845900	1.02300700
H	-2.67020500	0.34528900	-0.70287200
C	-0.60187700	-1.82826000	2.24123500
H	-1.35359900	-2.54103300	2.60447500
H	0.34073500	-2.05396700	2.74528700
H	-0.91924100	-0.82880900	2.54788100
C	1.73312600	0.88870000	-3.74848600
C	2.46990600	1.32839200	-4.84285700
C	3.19838700	2.52157500	-4.78085000
C	3.17140200	3.26946600	-3.60399300
C	2.43321000	2.83690500	-2.50108400
C	1.71001400	1.62992700	-2.55264000

H	1.18492200	-0.04651200	-3.79155700
H	2.48176600	0.73176400	-5.75142900
H	3.77368600	2.86121900	-5.63707000
H	3.72142400	4.20495200	-3.53963200
H	2.39552200	3.45335400	-1.60767500
N	0.86975900	1.23451400	-1.49532000
C	-1.52917300	3.69448800	2.33520800
C	-0.37384600	3.12161600	2.87689800
C	0.50368500	2.41229000	2.05879600
C	0.23415300	2.25812400	0.69016400
C	-0.91887800	2.84280100	0.15169400
C	-1.79539800	3.55669600	0.97180700
H	-2.21109400	4.25140100	2.97162200
H	-0.15529900	3.23215000	3.93537200
H	1.40336300	1.97040000	2.48210400
H	-1.10954000	2.73765400	-0.91125000
H	-2.68432900	4.01056100	0.54210800
C	1.21317000	1.54181100	-0.19563400
H	2.25581200	1.83796400	-0.02080500

BC-IN10i $E = -1511.67925654$ $\Delta H = 0.485472$ $\Delta G = 0.354366$

Ir	0.63269300	-1.13487800	-0.22198400
C	0.06878100	-3.30622600	-0.22968300
C	-1.09825500	-2.48866500	-0.06673600
C	-1.22339000	-1.64218000	-1.24840100
C	-0.11471800	-1.92241700	-2.12141100
C	0.70974100	-2.93103300	-1.46192700
Cl	1.66735800	-1.29192900	1.97985600
H	2.57624400	0.80074500	1.17774100
C	1.94131100	-3.55502100	-2.04317500
H	1.67246800	-4.41653800	-2.66901700
H	2.48858100	-2.84640700	-2.66960000
H	2.61932800	-3.90688800	-1.26240400
C	0.54637300	-4.35604400	0.72662500
H	0.31761300	-4.09077100	1.76039900
H	0.06156200	-5.31561300	0.50551800
H	1.62637600	-4.50280000	0.65731100
C	0.07266000	-1.42371800	-3.52083200
H	-0.37022200	-2.13310100	-4.23278500
H	-0.40386900	-0.45394200	-3.67394100
H	1.13013800	-1.31856900	-3.77352000
C	-2.39619000	-0.76242700	-1.55244100
H	-3.20393000	-1.36425100	-1.99008600
H	-2.78955200	-0.28996200	-0.64877400

H	-2.14027800	0.02293400	-2.26527100
C	-2.08783500	-2.56238200	1.05627900
H	-2.90894100	-3.24569000	0.80157200
H	-1.62427600	-2.92639800	1.97563000
H	-2.52483100	-1.58308200	1.26939400
C	1.99405600	1.46814900	-2.70265200
C	1.74539500	2.17207400	-3.88151900
C	0.52576200	2.82869600	-4.06644100
C	-0.43940800	2.77907700	-3.05829700
C	-0.19304100	2.07584200	-1.87606600
C	1.02285000	1.40154600	-1.68964100
H	2.94153400	0.95639500	-2.55619700
H	2.50611900	2.20670100	-4.65709800
H	0.33272800	3.37880700	-4.98303800
H	-1.38527900	3.29960400	-3.18412000
H	-0.93342500	2.05461200	-1.08317500
N	1.29826600	0.68754600	-0.47763700
C	0.17193100	4.77507500	2.40306800
C	1.16636300	5.02594800	1.45736100
C	1.80492600	3.96184600	0.81426300
C	1.46314800	2.63607100	1.10620900
C	0.46148000	2.39495200	2.05960200
C	-0.17835500	3.45461900	2.70226200
H	-0.32527700	5.60008800	2.90603900
H	1.44644000	6.04832200	1.21735900
H	2.57863400	4.16329200	0.07704200
H	0.19547700	1.36925800	2.29960000
H	-0.94619400	3.25107800	3.44432700
C	2.17261200	1.47583400	0.42548000
H	3.01315700	1.86922600	-0.16150300
B-TS12i	$E = -2376.05084186$	$\Delta H = 0.519858$	$\Delta G = 0.368054$
Ir	2.07302700	-1.45819200	-4.91911600
C	2.76080100	-3.01875800	-3.55546000
C	1.56362200	-3.46492900	-4.25387000
C	1.87931300	-3.49816800	-5.67364200
C	3.23270800	-3.04451400	-5.84095500
C	3.78939400	-2.76882100	-4.52073100
H	1.25734000	0.97700700	-6.66709700
C	5.20166600	-2.35984800	-4.23359900
H	5.86809300	-3.23142500	-4.27549000
H	5.55758800	-1.62781400	-4.96228000
H	5.29080800	-1.91761300	-3.23891900
C	2.89975000	-2.82325800	-2.07631500

H	3.35351600	-1.85303700	-1.85623800
H	1.92851700	-2.85382700	-1.57891600
H	3.52576200	-3.61562900	-1.64715200
C	3.99516100	-2.98340400	-7.12828700
H	4.51461600	-3.93498000	-7.30202000
H	3.33464500	-2.79961500	-7.97872500
H	4.74137400	-2.18718000	-7.10779200
C	0.98821000	-4.02324000	-6.75501100
H	1.10978800	-5.11147500	-6.83741000
H	-0.06299000	-3.81882000	-6.54518600
H	1.23419700	-3.58586000	-7.72558600
C	0.32682500	-4.02438800	-3.62153100
H	0.46172800	-5.09687900	-3.42562700
H	0.10108800	-3.53917300	-2.66976900
H	-0.54438700	-3.90841800	-4.26795500
C	-1.65438800	-1.69406500	-6.37136100
C	-2.85586200	-2.37957200	-6.17863000
C	-3.42953600	-2.46671700	-4.90879100
C	-2.78480400	-1.85260800	-3.83194000
C	-1.58637700	-1.16546200	-4.02063800
C	-0.99160800	-1.07652800	-5.29381200
H	-1.23172800	-1.63822400	-7.36899700
H	-3.34695800	-2.84333800	-7.03066700
H	-4.36830100	-2.99341600	-4.76313200
H	-3.22401500	-1.89418200	-2.83847100
H	-1.10314100	-0.67810600	-3.17968200
N	0.23228400	-0.34892600	-5.44245000
C	-2.65752200	3.73957200	-6.55307200
C	-2.64034500	2.83429800	-7.61423400
C	-1.70919600	1.79209600	-7.62833300
C	-0.77780000	1.64394100	-6.59330700
C	-0.79921900	2.56314300	-5.53128800
C	-1.73305900	3.59960600	-5.51340000
H	-3.38398200	4.54782600	-6.53478400
H	-3.35552800	2.93188900	-8.42705600
H	-1.70457100	1.08684600	-8.45649200
H	-0.07534800	2.47198800	-4.72334200
H	-1.73747300	4.30335200	-4.68463900
C	0.26204500	0.53453800	-6.63292600
H	0.14642900	-0.03467400	-7.56479000
Cl	3.51728200	0.34453600	-5.94961400
O	1.41897900	-0.00794500	-3.39173700
C	2.23078700	1.05965300	-2.97053800
O	1.81327000	2.20850800	-3.26244600

O	3.29077400	0.74622200	-2.38138000
K	4.31310600	2.61056200	-3.95594500
H	0.68330900	0.20335400	-4.21392000
Ph-TS12i	$E = -1858.31527295$	$\Delta H = 0.629200$	$\Delta G = 0.470487$
Ir	0.96058600	-0.62130700	-0.94612700
C	0.45003100	-2.62259600	-1.70409000
C	-0.74290300	-1.77660800	-1.70498300
C	-0.49564400	-0.67458000	-2.59497900
C	0.86497600	-0.78173700	-3.08530800
C	1.41539500	-2.03262600	-2.57343400
Cl	3.36008600	-0.27412300	-0.54400100
H	2.47973200	1.84587900	0.20077800
C	2.74980600	-2.60078200	-2.94331400
H	2.66177000	-3.14910200	-3.89037000
H	3.49738500	-1.81644000	-3.07135100
H	3.12286200	-3.29403600	-2.18694200
C	0.58335100	-3.92113900	-0.96905500
H	0.04938500	-3.89685300	-0.01609400
H	0.15984200	-4.73946800	-1.56598000
H	1.62833600	-4.16334200	-0.76376900
C	1.50730600	0.09560700	-4.11724900
H	1.29833900	-0.27826400	-5.12842500
H	1.13370900	1.12075600	-4.05639200
H	2.59146300	0.12861600	-3.98912700
C	-1.49234900	0.35124900	-3.03002200
H	-1.97350900	0.00772700	-3.95566200
H	-2.27316800	0.51080700	-2.28585500
H	-1.02176200	1.31351400	-3.24085700
C	-2.04555500	-2.12848500	-1.05506500
H	-2.61211400	-2.81353400	-1.69998100
H	-1.89335300	-2.62992000	-0.09584200
H	-2.66148700	-1.24497900	-0.88172100
C	-1.20801800	2.90907100	-0.65867600
C	-2.54113700	3.31811300	-0.74066300
C	-3.55819500	2.56430100	-0.15585900
C	-3.21939400	1.38942500	0.52319500
C	-1.89117900	0.97736800	0.60854400
C	-0.85408900	1.72394400	0.01303800
H	-0.44422300	3.52596000	-1.11685800
H	-2.77971100	4.23992000	-1.26515700
H	-4.59244800	2.89045200	-0.21431000
H	-3.99318100	0.79548700	1.00339100
H	-1.63834100	0.06967200	1.14631900

N	0.49206800	1.26458800	0.14234300
C	1.26409000	5.36494600	3.20086700
C	1.56061700	5.71926700	1.88402200
C	1.61287200	4.73934700	0.89052100
C	1.37694500	3.39098000	1.19080900
C	1.08675600	3.04754900	2.51900800
C	1.02697100	4.02435800	3.51356900
H	1.21669900	6.12514100	3.97578500
H	1.74544100	6.75899100	1.62668000
H	1.84123100	5.02544100	-0.13410100
H	0.89794500	2.01033800	2.77968900
H	0.79640100	3.73616900	4.53581300
C	1.51050700	2.33582200	0.10181500
H	1.52926400	2.83047000	-0.87860000
O	0.72212600	-0.84284400	1.27835800
C	1.73822800	-1.31473100	2.15677000
H	2.58279300	-0.61592200	2.18123300
H	2.12873800	-2.25521700	1.74906400
C	1.23183100	-1.55312700	3.56911000
C	-0.10081100	-1.34923000	3.93973700
C	2.14134300	-1.99631900	4.54195400
C	-0.51704200	-1.58300400	5.25438000
H	-0.81085100	-1.00393300	3.19631700
C	1.72741000	-2.23268800	5.85143200
H	3.18276500	-2.15492100	4.26873800
C	0.39272400	-2.02571100	6.21389900
H	-1.55623700	-1.41630500	5.52623300
H	2.44596700	-2.57570100	6.59113800
H	0.06913600	-2.20685000	7.23518900
H	0.64108000	0.27635600	1.10846600

B-TS2i	$E = -2164.98714845$	$\Delta H = 0.418837$	$\Delta G = 0.284489$
Ir	-0.12953600	-0.72844700	0.45379600
C	-0.67716600	-2.71560900	1.07971100
C	-1.84800300	-2.03661800	0.57750900
C	-1.60893300	-1.66028000	-0.80163600
C	-0.28759700	-2.15913000	-1.16512400
C	0.28638400	-2.80286600	-0.01623800
Cl	1.90799600	-0.35049000	1.82607800
O	-1.05247300	1.08712900	1.19227300
C	-0.68040800	1.64534800	2.42258100
O	-0.05629700	2.73704200	2.35295100
O	-0.97555700	0.99257300	3.45250500
K	1.43976600	1.65618200	4.20189200

O	0.30325100	1.10972900	-0.66586100
C	1.58711300	1.71834800	-0.76057000
H	2.34982500	0.94046600	-0.87945400
H	1.81424800	2.24736700	0.17480700
C	1.67235300	2.68770500	-1.92502400
C	0.53137700	3.25888100	-2.49970800
C	2.93185400	3.05717200	-2.41865600
C	0.64759700	4.17879900	-3.54493000
H	-0.44661800	2.97401100	-2.12601800
C	3.05025600	3.97906900	-3.45890200
H	3.82708000	2.61607300	-1.98432500
C	1.90545900	4.54389600	-4.02741600
H	-0.24846500	4.61279100	-3.98125900
H	4.03491200	4.25213100	-3.82956000
H	1.99428200	5.25989600	-4.83990500
H	-0.38251100	1.48574700	0.23822800
C	1.60646300	-3.50764900	0.04026000
H	1.47109100	-4.57870600	-0.15838700
H	2.30347300	-3.11307000	-0.70280100
H	2.07337500	-3.40127300	1.02148200
C	0.34498200	-2.03444600	-2.51628600
H	0.08340300	-2.90353200	-3.13383900
H	0.00288200	-1.13836800	-3.03776500
H	1.43405600	-1.98838800	-2.44488300
C	-2.58299600	-0.99130900	-1.72225900
H	-3.18634000	-1.73740600	-2.25555400
H	-3.26559800	-0.33972400	-1.17178600
H	-2.07007400	-0.37964900	-2.46818100
C	-3.10090600	-1.75933000	1.34657200
H	-3.82354500	-2.56754900	1.17417100
H	-2.90786100	-1.69712500	2.41870000
H	-3.56095800	-0.82006200	1.03450100
C	-0.52480300	-3.33668700	2.43477400
H	-0.88775900	-4.37295700	2.42450000
H	0.52065800	-3.35032400	2.74985100
H	-1.09227300	-2.78622600	3.18886600

S2.2 At the M06//B3PW91 level of calculations

A	$E = -1818.37398713$	$\Delta H = 0.275944$	$\Delta G = 0.169792$
Ir	0.56548100	0.53198600	-0.08634300
C	-0.21652700	-1.11169000	-1.26730200
C	-1.16156300	0.00177000	-1.29967700
C	-0.49446100	1.13128500	-1.87896100

C	0.87564100	0.74789400	-2.19341200
C	1.02184200	-0.65295200	-1.83108000
Cl	-0.39871200	-0.07100900	2.13059400
O	2.42898800	0.62720600	0.90133100
C	2.19582600	1.81261200	1.40632600
O	1.07194100	2.33298300	0.90899900
O	2.85493600	2.37616300	2.28939200
K	0.44381700	2.59039400	3.47821800
C	1.88615200	1.58431500	-2.90800500
H	1.80426300	1.45019600	-3.99448700
H	1.74932300	2.64644300	-2.69013100
H	2.90376600	1.31628300	-2.61297800
C	2.25871800	-1.46727600	-2.01716000
H	2.33306800	-2.25819900	-1.26743900
H	2.25427000	-1.93777600	-3.00839600
H	3.15737300	-0.85129300	-1.93998000
C	-0.52789900	-2.49792100	-0.80704900
H	-1.21468500	-2.48770200	0.04243100
H	-0.99616400	-3.07524900	-1.61482800
H	0.37500500	-3.02784000	-0.49452000
C	-2.58903200	-0.07268200	-0.86768200
H	-2.99657300	0.91898300	-0.65738100
H	-3.20500400	-0.53060200	-1.65227100
H	-2.69427000	-0.67271300	0.03932500
C	-1.09280600	2.47336900	-2.14369300
H	-0.35828800	3.27168800	-2.01253900
H	-1.46302700	2.52364800	-3.17552900
H	-1.93245200	2.67812800	-1.47547500

PhCH₂OH $E = -346.64279070$ $\Delta H = 0.145926$ $\Delta G = 0.089418$

C	0.35731400	1.95848800	0.19125900
H	-0.03932400	2.32370600	1.15266700
H	1.44032200	2.16960200	0.19908400
O	-0.27250400	2.59902300	-0.90204300
H	0.02062400	3.51698300	-0.90860900
C	0.15488700	0.46618600	0.10489300
C	-0.17670900	-0.15091200	-1.10341800
C	0.34106000	-0.32720100	1.24203200
C	-0.31954700	-1.53650300	-1.17226200
H	-0.33048700	0.46477300	-1.98354900
C	0.20556200	-1.71141800	1.17231500
H	0.59196900	0.14317800	2.19092900
C	-0.12589500	-2.32179900	-0.03754000
H	-0.58262400	-2.00325100	-2.11810500

H	0.35242600	-2.31374200	2.06509600
H	-0.23730300	-3.40135000	-0.09275000
PhNH ₂	$E = -287.48312188$	$\Delta H = 0.128154$	$\Delta G = 0.077662$
C	-2.02887300	-1.90620400	-0.15747500
C	-0.63972500	-1.84719100	-0.11675400
C	0.02075900	-0.62619200	0.01880700
C	-0.73729200	0.54108400	0.11200000
C	-2.12699900	0.49499100	0.07120200
C	-2.79681200	-0.73294300	-0.06492000
H	-2.53146600	-2.86470900	-0.26700200
H	-0.06878400	-2.76954300	-0.19065600
H	1.10539900	-0.58514900	0.05131200
H	-0.24256900	1.50318200	0.22049100
H	-2.70545300	1.41355400	0.14223800
N	-4.18137800	-0.77999700	-0.16265200
H	-4.60307800	-1.66463200	0.08270300
H	-4.67143100	-0.00077300	0.25373400
BN-TS2	$E = -2105.84323399$	$\Delta H = 0.401957$	$\Delta G = 0.274392$
Ir	-0.04136500	-1.02847000	-0.08458400
C	-0.48426900	-3.07289100	0.53651400
C	-1.70532700	-2.33717800	0.45850900
C	-1.86039100	-1.84547000	-0.90535600
C	-0.72845000	-2.33078900	-1.67368900
C	0.14205200	-3.05739100	-0.78446500
Cl	2.16271900	-0.88634600	1.04706400
C	1.30442400	1.31807000	-3.29613800
C	0.98382700	1.77212500	-4.57346500
C	-0.32408000	2.14209700	-4.88633400
C	-1.30733100	2.05985900	-3.89822100
C	-0.99249700	1.61247800	-2.61791200
C	0.32097000	1.22857500	-2.29746700
H	2.32707400	1.03191300	-3.05887700
H	1.76373500	1.83648900	-5.32843300
H	-0.57332800	2.49651800	-5.88254700
H	-2.32806900	2.36115800	-4.12150700
H	-1.75445000	1.57636000	-1.84468800
N	0.63819600	0.80205200	-0.99652700
H	-0.03091700	1.21663100	0.07410700
H	1.64430700	0.82774400	-0.84530900
O	-0.69338300	0.78664100	0.94931600
C	-0.27535100	1.02594000	2.25713100
O	0.42997600	2.04667200	2.42986700

O	-0.62561500	0.17910700	3.11734900
K	1.86847900	0.43456900	3.89541200
C	-3.06675500	-1.15282600	-1.44728100
H	-2.83473500	-0.60479000	-2.36279100
H	-3.85095500	-1.88371100	-1.68446400
H	-3.47847200	-0.44318800	-0.72541000
C	-0.53459100	-2.14920200	-3.14098000
H	-1.07818400	-2.93235300	-3.68491200
H	-0.90840700	-1.18086800	-3.48108100
H	0.51934600	-2.21781800	-3.41902100
C	1.38314300	-3.79786900	-1.15855100
H	1.14690500	-4.84508400	-1.38790400
H	1.86136600	-3.36060700	-2.03821700
H	2.11166000	-3.78591800	-0.34451200
C	0.04201900	-3.78031800	1.74075000
H	-0.20007100	-4.84978200	1.68850800
H	1.12796900	-3.68364900	1.81529200
H	-0.39746100	-3.37867000	2.65673900
C	-2.63359000	-2.07722700	1.60162000
H	-2.94021800	-3.02072200	2.06704900
H	-2.14202200	-1.44651600	2.35246000
H	-3.53477800	-1.55992300	1.26534000

KHCO_3 $E = -864.37768263$ $\Delta H = 0.037101$ $\Delta G = -0.012176$

C	-0.74644900	-0.12200100	0.00334600
O	-1.46793500	1.04694600	0.02261100
O	0.51260200	-0.00647300	-0.01306200
O	-1.41939300	-1.17846200	0.00313300
K	0.72540300	-2.55926200	-0.05857400
H	-0.79670000	1.74305300	0.01972000

C	$E = -1241.47240015$	$\Delta H = 0.367531$	$\Delta G = 0.259725$
Ir	0.14373800	-0.92515900	-0.54752500
C	-0.59189600	-2.50688600	0.83374300
C	-1.47158800	-1.37179000	0.83593700
C	-2.02007300	-1.21183400	-0.50728000
C	-1.42863600	-2.22277100	-1.33894500
C	-0.51581000	-3.00377200	-0.50949500
Cl	2.25844200	-0.63083500	0.55474700
C	1.18696200	2.32077100	-3.23987100
C	0.79203500	3.08677400	-4.32944900
C	-0.40290100	2.81022000	-4.99673400
C	-1.19428900	1.74964900	-4.55316200
C	-0.80628500	0.97866600	-3.46243100

C	0.39228200	1.24901800	-2.77989300
H	2.11961000	2.54395000	-2.72543800
H	1.42396700	3.90724600	-4.66033600
H	-0.71005700	3.40925900	-5.84911900
H	-2.12487400	1.51762100	-5.06600000
H	-1.41771600	0.15033700	-3.12759300
N	0.81818600	0.50530400	-1.69100500
H	1.73701300	0.81144200	-1.37758700
C	-1.85895000	-0.55296700	2.02239800
H	-2.09224000	0.47536200	1.73475700
H	-2.74943600	-0.97669800	2.50503400
H	-1.05855300	-0.52154900	2.76500400
C	0.13193500	-3.05682300	2.01824100
H	0.37076700	-2.27564500	2.74288900
H	-0.49047500	-3.80746100	2.52143800
H	1.07007400	-3.53541400	1.73022700
C	0.26528800	-4.18781900	-0.97435200
H	1.17307600	-4.32412400	-0.38226400
H	-0.33664800	-5.10169200	-0.88522100
H	0.56095800	-4.08213600	-2.02121200
C	-3.11563500	-0.26031400	-0.85895300
H	-4.05750400	-0.59591800	-0.40666500
H	-2.90770400	0.74649600	-0.48667600
H	-3.27341900	-0.19267700	-1.93668500
C	-1.77182300	-2.56033800	-2.75325500
H	-0.87785300	-2.66402400	-3.37421700
H	-2.31075500	-3.51565000	-2.78470900
H	-2.41589200	-1.80706500	-3.21095000
C-TS2i	$E = -1588.10769754$	$\Delta H = 0.511360$	$\Delta G = 0.374937$
Ir	0.06415900	-0.98798700	-0.32570100
C	-1.02707800	-2.85771600	-0.01593700
C	-1.74136300	-1.79127800	0.61255700
C	-2.10563900	-0.81052800	-0.40082200
C	-1.61595800	-1.30166200	-1.67034100
C	-0.91525500	-2.54206000	-1.43873100
Cl	2.29099500	-1.97656800	-0.26815400
C	1.21490900	1.75636400	-3.29917500
C	0.73910300	2.71508600	-4.19091600
C	-0.29785200	3.57240200	-3.82358200
C	-0.84810600	3.46324600	-2.54491500
C	-0.37390000	2.51043000	-1.64731000
C	0.66532800	1.63777200	-2.01217000
H	2.02549700	1.09250100	-3.59281000

H	1.18440100	2.79103500	-5.17989100
H	-0.66676000	4.32055900	-4.51944000
H	-1.64660700	4.13458700	-2.23802200
H	-0.79061500	2.44100400	-0.64652200
N	1.15817400	0.69665600	-1.09231700
H	2.05063100	0.31946100	-1.40403200
O	0.69819800	0.47100600	1.22157300
C	1.63010600	0.16346900	2.24208900
H	2.53614000	-0.28965100	1.81997300
H	1.17855400	-0.59569300	2.89616000
C	2.00407400	1.37583200	3.06827400
C	3.09278800	1.29347300	3.94598100
C	1.28976300	2.57379500	2.99649500
C	3.45497100	2.38117100	4.73614900
H	3.66321100	0.36833600	4.00669600
C	1.65571400	3.66738800	3.78286700
H	0.44915300	2.64559000	2.31365500
C	2.73716000	3.57582800	4.65639500
H	4.30403500	2.29957100	5.41022000
H	1.09303300	4.59487300	3.70931000
H	3.02274400	4.42789500	5.26763700
H	1.12879100	0.90017600	0.22554500
C	-0.51476200	-4.10077200	0.63279400
H	-1.21958300	-4.92747300	0.47735800
H	0.45149000	-4.39511900	0.21665500
H	-0.38443700	-3.96798100	1.70939500
C	-2.09207200	-1.68129100	2.05890900
H	-3.12696700	-2.00781900	2.22150100
H	-1.44342900	-2.30170800	2.68076700
H	-2.00855300	-0.64895500	2.40622600
C	-3.00657900	0.36083600	-0.18707600
H	-4.05583000	0.03709900	-0.19350700
H	-2.81719700	0.84517200	0.77463600
H	-2.88678200	1.10939400	-0.97318200
C	-1.84556800	-0.66069900	-2.99727500
H	-2.81404200	-0.98505100	-3.39888600
H	-1.85879200	0.42898500	-2.92546700
H	-1.07391700	-0.93994600	-3.71749100
C	-0.31763800	-3.43422800	-2.47579200
H	-1.04965100	-4.18503200	-2.80011300
H	-0.00099800	-2.86910300	-3.35561700
H	0.55816100	-3.95802800	-2.08671400

BC-IN4i $E = -1300.61745110$ $\Delta H = 0.385073$ $\Delta G = 0.270164$

Ir	0.06586900	-0.65783100	-0.69016100
C	-1.10013800	-2.34838900	-0.09100500
C	-1.87233600	-1.14824000	0.15173300
C	-2.02490300	-0.48698000	-1.12143500
C	-1.40905200	-1.31421700	-2.15773900
C	-0.84584100	-2.46384700	-1.52181300
O	0.71523700	0.55416500	0.72297000
C	1.98815600	1.17397300	0.78091300
H	2.17630800	1.78625800	-0.11124700
H	2.78842700	0.42116700	0.82262600
C	2.04264400	2.04343200	2.01507600
C	2.30243200	1.48124600	3.27062200
C	1.80826300	3.41983400	1.93516000
C	2.32782400	2.27309500	4.41682800
H	2.49271600	0.41263000	3.34471300
C	1.83442800	4.21828700	3.07869500
H	1.60886400	3.86958900	0.96461100
C	2.09399200	3.64593400	4.32330900
H	2.53645900	1.82126800	5.38354900
H	1.65507000	5.28753500	2.99748500
H	2.11862800	4.26598500	5.21582800
C	-0.71212900	-3.35856600	0.93501700
H	-1.50232000	-4.11523400	1.02574700
H	0.21258600	-3.87201700	0.66174000
H	-0.56887200	-2.90042900	1.91599500
C	-2.41970000	-0.69074700	1.46234000
H	-3.43191300	-1.08493300	1.61624200
H	-1.79780200	-1.02696800	2.29509100
H	-2.47106000	0.39912000	1.51367000
C	-2.76724400	0.78354200	-1.36575100
H	-3.81596300	0.56040200	-1.60125400
H	-2.74908100	1.43548600	-0.48978300
H	-2.34558200	1.33671500	-2.20828200
C	-1.41887400	-1.01270300	-3.61987700
H	-2.35691300	-1.35622000	-4.07399700
H	-1.32926200	0.06047900	-3.80643700
H	-0.59317800	-1.50556500	-4.13694900
C	-0.14130000	-3.60071400	-2.18536400
H	-0.83353200	-4.43558300	-2.35151700
H	0.27017100	-3.30600400	-3.15270200
H	0.68808700	-3.96650400	-1.57488500
Cl	2.09186900	-0.45655600	-1.89349300

BC-TS5i $E = -1300.59182287$ $\Delta H = 0.379844$ $\Delta G = 0.269233$

Ir	-0.36019200	-0.56661700	0.15847200
C	-0.81394100	-2.68716000	0.35991600
C	-2.01615400	-1.92035100	0.61896200
C	-2.35748900	-1.21040600	-0.60165900
C	-1.35364400	-1.48704500	-1.57876200
C	-0.37462700	-2.39913900	-0.98110800
O	-0.72677200	1.28740300	1.14637100
C	0.03292900	0.70741800	2.04697200
H	0.77427500	-0.40552500	1.39252400
H	-0.47419800	0.12868000	2.83682100
C	1.25856600	1.40178200	2.55972500
C	1.81273400	0.98696200	3.77537600
C	1.82122600	2.47956700	1.87004700
C	2.92655600	1.63822100	4.29802900
H	1.36353400	0.15545500	4.31588900
C	2.93221800	3.13267500	2.39781200
H	1.38096700	2.78305500	0.92646000
C	3.48779800	2.71329800	3.60781300
H	3.35148300	1.31310500	5.24393700
H	3.36946400	3.97081900	1.86180700
H	4.35585900	3.22544300	4.01464700
C	-0.16880200	-3.65274200	1.30090700
H	-0.60303600	-4.65149500	1.16660900
H	0.90595700	-3.72733900	1.12104900
H	-0.31525000	-3.36507700	2.34482500
C	-2.85992200	-1.97834600	1.85181100
H	-3.66382100	-2.71651900	1.73523900
H	-2.27471100	-2.26701900	2.72836700
H	-3.32663300	-1.01284500	2.06452800
C	-3.55905400	-0.34359800	-0.78088800
H	-4.42817800	-0.95848400	-1.04776000
H	-3.80412700	0.19818400	0.13586600
H	-3.41116100	0.39268200	-1.57360200
C	-1.30992900	-0.99748000	-2.98743900
H	-1.66653700	-1.77781000	-3.67162000
H	-1.93588600	-0.11341700	-3.12668200
H	-0.29067700	-0.72960200	-3.27565800
C	0.76752200	-3.02966200	-1.70846800
H	0.42596600	-3.90369000	-2.27788000
H	1.22292800	-2.32543500	-2.40829600
H	1.54790200	-3.35966900	-1.01869800
Cl	1.32273000	0.61749300	-1.11758200

BC-IN7i $E = -955.15463750$ $\Delta H = 0.257389$ $\Delta G = 0.172173$

Ir	0.54076600	0.37501900	0.12670400
C	0.25339400	-1.61347100	-0.57366400
C	-0.11911700	-1.55096000	0.81626700
C	-1.19094300	-0.58196800	0.89802200
C	-1.61288700	-0.22087600	-0.46647500
C	-0.72735300	-0.83910600	-1.36029800
H	1.80015000	0.51997800	1.10686400
C	1.30542500	-2.49050200	-1.16708900
H	0.86928000	-3.44911900	-1.47806600
H	1.75873300	-2.02966000	-2.04878500
H	2.10257400	-2.69956200	-0.45035500
C	0.44476400	-2.36004400	1.93846000
H	-0.11659600	-3.29669900	2.05077000
H	1.49247600	-2.61433200	1.76224000
H	0.39218300	-1.82052600	2.88702900
C	-1.92202300	-0.18651400	2.13698500
H	-2.78239100	-0.85160200	2.29102300
H	-1.28175600	-0.25307500	3.01928700
H	-2.29942000	0.83686200	2.06803400
C	-2.75378200	0.68624400	-0.78622700
H	-3.70998300	0.16148900	-0.66587900
H	-2.77037200	1.55606100	-0.12311100
H	-2.69984600	1.05634900	-1.81239700
C	-0.70958600	-0.74015000	-2.84868300
H	-1.05773200	-1.67817200	-3.29901100
H	-1.35225300	0.06567000	-3.20852000
H	0.30161800	-0.55267600	-3.22225400
Cl	1.00315800	2.54744100	-0.60779900

PhCHO	$E = -345.44172585$	$\Delta H = 0.121536$	$\Delta G = 0.068246$
C	2.21227500	-0.25048400	-0.00000100
C	1.73207100	1.05902900	-0.00000100
C	0.35935800	1.29033400	0.00000000
C	-0.53330500	0.21245000	0.00000100
C	-0.04515000	-1.10131900	0.00000100
C	1.32438900	-1.33040800	0.00000000
H	3.28350400	-0.43295100	-0.00000200
H	2.42695300	1.89388300	-0.00000200
H	-0.02751600	2.30723100	0.00000000
H	-0.75651700	-1.92187400	0.00000200
H	1.70690000	-2.34712400	0.00000000
C	-1.98642100	0.47123700	0.00000300
H	-2.26464900	1.54818000	0.00000200
O	-2.84487500	-0.39061900	0.00000400

BC-TS9i	$E = -1511.65725556$	$\Delta H = 0.480953$	$\Delta G = 0.353248$
Ir	0.81556500	-0.69205500	-0.57001100
C	0.44931300	-2.76656100	0.02973400
C	-0.46362500	-1.93178000	0.75100800
C	-1.30130500	-1.23807700	-0.20783400
C	-0.94679000	-1.71294400	-1.52935700
C	0.14563100	-2.62430400	-1.39768100
Cl	3.16953400	-0.94143300	-1.08356600
H	1.47466900	0.27143300	0.60086200
C	0.81309900	-3.40339900	-2.48241000
H	0.44646200	-4.43767400	-2.48781500
H	0.62018400	-2.97416100	-3.46809700
H	1.89605300	-3.42831100	-2.33710000
C	1.44266200	-3.72387900	0.60111100
H	1.74059800	-3.43512900	1.61179400
H	1.01932800	-4.73546200	0.64892000
H	2.34735400	-3.76356200	-0.01034600
C	-1.63579000	-1.30993600	-2.79142700
H	-2.59555800	-1.83540500	-2.87766800
H	-1.83956500	-0.23620500	-2.81024600
H	-1.04258800	-1.55611200	-3.67439200
C	-2.47548600	-0.37492900	0.11673400
H	-3.37443200	-0.99238800	0.24512600
H	-2.32382700	0.18751500	1.04045400
H	-2.67745600	0.34209400	-0.68203600
C	-0.58384200	-1.83018400	2.23730900
H	-1.32591100	-2.55170300	2.60220600
H	0.36485600	-2.04779000	2.73346400
H	-0.90862000	-0.83481900	2.54915100
C	1.74611400	0.86197600	-3.73140300
C	2.48970700	1.29837600	-4.81998400
C	3.20517900	2.49730500	-4.76087400
C	3.15870300	3.25382000	-3.59222400
C	2.41328400	2.82457300	-2.49537600
C	1.70177600	1.61293800	-2.54501000
H	1.20790000	-0.07982500	-3.76911100
H	2.51853600	0.69288200	-5.72270700
H	3.78739100	2.83472800	-5.61371700
H	3.70020100	4.19479100	-3.52966300
H	2.35959200	3.44766600	-1.60650900
N	0.85517100	1.22486800	-1.49825800
C	-1.52799300	3.69723800	2.31498700
C	-0.38593700	3.10995300	2.86414300

C	0.48782300	2.39165600	2.05299100
C	0.22717300	2.24379600	0.68425700
C	-0.91191800	2.84271900	0.13797900
C	-1.78495100	3.56488800	0.95116600
H	-2.20802700	4.26205100	2.94706600
H	-0.17436300	3.21619400	3.92485600
H	1.37876000	1.93716100	2.48268300
H	-1.09303000	2.74038600	-0.92776400
H	-2.66503400	4.03072200	0.51522200
C	1.20114000	1.52013300	-0.19599700
H	2.24692300	1.81396000	-0.02543500

H ₂ O	$E = -76.42674396$	$\Delta H = 0.026338$	$\Delta G = -0.003276$
O	-1.07192000	-0.38565800	0.00000000
H	-0.10958600	-0.33567000	0.00000000
H	-1.34604700	0.53818000	0.00000000

BC-IN10i	$E = -1511.69060792$	$\Delta H = 0.486239$	$\Delta G = 0.354981$
Ir	0.62885300	-1.13650500	-0.22096000
C	0.07224900	-3.29751600	-0.22928400
C	-1.09533400	-2.48153000	-0.06305500
C	-1.22165800	-1.63215100	-1.24162500
C	-0.11462800	-1.90967900	-2.11721600
C	0.71098400	-2.91854100	-1.46183500
Cl	1.65622400	-1.28923500	1.96026100
H	2.56459200	0.78636300	1.17765900
C	1.94092500	-3.53494300	-2.04102000
H	1.67488300	-4.39642400	-2.66757200
H	2.48606600	-2.82300300	-2.66541500
H	2.61967500	-3.88425100	-1.25970800
C	0.55221700	-4.34253500	0.72266100
H	0.32770300	-4.07528100	1.75710000
H	0.06670300	-5.30202900	0.50407500
H	1.63218300	-4.48814200	0.64991700
C	0.07100700	-1.40505600	-3.50879300
H	-0.38706000	-2.10233000	-4.22263800
H	-0.39069200	-0.42608500	-3.65118900
H	1.12858600	-1.31375900	-3.76625200
C	-2.39065300	-0.75524100	-1.54179600
H	-3.19978300	-1.35873600	-1.97387600
H	-2.77959300	-0.27883500	-0.63838500
H	-2.13624300	0.02676800	-2.25917500
C	-2.07781200	-2.55569000	1.05903200
H	-2.89797700	-3.24060000	0.80678800

H	-1.61023500	-2.91740000	1.97731700
H	-2.51467400	-1.57656500	1.27272300
C	1.99180400	1.46183500	-2.69425900
C	1.74118900	2.16448600	-3.87109500
C	0.52110600	2.81642200	-4.05553700
C	-0.44283000	2.76330400	-3.04895100
C	-0.19481600	2.06091900	-1.86902300
C	1.02131500	1.39118500	-1.68355600
H	2.94045800	0.95135100	-2.54720700
H	2.50197500	2.20185000	-4.64700200
H	0.32655500	3.36680100	-4.97206800
H	-1.39013900	3.28207600	-3.17429100
H	-0.93313000	2.03686800	-1.07356400
N	1.29641800	0.68156900	-0.47711300
C	0.17001600	4.76067900	2.38277200
C	1.18076900	5.00862800	1.45652800
C	1.81901300	3.94470900	0.81706800
C	1.46008800	2.62230400	1.09351400
C	0.44165100	2.38395700	2.02628100
C	-0.19764500	3.44336100	2.66563300
H	-0.32778000	5.58706100	2.88364800
H	1.47385800	6.03042700	1.22837200
H	2.60648600	4.14360700	0.09317400
H	0.16251800	1.35775100	2.25216200
H	-0.97998700	3.24184500	3.39346800
C	2.16674500	1.46189200	0.42013200
H	3.01269600	1.85144600	-0.16326000
B-TS12i	$E = -2376.06190638$	$\Delta H = 0.520915$	$\Delta G = 0.369573$
Ir	2.03830300	-1.44777500	-4.78125600
C	3.00886700	-2.95838400	-3.51158700
C	1.68534900	-3.41028100	-3.93172700
C	1.69284500	-3.51087100	-5.37240400
C	2.97866200	-3.05222200	-5.85173100
C	3.79854300	-2.75384400	-4.67922300
H	1.38561300	1.04756900	-6.44718600
C	5.23242500	-2.34271900	-4.70333900
H	5.87148700	-3.23416700	-4.74734200
H	5.45657100	-1.72036200	-5.57149700
H	5.49812900	-1.77546100	-3.80888100
C	3.44232700	-2.73596600	-2.09653900
H	3.28421500	-1.68904600	-1.80760100
H	2.87373600	-3.37397100	-1.41409300
H	4.50272000	-2.97480100	-1.97278600

C	3.46029000	-3.07918700	-7.26544200
H	3.94585100	-4.03804700	-7.48971800
H	2.63486200	-2.94857700	-7.96946200
H	4.18526700	-2.28360900	-7.45281300
C	0.60093100	-4.07346500	-6.21556700
H	0.76962800	-5.14980500	-6.35156000
H	-0.37949100	-3.94107000	-5.75590900
H	0.57506900	-3.61285300	-7.20542000
C	0.61614100	-3.88450600	-3.00545500
H	0.82754000	-4.91429600	-2.68829300
H	0.56143900	-3.26347000	-2.10802500
H	-0.36478300	-3.87477800	-3.48251400
C	-1.65704600	-1.41360500	-6.67149800
C	-2.85473300	-2.12809000	-6.64172800
C	-3.39917500	-2.55791500	-5.43408200
C	-2.72691100	-2.25353500	-4.24827600
C	-1.53354900	-1.53879600	-4.27185200
C	-0.96710500	-1.10683400	-5.48635000
H	-1.26537900	-1.08990100	-7.62925600
H	-3.36651400	-2.34332200	-7.57684900
H	-4.33747600	-3.10525400	-5.41325900
H	-3.14312200	-2.56081800	-3.29165600
H	-1.03034500	-1.29015300	-3.34225400
N	0.24085900	-0.35690500	-5.45318600
C	-2.51875400	3.77755000	-6.71394100
C	-2.28637400	2.99066700	-7.83998100
C	-1.35996700	1.94883500	-7.78293100
C	-0.64578100	1.68294500	-6.61040200
C	-0.87828400	2.48652400	-5.48497600
C	-1.80968100	3.52157300	-5.53886300
H	-3.24532400	4.58542900	-6.75083700
H	-2.83178200	3.17980100	-8.76146200
H	-1.18587500	1.33609000	-8.66557600
H	-0.31183800	2.31385000	-4.57040100
H	-1.97995200	4.13506800	-4.65721200
C	0.40347600	0.58877800	-6.57004300
H	0.43461400	0.07010500	-7.53843100
Cl	3.48085500	0.44300900	-5.49720900
O	1.14258000	-0.12434200	-3.25663900
C	1.85287600	0.92857400	-2.68381600
O	1.42085000	2.08010500	-2.93416900
O	2.85651100	0.61590900	-2.00186600
K	3.94252500	2.64549500	-3.29096000
H	0.51695600	0.11103700	-4.17915900

PhCH ₂ NHPh	$E = -557.70952431$	$\Delta H = 0.247501$	$\Delta G = 0.172658$
H	-0.13644000	-0.87674400	0.89829200
H	0.30277800	-0.54272800	-1.67464100
C	-2.65901900	-0.63795000	1.12503400
C	-4.04129700	-0.56569900	1.02556500
C	-4.64832700	0.04702000	-0.07353300
C	-3.83869600	0.57906400	-1.07334700
C	-2.44887800	0.50720000	-0.99148900
C	-1.83321800	-0.09641600	0.11931600
H	-2.19821900	-1.11073600	1.98991700
H	-4.65228300	-0.99330100	1.81676100
H	-5.73018700	0.10298200	-0.14790100
H	-4.28939600	1.05366000	-1.94163500
H	-1.84736900	0.91996700	-1.79475000
N	-0.45732500	-0.14787800	0.27547700
C	4.57171900	-0.05488600	0.47017300
C	3.63347300	0.65514000	1.22015700
C	2.30420400	0.71009500	0.80874000
C	1.89169700	0.05247000	-0.35694800
C	2.83748700	-0.66136900	-1.09783800
C	4.17042000	-0.71246900	-0.69064300
H	5.60910600	-0.09629900	0.79086200
H	3.93897400	1.17062300	2.12686600
H	1.57299700	1.26279500	1.39297100
H	2.52707700	-1.18273300	-2.00055400
H	4.89319100	-1.27193900	-1.27854000
C	0.45420900	0.13281500	-0.81647800
H	0.25245300	1.14938200	-1.18119300
Ph-TS12i	$E = -1858.32663540$	$\Delta H = 0.630386$	$\Delta G = 0.472340$
Ir	0.94154000	-0.62141600	-0.92359400
C	0.42398500	-2.60530000	-1.70409600
C	-0.75679100	-1.74621600	-1.72606800
C	-0.47030100	-0.63459700	-2.59349800
C	0.89712100	-0.75863000	-3.05714900
C	1.41807600	-2.02128100	-2.54394800
Cl	3.31725000	-0.26342800	-0.52483500
H	2.44402700	1.84127900	0.16098600
C	2.74784600	-2.60390200	-2.88478000
H	2.66917500	-3.16129200	-3.82705400
H	3.50470300	-1.82767300	-3.00872200
H	3.10186700	-3.29181900	-2.11431300
C	0.52186000	-3.90652000	-0.97936800

H	-0.00884400	-3.87247500	-0.02487800
H	0.07381700	-4.70769700	-1.58113200
H	1.56023300	-4.17894300	-0.77862000
C	1.58204500	0.12109400	-4.05127600
H	1.43898900	-0.26112900	-5.07033000
H	1.18981800	1.14036700	-4.01739800
H	2.65600200	0.17272300	-3.85753800
C	-1.43769000	0.41136200	-3.02855400
H	-1.91473700	0.08663800	-3.96265100
H	-2.22314200	0.57935300	-2.29022500
H	-0.94515500	1.36626000	-3.22270400
C	-2.07875500	-2.09987900	-1.13088700
H	-2.61461600	-2.78580800	-1.80023600
H	-1.96474300	-2.60261300	-0.16698500
H	-2.70458000	-1.21871500	-0.98281300
C	-1.25507800	2.88813200	-0.57685200
C	-2.59335200	3.27677100	-0.64043300
C	-3.59532500	2.48484100	-0.08567500
C	-3.23544300	1.29208400	0.54608100
C	-1.90266000	0.89906800	0.61138800
C	-0.88078900	1.68410400	0.04426600
H	-0.50236400	3.53865300	-1.00756400
H	-2.84804300	4.21557800	-1.12639800
H	-4.63523900	2.79607700	-0.12924900
H	-3.99786700	0.66716900	1.00549200
H	-1.63144600	-0.02378200	1.11508600
N	0.46657300	1.24575600	0.15631500
C	1.29494700	5.39286800	3.12479400
C	1.68358100	5.70259100	1.82231100
C	1.70753500	4.70866000	0.84519900
C	1.35271300	3.38868200	1.14791100
C	0.96822100	3.08956500	2.45996100
C	0.93691600	4.08195100	3.43816800
H	1.26915100	6.16597700	3.88829000
H	1.96261300	6.72094200	1.56299400
H	2.00744400	4.96083900	-0.17048300
H	0.68381700	2.07395700	2.72029600
H	0.63202600	3.82761300	4.45022200
C	1.46531100	2.31910400	0.07747100
H	1.45777600	2.79707200	-0.91244800
O	0.70869600	-0.85621800	1.28625700
C	1.73538400	-1.31843400	2.14647100
H	2.57618100	-0.61403700	2.16029700
H	2.12759200	-2.25746100	1.73642500

C	1.24954800	-1.55627200	3.56090800
C	-0.07886200	-1.36167000	3.94372400
C	2.17080800	-1.98957300	4.52416200
C	-0.47971600	-1.59352000	5.26120300
H	-0.79824000	-1.02425400	3.20467000
C	1.77210100	-2.22445100	5.83670000
H	3.21102900	-2.14114100	4.24105900
C	0.44166100	-2.02600400	6.21162700
H	-1.51761800	-1.43332800	5.54306400
H	2.50085600	-2.55993400	6.57036400
H	0.12962100	-2.20589800	7.23706200
H	0.63054800	0.25938200	1.11951400
B-TS2i	$E = -2164.99867035$	$\Delta H = 0.419697$	$\Delta G = 0.284906$
Ir	-0.13035100	-0.72443000	0.44665800
C	-0.67497300	-2.70123900	1.08102600
C	-1.84625700	-2.02392900	0.57613300
C	-1.60941100	-1.65525900	-0.80403300
C	-0.28802200	-2.15300000	-1.16517400
C	0.28653800	-2.79334700	-0.01493000
Cl	1.89099800	-0.34725000	1.79103000
O	-1.04261000	1.08186600	1.19079600
C	-0.66622100	1.62250900	2.41900600
O	-0.05349800	2.71904600	2.36017800
O	-0.95424200	0.96022900	3.44245600
K	1.44392100	1.64210600	4.19934200
O	0.29474300	1.10906300	-0.67356200
C	1.57902000	1.69755700	-0.77206900
H	2.33112200	0.91096800	-0.90569400
H	1.82580900	2.21498600	0.16519400
C	1.66744400	2.67475700	-1.92407400
C	0.52810300	3.23746900	-2.50495900
C	2.92622200	3.05913900	-2.40278500
C	0.64474100	4.16381700	-3.54188500
H	-0.45020900	2.93937200	-2.14086100
C	3.04489300	3.98665800	-3.43524900
H	3.82210100	2.62441000	-1.96238600
C	1.90150100	4.54343800	-4.01010000
H	-0.25176500	4.59233800	-3.98354300
H	4.03052000	4.27161900	-3.79520000
H	1.99084200	5.26551400	-4.81756900
H	-0.37038600	1.48147200	0.23124800
C	1.60243000	-3.49446600	0.04292000
H	1.46635900	-4.56633800	-0.14925400

H	2.29809200	-3.10338800	-0.70318900
H	2.07100100	-3.38136600	1.02279100
C	0.34196600	-2.03462500	-2.51224400
H	0.08236500	-2.90831800	-3.12362800
H	-0.00237800	-1.14240300	-3.03881400
H	1.43079600	-1.98444400	-2.44095400
C	-2.58106900	-0.99443100	-1.72442600
H	-3.18386500	-1.74461000	-2.25204400
H	-3.26308400	-0.33939600	-1.17740900
H	-2.06902300	-0.38678100	-2.47418400
C	-3.09411200	-1.74520300	1.34241900
H	-3.81407500	-2.55664500	1.17586600
H	-2.89957600	-1.67455400	2.41364200
H	-3.55643600	-0.80892100	1.02490700
C	-0.52233400	-3.31446200	2.43367000
H	-0.88388400	-4.35096300	2.42663600
H	0.52336000	-3.32444100	2.74838900
H	-1.08964200	-2.76098900	3.18559100

S2.3 At the M06//PBE1PBE level of calculations

A	$E = -1818.37490216$	$\Delta H = 0.277093$	$\Delta G = 0.172122$
Ir	0.56092000	0.52812900	-0.10179900
C	-0.21710500	-1.11120900	-1.27208400
C	-1.16091700	0.00056300	-1.30468500
C	-0.49551700	1.12829200	-1.88455100
C	0.87248100	0.74552600	-2.19876000
C	1.01921400	-0.65291300	-1.83638700
Cl	-0.40634200	-0.06795000	2.10257400
O	2.41763200	0.61459000	0.88310800
C	2.18657900	1.79665400	1.38966000
O	1.07037200	2.32221400	0.88838300
O	2.84012400	2.35273300	2.27844700
K	0.43614500	2.57784400	3.44402200
C	1.88403500	1.58332500	-2.90444800
H	1.80472200	1.45627000	-3.99155400
H	1.74739400	2.64388400	-2.67910800
H	2.89989900	1.31098400	-2.60747000
C	2.26102300	-1.45746200	-2.01015900
H	2.31786400	-2.26649400	-1.27870300
H	2.28637700	-1.90073000	-3.01307400
H	3.15309100	-0.83849700	-1.89062900
C	-0.52778000	-2.49030300	-0.79857600
H	-1.19133600	-2.46748200	0.06906900

H	-1.02204700	-3.06695100	-1.59053200
H	0.37861100	-3.02565200	-0.50642800
C	-2.58210200	-0.07241800	-0.86101700
H	-2.98921600	0.92098100	-0.65855600
H	-3.20287500	-0.54081600	-1.63492000
H	-2.67595500	-0.66190700	0.05421300
C	-1.08903500	2.47126100	-2.14044800
H	-0.35152700	3.26556700	-2.00180600
H	-1.45714400	2.52976000	-3.17215700
H	-1.92863900	2.67264900	-1.47132500

PhNH₂ $E = -287.48329470$ $\Delta H = 0.128711$ $\Delta G = 0.078287$

C	-2.02909400	-1.90462600	-0.15760000
C	-0.64158800	-1.84576400	-0.11664500
C	0.01817800	-0.62629500	0.01890200
C	-0.73907400	0.53950800	0.11192300
C	-2.12712700	0.49336100	0.07088300
C	-2.79586900	-0.73292100	-0.06526900
H	-2.53228400	-2.86267400	-0.26709800
H	-0.07076300	-2.76793200	-0.19039800
H	1.10255700	-0.58529000	0.05169000
H	-0.24447800	1.50140900	0.22049100
H	-2.70618200	1.41139700	0.14171000
N	-4.17763200	-0.77985700	-0.16257400
H	-4.59808000	-1.66402200	0.08319200
H	-4.66626400	-0.00081600	0.25381800

PhCH₂OH $E = -346.64305551$ $\Delta H = 0.146525$ $\Delta G = 0.089568$

C	0.35108400	1.95615300	0.19232500
H	-0.08294800	2.32264000	1.13685000
H	1.43265200	2.16768700	0.24164900
O	-0.23600300	2.58705200	-0.92312400
H	0.03638000	3.50968600	-0.91261800
C	0.15450000	0.46570800	0.10464100
C	-0.18503000	-0.14876300	-1.10039400
C	0.34916000	-0.32700100	1.23870700
C	-0.32673300	-1.53306200	-1.16933000
H	-0.34469200	0.46871300	-1.97815800
C	0.21382000	-1.70934700	1.16895900
H	0.60673900	0.14365400	2.18561100
C	-0.12507300	-2.31811300	-0.03801900
H	-0.59559700	-1.99930300	-2.11353300
H	0.36731900	-2.31244600	2.05982300
H	-0.23580900	-3.39749600	-0.09338800

BN-TS2	$E = -2105.84452624$	$\Delta H = 0.403644$	$\Delta G = 0.276265$
Ir	-0.03690000	-1.02266500	-0.08128900
C	-0.48638700	-3.06177300	0.52078200
C	-1.70267600	-2.32280000	0.43779100
C	-1.84352500	-1.81963000	-0.92149700
C	-0.70771900	-2.30129300	-1.68261300
C	0.15177900	-3.03585900	-0.79200900
Cl	2.15017600	-0.89382800	1.05939200
C	1.27343100	1.24954300	-3.29778800
C	0.93367900	1.67565100	-4.57817100
C	-0.37086500	2.06723700	-4.87067200
C	-1.33052500	2.03730600	-3.85894300
C	-0.99604100	1.61815700	-2.57579700
C	0.31333000	1.21112100	-2.27651700
H	2.29386100	0.94414800	-3.07574100
H	1.69659800	1.70078000	-5.35223400
H	-0.63522500	2.40012600	-5.87009900
H	-2.34875100	2.35681700	-4.06673500
H	-1.74001700	1.61946200	-1.78401500
N	0.64488300	0.80148300	-0.97632700
H	-0.02884200	1.21369800	0.09408500
H	1.65161500	0.82693000	-0.83420300
O	-0.69747900	0.77774600	0.95606800
C	-0.28317800	0.99672200	2.26257500
O	0.42544600	2.00908900	2.45209900
O	-0.63683700	0.13960100	3.10846000
K	1.84406400	0.38113100	3.89931100
C	-3.03802000	-1.11311700	-1.46466900
H	-2.79418500	-0.55937600	-2.37365300
H	-3.82676800	-1.83506600	-1.71200000
H	-3.44667700	-0.40602000	-0.73857100
C	-0.49591900	-2.10302500	-3.14274800
H	-1.02350100	-2.88673600	-3.70070400
H	-0.87559600	-1.13525100	-3.47787000
H	0.56268100	-2.15785300	-3.40600200
C	1.39843700	-3.76657300	-1.15613300
H	1.17051500	-4.81344300	-1.39322000
H	1.88291700	-3.32056200	-2.02789100
H	2.11710700	-3.75327700	-0.33331800
C	0.03294800	-3.76967200	1.72459600
H	-0.18993600	-4.84220400	1.66022000
H	1.11593600	-3.65341700	1.81436800
H	-0.42686000	-3.38191800	2.63660000

C	-2.63229500	-2.05861500	1.57564200
H	-2.93374200	-2.99951700	2.04873300
H	-2.14232700	-1.41851500	2.32055000
H	-3.53550300	-1.54932100	1.23253900

C	$E = -1241.47327089$	$\Delta H = 0.368958$	$\Delta G = 0.261245$
Ir	0.14248500	-0.93676500	-0.54540500
C	-0.60049700	-2.50535100	0.82868100
C	-1.47297400	-1.36700500	0.82546800
C	-2.01407400	-1.20544300	-0.51828800
C	-1.42565700	-2.21905400	-1.34501100
C	-0.52126600	-3.00233200	-0.51204900
Cl	2.24359000	-0.65296700	0.56362400
C	1.17453600	2.30910600	-3.22555000
C	0.77072000	3.07545900	-4.30961400
C	-0.42355300	2.79405400	-4.97250300
C	-1.20488700	1.72779800	-4.53028300
C	-0.80765000	0.95644800	-3.44509000
C	0.38984000	1.23243100	-2.76689300
H	2.10742600	2.53625800	-2.71351200
H	1.39578400	3.90114200	-4.63979100
H	-0.73799900	3.39416000	-5.82112400
H	-2.13569500	1.49116900	-5.04017500
H	-1.41134400	0.12260700	-3.11013600
N	0.82190200	0.48904800	-1.68319700
H	1.73971500	0.79676600	-1.37102700
C	-1.85493900	-0.54150000	2.00566900
H	-2.08632500	0.48510900	1.71078200
H	-2.74470700	-0.96067400	2.49258600
H	-1.05141600	-0.50796400	2.74481600
C	0.12475800	-3.04952600	2.01155000
H	0.35042900	-2.26654400	2.73845100
H	-0.48860500	-3.81016900	2.50983000
H	1.07058300	-3.51262200	1.72312000
C	0.26023200	-4.18388200	-0.97407300
H	1.16377200	-4.32110300	-0.37578000
H	-0.34313700	-5.09689200	-0.89092500
H	0.56217800	-4.07452000	-2.01870200
C	-3.09216100	-0.24013100	-0.87684800
H	-4.03122400	-0.53692700	-0.39387900
H	-2.85021800	0.77259500	-0.54274600
H	-3.27075500	-0.20405100	-1.95284200
C	-1.75681200	-2.55358500	-2.76029000
H	-0.85802500	-2.63840500	-3.37715000

H	-2.27896200	-3.51746200	-2.79828500
H	-2.41174900	-1.80852500	-3.21601200
KHCO ₃	$E = -864.37787345$	$\Delta H = 0.037367$	$\Delta G = -0.011781$
C	-0.74650300	-0.12216900	0.00368500
O	-1.46496200	1.04242500	0.02209100
O	0.51037200	-0.00723900	-0.01227200
O	-1.41755000	-1.17721400	0.00355200
K	0.72075000	-2.54918300	-0.05904800
H	-0.79458000	1.73717900	0.01916700
C-TS2i	$E = -1588.10913960$	$\Delta H = 0.513372$	$\Delta G = 0.376328$
Ir	0.07543500	-0.97745200	-0.32578100
C	-1.02037400	-2.83395900	-0.02098600
C	-1.72738800	-1.76450600	0.60576300
C	-2.08115300	-0.78132200	-0.40658200
C	-1.59385300	-1.27527200	-1.67379200
C	-0.90229100	-2.51828100	-1.44120100
Cl	2.28472200	-1.97849800	-0.25388800
C	1.16750300	1.71263800	-3.31568100
C	0.65902000	2.65138000	-4.20827800
C	-0.36759800	3.51076500	-3.82355300
C	-0.87299400	3.42560100	-2.52634200
C	-0.36578200	2.49300300	-1.62816300
C	0.66113200	1.61677300	-2.01168100
H	1.96910100	1.04414900	-3.62290300
H	1.07018400	2.70959000	-5.21281800
H	-0.76258600	4.24363400	-4.52092900
H	-1.66279100	4.10055800	-2.20594700
H	-0.74861800	2.43948100	-0.61266400
N	1.17536600	0.68811800	-1.09511900
H	2.06293000	0.31050500	-1.41775800
O	0.70386200	0.47272800	1.21090200
C	1.61533400	0.15290600	2.23989900
H	2.52246900	-0.30913000	1.82993700
H	1.14672800	-0.60266200	2.88640500
C	1.98855000	1.35789700	3.07128200
C	3.06052400	1.26428300	3.96509800
C	1.28894700	2.56146400	2.98592800
C	3.42056500	2.34743900	4.75938100
H	3.61966400	0.33303900	4.03466200
C	1.65279300	3.65045600	3.77672300
H	0.46120500	2.64022600	2.28818100
C	2.71734000	3.54795700	4.66695000

H	4.25724000	2.25792700	5.44735000
H	1.10161600	4.58369000	3.69343700
H	3.00165700	4.39722400	5.28220100
H	1.14793400	0.89672500	0.22354200
C	-0.50770400	-4.07373700	0.62767900
H	-1.21028100	-4.90158100	0.47124900
H	0.46011800	-4.36413600	0.21229700
H	-0.37881800	-3.93877100	1.70413700
C	-2.06928600	-1.64556300	2.05097800
H	-3.11072400	-1.94648300	2.21846900
H	-1.43224300	-2.28098300	2.66967600
H	-1.95871000	-0.61465700	2.39550300
C	-2.96474000	0.39963400	-0.19097800
H	-4.01750100	0.08889800	-0.19040100
H	-2.76245700	0.88259000	0.76886700
H	-2.83845900	1.14452700	-0.97952300
C	-1.80645900	-0.62825600	-2.99781900
H	-2.76730000	-0.95452500	-3.41479900
H	-1.82409600	0.46097000	-2.91919200
H	-1.02236500	-0.90068200	-3.70726300
C	-0.29720700	-3.40879100	-2.47162500
H	-1.01496800	-4.17964700	-2.77877300
H	-0.00212400	-2.84673400	-3.36079700
H	0.59428100	-3.90650500	-2.08334300

BC-IN4i $E = -1300.61839939$ $\Delta H = 0.386486$ $\Delta G = 0.271848$

Ir	0.05501500	-0.65927900	-0.69065000
C	-1.10041200	-2.34252300	-0.08565200
C	-1.87163300	-1.14396800	0.15460200
C	-2.02665800	-0.48764000	-1.11843300
C	-1.41091800	-1.31496100	-2.15162100
C	-0.84707100	-2.46106800	-1.51429900
O	0.70281300	0.55184500	0.71737000
C	1.96958700	1.17226100	0.76686600
H	2.15055800	1.78997800	-0.12338800
H	2.77397200	0.42313900	0.79988700
C	2.02993300	2.03505500	2.00218200
C	2.28121100	1.46472500	3.25374600
C	1.80585800	3.41143500	1.92847200
C	2.30839000	2.24922100	4.40281400
H	2.46327300	0.39433200	3.32152200
C	1.83375800	4.20278400	3.07501700
H	1.61283000	3.86670100	0.95932700
C	2.08487300	3.62261000	4.31577800

H	2.51036800	1.79105300	5.36767900
H	1.66203600	5.27341500	2.99912000
H	2.11069000	4.23751800	5.21151600
C	-0.70234900	-3.34350200	0.94169300
H	-1.48487300	-4.10707400	1.03610700
H	0.22702000	-3.84800800	0.66772700
H	-0.56208100	-2.87925700	1.92015200
C	-2.40470500	-0.67681200	1.46457600
H	-3.41454600	-1.06993300	1.63284600
H	-1.77211600	-1.00534800	2.29227100
H	-2.45495400	0.41349900	1.50596300
C	-2.76210600	0.78356500	-1.36363200
H	-3.81310000	0.56480700	-1.59114100
H	-2.73347800	1.43882400	-0.49047600
H	-2.34196400	1.32927300	-2.21165900
C	-1.41235900	-1.01150200	-3.61067200
H	-2.34742300	-1.35381100	-4.07073000
H	-1.32087300	0.06216200	-3.79317300
H	-0.58284400	-1.50331600	-4.12247900
C	-0.13365100	-3.59190500	-2.17270600
H	-0.81924000	-4.43143300	-2.34011400
H	0.27957600	-3.29441400	-3.13839500
H	0.69587300	-3.95000100	-1.55793500
Cl	2.07275500	-0.46055400	-1.89380900

BC-TS5i $E = -1300.59246892$ $\Delta H = 0.381268$ $\Delta G = 0.270888$

Ir	-0.35981400	-0.57242300	0.16040300
C	-0.80674300	-2.68562000	0.36166300
C	-2.00564900	-1.91853200	0.62502500
C	-2.35065900	-1.20918200	-0.59288100
C	-1.35177500	-1.48485700	-1.57220800
C	-0.37225300	-2.39541300	-0.97805400
O	-0.73678800	1.28212300	1.12328900
C	0.00886100	0.70325400	2.03156400
H	0.76604300	-0.41952800	1.39371900
H	-0.50806100	0.13309100	2.82146800
C	1.23581700	1.38989500	2.54500500
C	1.77718200	0.98258700	3.76644600
C	1.81131600	2.45320700	1.84745000
C	2.89349700	1.62714100	4.28788500
H	1.31535800	0.16184600	4.31263500
C	2.92475000	3.09961700	2.37405400
H	1.37846400	2.74964000	0.89809300
C	3.46853400	2.68772700	3.59007200

H	3.30972500	1.30828100	5.23947800
H	3.37362500	3.92736600	1.83203500
H	4.33929300	3.19528100	3.99625700
C	-0.15617900	-3.64496500	1.30105900
H	-0.58952400	-4.64451600	1.17316500
H	0.91758400	-3.71721800	1.11500300
H	-0.29772300	-3.35183600	2.34405800
C	-2.84006100	-1.97039400	1.86132800
H	-3.64439900	-2.70893200	1.75404300
H	-2.24815600	-2.25428900	2.73495600
H	-3.30504800	-1.00337200	2.07095900
C	-3.54341300	-0.33204300	-0.75903100
H	-4.42510200	-0.93897000	-0.99964100
H	-3.76053900	0.22356800	0.15654500
H	-3.40161600	0.39268000	-1.56319400
C	-1.30154700	-0.98867800	-2.97572500
H	-1.62476300	-1.77522500	-3.66853600
H	-1.94985400	-0.12175700	-3.11996600
H	-0.28496800	-0.69090000	-3.24470800
C	0.77237600	-3.01275900	-1.70720600
H	0.43409200	-3.87579400	-2.29426400
H	1.23174800	-2.29466200	-2.39034800
H	1.54747400	-3.35471700	-1.01743500
Cl	1.32476600	0.59505100	-1.10977800

BC-IN7i $E = -955.15523745$ $\Delta H = 0.258324$ $\Delta G = 0.173261$

Ir	0.52605200	0.36367600	0.11992700
C	0.24731300	-1.61977600	-0.57308700
C	-0.12395900	-1.55580500	0.81472600
C	-1.19485800	-0.58920200	0.89654700
C	-1.61401400	-0.22579800	-0.46482700
C	-0.72879300	-0.84375500	-1.35797700
H	1.78830900	0.51210700	1.09602800
C	1.30077600	-2.49134900	-1.16525900
H	0.86724800	-3.44988500	-1.47877600
H	1.75350600	-2.02642000	-2.04500000
H	2.09682100	-2.69899200	-0.44699700
C	0.44667700	-2.35521900	1.93675800
H	-0.10911800	-3.29392900	2.05526100
H	1.49518600	-2.60346600	1.75728400
H	0.39422600	-1.81021800	2.88209300
C	-1.92134300	-0.19009800	2.13382500
H	-2.78066000	-0.85498000	2.29188000
H	-1.27797000	-0.25318400	3.01403900

H	-2.29868600	0.83293900	2.06072900
C	-2.74524600	0.68954300	-0.78321500
H	-3.70564600	0.17375700	-0.66118300
H	-2.75148100	1.55964600	-0.12032700
H	-2.68776100	1.05814300	-1.80964600
C	-0.70399100	-0.73696300	-2.84315200
H	-1.04926400	-1.67247900	-3.29993700
H	-1.34492100	0.07122800	-3.20054200
H	0.30946500	-0.54682200	-3.20907000
Cl	0.97061400	2.53340000	-0.61703000

PhCHO $E = -345.44198135$ $\Delta H = 0.122081$ $\Delta G = 0.068863$

C	2.20942300	-0.25020700	-0.00000100
C	1.73073800	1.05809100	-0.00000100
C	0.35958100	1.28971300	0.00000000
C	-0.53117400	0.21318500	0.00000100
C	-0.04544900	-1.09916600	0.00000100
C	1.32244500	-1.32876600	0.00000000
H	3.28040500	-0.43309500	-0.00000200
H	2.42611800	1.89226000	-0.00000200
H	-0.02782700	2.30632200	0.00000000
H	-0.75879100	-1.91803900	0.00000200
H	1.70474500	-2.34534400	0.00000000
C	-1.98310600	0.46995500	0.00000300
H	-2.26356600	1.54583800	0.00000200
O	-2.83652700	-0.39318600	0.00000400

BC-TS9i $E = -1511.65859301$ $\Delta H = 0.482904$ $\Delta G = 0.356224$

Ir	0.81779500	-0.68066700	-0.56871600
C	0.45186700	-2.74565000	0.02855600
C	-0.45226700	-1.90820100	0.75470800
C	-1.28862500	-1.20839200	-0.19814400
C	-0.94321200	-1.68289700	-1.52061000
C	0.14320800	-2.59962400	-1.39513000
Cl	3.15646100	-0.93781600	-1.09592600
H	1.48821300	0.27544600	0.59799600
C	0.81398900	-3.36676600	-2.48300500
H	0.47475500	-4.40983400	-2.47855400
H	0.59566700	-2.94638600	-3.46722900
H	1.89932600	-3.36023900	-2.35157200
C	1.44974500	-3.69999200	0.59014500
H	1.74837600	-3.41524100	1.60170000
H	1.03232500	-4.71383800	0.63184000
H	2.35254900	-3.72855500	-0.02491600

C	-1.62722900	-1.26422600	-2.77721000
H	-2.59688800	-1.77072500	-2.86123400
H	-1.80986700	-0.18659400	-2.79131700
H	-1.04099900	-1.51935000	-3.66234600
C	-2.44620600	-0.32944200	0.13169600
H	-3.35377700	-0.93247100	0.26451600
H	-2.27940900	0.23100100	1.05412300
H	-2.63920600	0.39093200	-0.66635700
C	-0.56007500	-1.79989300	2.23884600
H	-1.30911500	-2.50960500	2.61144800
H	0.38980200	-2.02855300	2.72752400
H	-0.86889200	-0.79832000	2.54769700
C	1.74515800	0.82835700	-3.72067700
C	2.49162000	1.24819700	-4.81163800
C	3.20622700	2.44635100	-4.76719500
C	3.15570400	3.21929200	-3.61160300
C	2.40675700	2.80677300	-2.51251500
C	1.69715700	1.59656000	-2.54794000
H	1.20678600	-0.11416800	-3.74483300
H	2.52396300	0.62971100	-5.70505100
H	3.79162700	2.77083800	-5.62252000
H	3.69708500	4.16072200	-3.56127100
H	2.34890400	3.44158900	-1.63211300
N	0.84892700	1.22292200	-1.50000200
C	-1.56803600	3.62992900	2.31509600
C	-0.43779400	3.02773400	2.86876400
C	0.45008000	2.33287500	2.05533700
C	0.21500000	2.22455700	0.68031400
C	-0.91191700	2.83725100	0.12954500
C	-1.79935700	3.53585100	0.94531500
H	-2.26007000	4.17642300	2.94982100
H	-0.24680800	3.10387100	3.93570100
H	1.33222100	1.86393800	2.48786000
H	-1.07379900	2.76060500	-0.94161700
H	-2.67173800	4.01290000	0.50665000
C	1.19763500	1.51832700	-0.20142000
H	2.24099100	1.82228300	-0.03332900

H ₂ O	$E = -76.42676530$	$\Delta H = 0.026479$	$\Delta G = -0.003129$
O	-1.07147800	-0.38503000	0.00000000
H	-0.11067900	-0.33536700	0.00000000
H	-1.34539600	0.53725000	0.00000000

BC-IN10i $E = -1511.69183989$ $\Delta H = 0.488137$ $\Delta G = 0.357185$

Ir	0.63934300	-1.13986600	-0.21890100
C	0.06676700	-3.28468100	-0.23689400
C	-1.09019200	-2.45821100	-0.06356400
C	-1.20932700	-1.60059500	-1.23442900
C	-0.10869300	-1.88395400	-2.11291400
C	0.70566300	-2.90496800	-1.46692400
Cl	1.65569500	-1.29913100	1.95734100
H	2.58107800	0.77799900	1.18202800
C	1.92966300	-3.52357100	-2.04953400
H	1.65707900	-4.37300900	-2.68890000
H	2.48247200	-2.80687100	-2.66154100
H	2.60179700	-3.88967100	-1.27035400
C	0.54149400	-4.33007500	0.71334600
H	0.34582400	-4.04480600	1.74896500
H	0.02982900	-5.27991600	0.51562200
H	1.61621100	-4.49995900	0.61872000
C	0.08557500	-1.36393200	-3.49496900
H	-0.37651700	-2.04814600	-4.21817300
H	-0.36610400	-0.37838500	-3.62540700
H	1.14512200	-1.27907700	-3.74654800
C	-2.35927400	-0.69900800	-1.52126300
H	-3.17722700	-1.27926200	-1.96729500
H	-2.74124100	-0.23345000	-0.60928700
H	-2.08526400	0.09196700	-2.22164300
C	-2.06285600	-2.52286800	1.06408000
H	-2.88793500	-3.20446200	0.82094100
H	-1.58809800	-2.88290400	1.97934200
H	-2.49207100	-1.54014700	1.27630900
C	1.99599100	1.42911500	-2.69582800
C	1.73552900	2.11863500	-3.87640500
C	0.51743600	2.77266500	-4.05422700
C	-0.43298900	2.73866700	-3.03613200
C	-0.17457800	2.04993400	-1.85233000
C	1.03754200	1.37433900	-1.67559500
H	2.94282700	0.91396400	-2.55279700
H	2.48693400	2.14325300	-4.66157100
H	0.31444200	3.31208400	-4.97514100
H	-1.37874800	3.26092600	-3.15666700
H	-0.90304900	2.03666400	-1.04728600
N	1.31701700	0.66835700	-0.47211100
C	0.12160300	4.71848600	2.35770000
C	1.11575300	4.98022700	1.41993200
C	1.77710200	3.92596600	0.79139200
C	1.45807000	2.60067600	1.09158100

C	0.45497300	2.34781900	2.03454800
C	-0.20676000	3.39747100	2.66334400
H	-0.39430600	5.53807400	2.85079900
H	1.37794700	6.00596200	1.17381900
H	2.55180900	4.13430100	0.05656900
H	0.20649300	1.31701000	2.27596000
H	-0.97692300	3.18590900	3.40088100
C	2.17921500	1.45004700	0.42342100
H	3.02269400	1.84780700	-0.15844800
B-TS12i	$E = -2376.06323916$	$\Delta H = 0.523074$	$\Delta G = 0.373398$
Ir	2.03303900	-1.44594300	-4.77526900
C	3.00293900	-2.94562800	-3.51074400
C	1.67411400	-3.39138200	-3.91324500
C	1.66299900	-3.49910300	-5.35073900
C	2.94552200	-3.05165100	-5.84664200
C	3.77955500	-2.75450000	-4.68692200
H	1.40387100	1.05437900	-6.43345300
C	5.21039100	-2.34408700	-4.73056800
H	5.84796100	-3.23583000	-4.77952300
H	5.42149900	-1.72429800	-5.60375100
H	5.48595100	-1.77324600	-3.84142400
C	3.44659600	-2.71157200	-2.10346500
H	3.27553900	-1.66528700	-1.81796700
H	2.89278400	-3.35570100	-1.41457200
H	4.51121400	-2.93488800	-1.98951000
C	3.40777100	-3.08074000	-7.26396900
H	3.88806300	-4.04024800	-7.49469200
H	2.57246100	-2.94794000	-7.95579500
H	4.13129600	-2.28573700	-7.45963100
C	0.55644800	-4.04719600	-6.18010500
H	0.72090800	-5.12154700	-6.33301500
H	-0.41592400	-3.91677900	-5.70254100
H	0.51535000	-3.57218700	-7.16273500
C	0.61411100	-3.84086800	-2.96853000
H	0.84471600	-4.85054500	-2.60509200
H	0.54969600	-3.17918600	-2.10106700
H	-0.36587100	-3.87034400	-3.44635100
C	-1.62719500	-1.40528900	-6.69595700
C	-2.81111300	-2.13986700	-6.68099300
C	-3.34998300	-2.59935800	-5.48377700
C	-2.68841400	-2.30101500	-4.29221800
C	-1.50896500	-1.56644100	-4.30089600
C	-0.94528100	-1.11052600	-5.50563800

H	-1.23884400	-1.05878600	-7.64709200
H	-3.31695200	-2.34812200	-7.62060300
H	-4.27791400	-3.16385900	-5.47497200
H	-3.10209500	-2.63018500	-3.34199900
H	-1.01129800	-1.32447200	-3.36623700
N	0.25614600	-0.35692600	-5.45752000
C	-2.50792200	3.76164500	-6.69096800
C	-2.27375900	2.98302400	-7.82026100
C	-1.34329600	1.94664200	-7.76992000
C	-0.62723100	1.67961700	-6.60125000
C	-0.86169600	2.47389800	-5.47169000
C	-1.79721300	3.50325600	-5.51925100
H	-3.23819800	4.56603700	-6.72265600
H	-2.82144300	3.17442100	-8.73958800
H	-1.16695700	1.33849700	-8.65522400
H	-0.29181400	2.29883000	-4.55907200
H	-1.96957400	4.11135200	-4.63457400
C	0.42450700	0.59215600	-6.56449600
H	0.46322500	0.07943500	-7.53598800
Cl	3.48093100	0.43005200	-5.47746500
O	1.12953900	-0.13304000	-3.25506700
C	1.84097800	0.91576300	-2.69129300
O	1.41997000	2.06649900	-2.95373600
O	2.83930400	0.60400700	-2.00447800
K	3.93628800	2.61593200	-3.28720200
H	0.51293900	0.10478700	-4.18309500

PhCH₂NHPh $E = -557.70986844$ $\Delta H = 0.248607$ $\Delta G = 0.174139$

H	-0.13436400	-0.86437500	0.91016100
H	0.29584900	-0.55189200	-1.66384100
C	-2.65475200	-0.62038000	1.13322000
C	-4.03518000	-0.55154000	1.02894800
C	-4.63897800	0.04506900	-0.07874600
C	-3.82813300	0.56394000	-1.08207400
C	-2.43996600	0.49499000	-0.99539000
C	-1.82830800	-0.09198000	0.12397200
H	-2.19496000	-1.08073400	2.00513100
H	-4.64791500	-0.96911200	1.82380600
H	-5.72043700	0.09872600	-0.15693300
H	-4.27694700	1.02624400	-1.95765100
H	-1.83605700	0.89725000	-1.80207300
N	-0.45503300	-0.13947200	0.28356500
C	4.56411500	-0.05423100	0.46556600
C	3.62389800	0.63754700	1.22696400

C	2.29528200	0.69103500	0.81857500
C	1.88632600	0.05033400	-0.35553100
C	2.83356200	-0.64585300	-1.10782400
C	4.16568900	-0.69525500	-0.70362100
H	5.60190400	-0.09480200	0.78433100
H	3.92764400	1.14008100	2.14124600
H	1.56042700	1.22961800	1.41129000
H	2.52387200	-1.15534800	-2.01741600
H	4.89086400	-1.24144700	-1.30058000
C	0.45057200	0.12974600	-0.81110500
H	0.25015300	1.14390700	-1.18334800

Ph-TS12i $E = -1858.32812852$ $\Delta H = 0.632788$ $\Delta G = 0.475067$

Ir	0.93951100	-0.62865200	-0.92323500
C	0.41413600	-2.59678500	-1.70699600
C	-0.76069700	-1.73326400	-1.72371700
C	-0.46894800	-0.61875800	-2.58277800
C	0.89498000	-0.74793100	-3.04865700
C	1.40899300	-2.01435300	-2.54400100
Cl	3.30716700	-0.27959700	-0.52885500
H	2.45072500	1.82723600	0.15630900
C	2.73711300	-2.59593500	-2.88155400
H	2.66253300	-3.14503200	-3.82852800
H	3.49533300	-1.81917600	-2.99327200
H	3.08413700	-3.29033200	-2.11370400
C	0.50882700	-3.89483500	-0.98136600
H	-0.01300900	-3.85300600	-0.02216600
H	0.04930500	-4.69396700	-1.57646400
H	1.54745000	-4.17295600	-0.78998200
C	1.58772100	0.13846300	-4.02741100
H	1.45090700	-0.23229700	-5.05109800
H	1.19729200	1.15813600	-3.98377200
H	2.66016700	0.18443400	-3.82367800
C	-1.42453200	0.44163600	-3.00057200
H	-1.90024300	0.13817600	-3.94204100
H	-2.21021400	0.60440900	-2.26092400
H	-0.92094600	1.39480100	-3.17440800
C	-2.07907400	-2.08062900	-1.12323400
H	-2.61817600	-2.76805100	-1.78778600
H	-1.96107400	-2.57977600	-0.15782600
H	-2.70120900	-1.19674900	-0.97584400
C	-1.24605100	2.86899200	-0.56153400
C	-2.58522900	3.24758800	-0.63140600
C	-3.58420200	2.44379400	-0.09264400

C	-3.22030900	1.25071600	0.53269000
C	-1.88668000	0.86757600	0.60447000
C	-0.86884500	1.66252300	0.04841700
H	-0.49457300	3.52884100	-0.98023900
H	-2.84346900	4.18871200	-1.11036300
H	-4.62587400	2.74726300	-0.14191400
H	-3.98117200	0.61644400	0.98133800
H	-1.61163900	-0.05857500	1.10088400
N	0.47689900	1.22820500	0.15521900
C	1.27003000	5.36078400	3.12198300
C	1.66694900	5.67545500	1.82496400
C	1.70229000	4.68549800	0.84654200
C	1.35061100	3.36550400	1.14335800
C	0.95665000	3.06099700	2.44940500
C	0.91462700	4.04933500	3.42887200
H	1.23548200	6.13154700	3.88712200
H	1.94377500	6.69544000	1.57086300
H	2.00799400	4.94049900	-0.16659900
H	0.67296700	2.04333100	2.70357100
H	0.60295000	3.79140900	4.43765300
C	1.46965500	2.30038100	0.07362600
H	1.45903900	2.77897800	-0.91635600
O	0.70961100	-0.87248400	1.27233700
C	1.73233800	-1.34148900	2.12565400
H	2.58685200	-0.65341800	2.12405800
H	2.10381000	-2.29345500	1.72533400
C	1.25224900	-1.54925800	3.54336600
C	-0.06748200	-1.31739800	3.92935500
C	2.16792200	-1.98892600	4.50616300
C	-0.46544500	-1.52046600	5.25075200
H	-0.78231100	-0.97265300	3.18885300
C	1.77191000	-2.19493900	5.82245900
H	3.20231100	-2.16852900	4.21858200
C	0.45006700	-1.96029400	6.20099300
H	-1.49722100	-1.33145200	5.53616700
H	2.49656900	-2.53631800	6.55707300
H	0.13997300	-2.11778200	7.23041600
H	0.63839800	0.24361600	1.11406000
B-TS2i	$E = -2165.00036033$	$\Delta H = 0.421042$	$\Delta G = 0.285947$
Ir	-0.14014800	-0.69676900	0.40266500
C	-0.62667200	-2.66647100	1.06025200
C	-1.82083400	-2.00919300	0.60006100
C	-1.63882900	-1.64299700	-0.79151700

C	-0.32615300	-2.12186600	-1.19474900
C	0.30093600	-2.74635400	-0.06304800
Cl	1.79078600	-0.28753900	1.85192300
O	-1.09071000	1.09590800	1.10023600
C	-0.90515800	1.50117900	2.41170500
O	-0.33264900	2.60199800	2.57348800
O	-1.30597900	0.70868000	3.29803300
K	0.96795700	1.30531000	4.41710500
O	0.33272800	1.12484800	-0.67546000
C	1.63303700	1.65345600	-0.80076900
H	2.34600300	0.83609600	-0.96653900
H	1.94069200	2.14671300	0.13203600
C	1.73176400	2.63664400	-1.94382200
C	0.59751600	3.19843500	-2.53036400
C	2.99244700	3.01987900	-2.41290700
C	0.72093100	4.12456200	-3.56479500
H	-0.38229100	2.89905000	-2.17137200
C	3.11752700	3.94538200	-3.44379400
H	3.88475500	2.58524600	-1.96553200
C	1.97909600	4.50240000	-4.02487200
H	-0.17235500	4.55389700	-4.01153000
H	4.10509500	4.23009900	-3.79771400
H	2.07387100	5.22424100	-4.83156500
H	-0.34964000	1.51585900	0.22957200
C	1.62658900	-3.42517400	-0.04083700
H	1.50281600	-4.50340100	-0.20140700
H	2.28550000	-3.04108400	-0.82298000
H	2.12860800	-3.27891400	0.91833800
C	0.25950500	-1.98397000	-2.55704000
H	-0.01433000	-2.85126100	-3.17048600
H	-0.10726100	-1.08666400	-3.05962800
H	1.34976500	-1.92733500	-2.51858000
C	-2.64207000	-0.98358000	-1.67446600
H	-3.25106000	-1.73172500	-2.19680100
H	-3.31339200	-0.34222900	-1.09914400
H	-2.15554600	-0.35879400	-2.42745400
C	-2.99849300	-1.69348000	1.45901000
H	-3.46492600	-2.61882300	1.81589100
H	-2.68652200	-1.08988400	2.31909900
H	-3.75003500	-1.12455300	0.90852800
C	-0.40798200	-3.23902100	2.41803200
H	-0.67411100	-4.30354600	2.43115100
H	0.63797200	-3.14645900	2.71978900
H	-1.02128700	-2.72565900	3.16193900

S2.4 At the M06//M06 level of calculations

A	$E = -1818.37514690$	$\Delta H = 0.274737$	$\Delta G = 0.170014$
Ir	0.55808400	0.51200800	-0.11895000
C	-0.23906200	-1.13028000	-1.29823000
C	-1.17248900	-0.01285000	-1.32115200
C	-0.49657700	1.10976400	-1.90525700
C	0.86265900	0.71539300	-2.22268900
C	0.99944900	-0.68443000	-1.86245100
Cl	-0.28042700	-0.20148800	2.13753200
O	2.46383600	0.76343500	0.79055400
C	2.14748900	1.91033900	1.32619200
O	0.96852300	2.34474300	0.88649800
O	2.78109100	2.50862600	2.20148200
K	0.44002400	2.54216800	3.46040600
C	1.90031700	1.55475500	-2.87952800
H	1.84976300	1.46936300	-3.97343700
H	1.77977100	2.61187300	-2.61928700
H	2.90641400	1.25597000	-2.56598600
C	2.24734100	-1.47768000	-2.01460700
H	2.24290700	-2.36270100	-1.37119000
H	2.36947900	-1.81275000	-3.05298300
H	3.12619000	-0.88169000	-1.74612500
C	-0.54629100	-2.49797000	-0.80107200
H	-1.21950700	-2.46712700	0.06124300
H	-1.02751000	-3.09802800	-1.58495900
H	0.36143800	-3.02090300	-0.48330400
C	-2.58705900	-0.06457000	-0.86359600
H	-2.95124200	0.92819200	-0.57894500
H	-3.24485100	-0.45221300	-1.65319700
H	-2.69478600	-0.71218400	0.01252300
C	-1.06363800	2.46735900	-2.11930800
H	-0.30482100	3.24368200	-1.97463800
H	-1.45388700	2.56533300	-3.14094400
H	-1.88368100	2.67430600	-1.42429700
PhNH ₂	$E = -287.48338242$	$\Delta H = 0.127432$	$\Delta G = 0.076834$
C	-2.02890900	-1.90267500	-0.15802300
C	-0.64274400	-1.84525500	-0.11625100
C	0.01666100	-0.62685500	0.01951100
C	-0.73893800	0.53869000	0.11087300
C	-2.12568600	0.49402300	0.06884100
C	-2.79216900	-0.73133200	-0.06632300

H	-2.53669000	-2.86042900	-0.26787300
H	-0.07106400	-2.76844900	-0.18911700
H	1.10221800	-0.58564700	0.05359800
H	-0.24322000	1.50145500	0.22010200
H	-2.70902600	1.41166100	0.13844500
N	-4.17536500	-0.77954900	-0.15849400
H	-4.59593200	-1.66811700	0.07706000
H	-4.66683700	-0.00204400	0.26067600
PhCH ₂ OH	$E = -346.64317421$	$\Delta H = 0.145231$	$\Delta G = 0.088733$
C	0.35437300	1.95024200	0.18988800
H	-0.06738700	2.31189600	1.14495000
H	1.43846100	2.16154500	0.23509800
O	-0.23973700	2.58769100	-0.91383500
H	0.01802800	3.51464800	-0.89613200
C	0.15491100	0.46493500	0.09770400
C	-0.18145500	-0.15124600	-1.10545400
C	0.34678900	-0.32340600	1.23330700
C	-0.32418400	-1.53443500	-1.16947700
H	-0.33864500	0.46429500	-1.98704600
C	0.21043300	-1.70430300	1.16873700
H	0.60261500	0.15500600	2.17918200
C	-0.12631800	-2.31534700	-0.03626600
H	-0.59094300	-2.00432500	-2.11393700
H	0.36137100	-2.30556600	2.06270000
H	-0.23854000	-3.39586900	-0.08942100
BN-TS2	$E = -2105.84519914$	$\Delta H = 0.399994$	$\Delta G = 0.275453$
Ir	-0.02028100	-1.01543200	-0.07270000
C	-0.48159800	-3.06605600	0.48465000
C	-1.69811400	-2.32674800	0.39706400
C	-1.82157800	-1.80584200	-0.95365500
C	-0.67929400	-2.27785700	-1.70765100
C	0.16880700	-3.02747500	-0.81911500
Cl	2.18020200	-0.87464200	1.11103000
C	1.22598600	1.15699500	-3.28896200
C	0.85105300	1.49822200	-4.58347800
C	-0.45031200	1.91283000	-4.85569100
C	-1.37048800	1.99508700	-3.81216400
C	-1.00037200	1.66174800	-2.51455100
C	0.30393300	1.23128000	-2.23803000
H	2.24206100	0.82341800	-3.07688000
H	1.58338600	1.43686200	-5.38626000
H	-0.74195800	2.17958800	-5.86874600

H	-2.38647100	2.33336800	-4.00779200
H	-1.71316700	1.74457600	-1.69466100
N	0.65758300	0.86697400	-0.92831900
H	-0.01680400	1.23814300	0.07938600
H	1.66471000	0.91385100	-0.78319600
O	-0.73643600	0.77316200	0.97220500
C	-0.31836600	0.94871100	2.27761900
O	0.37746400	1.96356800	2.50095200
O	-0.64782100	0.05608200	3.09795700
K	1.78614400	0.35611700	3.98525400
C	-2.98472700	-1.04481900	-1.48421600
H	-2.72779200	-0.50538000	-2.40245500
H	-3.82057200	-1.71978100	-1.71346400
H	-3.34200400	-0.30807000	-0.75575100
C	-0.43881700	-2.03009600	-3.15226300
H	-0.97949000	-2.76942400	-3.75795000
H	-0.78182600	-1.03362100	-3.45283000
H	0.62461800	-2.10312900	-3.40287000
C	1.42801600	-3.73205900	-1.17938800
H	1.22192600	-4.76557700	-1.48875500
H	1.94615500	-3.22951100	-2.00299100
H	2.12022600	-3.76546000	-0.33216300
C	0.01721900	-3.75683900	1.70302000
H	-0.37570600	-4.78137300	1.75657600
H	1.11012400	-3.81318100	1.71456800
H	-0.30026100	-3.22478100	2.60682300
C	-2.62640000	-2.06943600	1.53156200
H	-2.96530600	-3.01497800	1.97360700
H	-2.12048900	-1.47012200	2.30345700
H	-3.51005600	-1.51347400	1.20360000

C	$E = -1241.47361272$	$\Delta H = 0.365411$	$\Delta G = 0.258903$
Ir	0.13810500	-0.91832000	-0.50767300
C	-0.63548100	-2.52371900	0.82569800
C	-1.50806300	-1.38847200	0.83422200
C	-2.03642500	-1.20094300	-0.50946400
C	-1.44119200	-2.19565000	-1.34947200
C	-0.54117900	-2.98850400	-0.52399500
Cl	2.24200100	-0.66032300	0.64756700
C	1.19086300	2.28046800	-3.25813300
C	0.77386500	3.00227100	-4.36616600
C	-0.43538500	2.70670000	-4.99284700
C	-1.22043300	1.67274600	-4.48820200
C	-0.81026800	0.94567700	-3.37921400

C	0.40485500	1.23401900	-2.73975700
H	2.13747600	2.51615100	-2.77199000
H	1.40234200	3.80607400	-4.74478400
H	-0.75915700	3.27388700	-5.86201200
H	-2.16636100	1.42709600	-4.96804800
H	-1.42009900	0.13614100	-2.99020700
N	0.84254600	0.52286800	-1.63676400
H	1.76236200	0.83704900	-1.33008500
C	-1.87864800	-0.56572200	2.01605500
H	-2.14606000	0.45363200	1.71777100
H	-2.74118100	-0.99943400	2.54026400
H	-1.05052800	-0.49620300	2.72915200
C	0.09058400	-3.08864000	1.99416200
H	0.22254200	-2.34473600	2.78593200
H	-0.46632700	-3.93560900	2.41574100
H	1.08723900	-3.44439400	1.71421000
C	0.27418500	-4.13405200	-1.00659100
H	1.20417500	-4.22763700	-0.43588900
H	-0.27938000	-5.07816500	-0.90973700
H	0.54351100	-4.00898300	-2.06072200
C	-3.08283300	-0.20130000	-0.86032000
H	-4.00167800	-0.39888400	-0.29275100
H	-2.75939300	0.81956400	-0.62404300
H	-3.33914100	-0.22710000	-1.92352500
C	-1.72948500	-2.49153000	-2.78014300
H	-0.82087900	-2.45764100	-3.39306300
H	-2.15553100	-3.49911400	-2.87638000
H	-2.44822500	-1.78851500	-3.21140200
KHCO ₃	$E = -864.37800704$	$\Delta H = 0.037437$	$\Delta G = -0.011581$
C	-0.74827400	-0.12353800	0.00897500
O	-1.46425800	1.04461500	0.01727000
O	0.50588800	-0.00919600	-0.00041500
O	-1.42217900	-1.17362900	0.00948500
K	0.72953200	-2.55415200	-0.06948800
H	-0.79318100	1.73970000	0.01134600
C-TS2i	$E = -1588.11006436$	$\Delta H = 0.508407$	$\Delta G = 0.373858$
Ir	0.11975500	-0.99324000	-0.33902500
C	-1.01346300	-2.83326500	-0.06203500
C	-1.68946700	-1.76252800	0.59585000
C	-2.04120300	-0.75772000	-0.39339800
C	-1.58890600	-1.23756800	-1.67452700
C	-0.91363400	-2.49634100	-1.47613700

C1	2.33227500	-2.03818200	-0.18475700
C	1.06626600	1.59982500	-3.38072400
C	0.46992900	2.49217800	-4.26499500
C	-0.51353000	3.37348600	-3.82403800
C	-0.88749700	3.36009400	-2.48117900
C	-0.29207900	2.47460500	-1.59148500
C	0.69001000	1.57773400	-2.03338000
H	1.83020600	0.90395700	-3.72764600
H	0.77634000	2.49664300	-5.30912100
H	-0.97761700	4.07104400	-4.51711100
H	-1.64420500	4.05404500	-2.11948600
H	-0.57625400	2.46682100	-0.53902900
N	1.26474400	0.67271500	-1.12566800
H	2.14835300	0.29893500	-1.46765300
O	0.73650300	0.50742000	1.17494300
C	1.61892800	0.19078600	2.21838500
H	2.55837100	-0.23732200	1.82890000
H	1.17031300	-0.60186100	2.84427000
C	1.94531100	1.38027300	3.08414800
C	2.86688500	1.22170200	4.12363500
C	1.37108000	2.63284100	2.88146000
C	3.20701400	2.29126900	4.94107700
H	3.32515600	0.24453800	4.28282800
C	1.71274000	3.70801000	3.69946400
H	0.65569800	2.76223200	2.07285900
C	2.62959600	3.54236800	4.73088200
H	3.92958700	2.15184000	5.74283000
H	1.25833100	4.68195100	3.52687900
H	2.89783500	4.38292100	5.36736600
H	1.22665300	0.90055000	0.12162000
C	-0.48773500	-4.07148600	0.57183400
H	-1.22374200	-4.88340000	0.50379500
H	0.43608300	-4.40485200	0.08941700
H	-0.25731600	-3.90849600	1.63029400
C	-1.97505500	-1.64360600	2.04976300
H	-3.03110900	-1.86283500	2.25636100
H	-1.36562500	-2.33677100	2.63801500
H	-1.76859000	-0.62800300	2.40531200
C	-2.84352600	0.46503000	-0.12150200
H	-3.91339100	0.22239900	-0.06250600
H	-2.55605000	0.92289200	0.83217400
H	-2.71440400	1.21731400	-0.90704900
C	-1.78633700	-0.55325200	-2.97808600
H	-2.73058300	-0.88089300	-3.43268900

H	-1.82665600	0.53525200	-2.86360500
H	-0.97912800	-0.78370200	-3.68104700
C	-0.33000100	-3.36143700	-2.53578900
H	-1.07676200	-4.06802000	-2.92246500
H	0.03842500	-2.76538200	-3.37755200
H	0.51682900	-3.93886500	-2.15276400
BC-IN4i	$E = -1300.61872793$	$\Delta H = 0.382580$	$\Delta G = 0.268082$
Ir	0.03291900	-0.68634400	-0.66508600
C	-1.08956500	-2.43180400	-0.12310800
C	-1.88041100	-1.26120500	0.18333300
C	-2.07192100	-0.55379800	-1.05298600
C	-1.44638600	-1.31612900	-2.12924000
C	-0.85273000	-2.47995000	-1.55471200
O	0.65677300	0.54947300	0.75123200
C	1.91019400	1.18341300	0.79031800
H	2.10259600	1.77590900	-0.11950500
H	2.72279900	0.43629100	0.84093500
C	1.97673000	2.08441200	1.99421300
C	1.78853900	1.56479500	3.27809900
C	2.22886000	3.44806600	1.85512700
C	1.85300500	2.38989400	4.39414400
H	1.59004500	0.49968100	3.39306900
C	2.29851300	4.27910300	2.97094300
H	2.37157600	3.86229700	0.85717100
C	2.10932800	3.75196200	4.24335800
H	1.70739200	1.97059200	5.38803600
H	2.49690700	5.34163800	2.84421300
H	2.16111500	4.39800800	5.11730100
C	-0.62641700	-3.44379200	0.85966200
H	-1.38114700	-4.23300400	0.97792500
H	0.30611500	-3.91705700	0.53689200
H	-0.45164300	-2.99404400	1.84225500
C	-2.37259300	-0.85346000	1.52531300
H	-3.38040500	-1.24562800	1.71272400
H	-1.71448900	-1.22291800	2.31849700
H	-2.41005100	0.23619100	1.62270600
C	-2.81330000	0.72103500	-1.22825500
H	-3.86740900	0.51878500	-1.46145900
H	-2.77843000	1.33442900	-0.32267100
H	-2.39716500	1.31415300	-2.04898500
C	-1.44470400	-0.92345400	-3.56378800
H	-2.39331600	-1.19422400	-4.04552300
H	-1.30483500	0.15689800	-3.67937800

H	-0.63344400	-1.41248700	-4.11122100
C	-0.09460300	-3.54507200	-2.26493100
H	-0.72216000	-4.43032400	-2.42995400
H	0.26571100	-3.19895000	-3.23815700
H	0.78496300	-3.85679600	-1.69112000
Cl	2.07407700	-0.47468900	-1.87111900
BC-TS5i	$E = -1300.59304783$	$\Delta H = 0.377341$	$\Delta G = 0.267579$
Ir	-0.36373800	-0.59429300	0.15226400
C	-0.82432800	-2.71219500	0.34173500
C	-2.01841700	-1.94257100	0.59793800
C	-2.35938700	-1.23397700	-0.62111100
C	-1.36016400	-1.51086700	-1.59514500
C	-0.38204800	-2.41749700	-0.99575100
O	-0.77780500	1.24225800	1.19934500
C	-0.00044200	0.68187400	2.07803700
H	0.78215600	-0.44582200	1.40122600
H	-0.47188400	0.05605300	2.86347700
C	1.21943400	1.38320400	2.57162200
C	1.78653900	0.97383000	3.77887000
C	1.77371500	2.45152600	1.86599000
C	2.90521200	1.62489600	4.28304600
H	1.33782600	0.14330000	4.32533300
C	2.89049500	3.10330400	2.37442800
H	1.32507800	2.74645100	0.92080200
C	3.45748300	2.69193000	3.57883100
H	3.34247500	1.30525600	5.22632900
H	3.32600300	3.93587400	1.82656900
H	4.33249000	3.20564200	3.97137100
C	-0.16018100	-3.64064500	1.29706700
H	-0.57863800	-4.65147100	1.20578200
H	0.91605000	-3.70341300	1.10754300
H	-0.29389000	-3.31643400	2.33486700
C	-2.84369900	-1.94595500	1.83737800
H	-3.68336500	-2.64872100	1.75038000
H	-2.25864200	-2.23905400	2.71540500
H	-3.26450300	-0.95296300	2.03470900
C	-3.52296600	-0.31758000	-0.75395000
H	-4.46188800	-0.88598300	-0.78588400
H	-3.58002900	0.37017200	0.09774400
H	-3.46280200	0.28738400	-1.66299200
C	-1.28476100	-0.99612300	-2.98723200
H	-1.58809800	-1.77150800	-3.70310000
H	-1.93218600	-0.12593000	-3.13212500

H	-0.26325200	-0.68676300	-3.23358100
C	0.77084400	-3.02520900	-1.71389600
H	0.46399700	-3.93065200	-2.25489000
H	1.19246100	-2.32481400	-2.44175400
H	1.57494800	-3.29819600	-1.02266700
Cl	1.30578000	0.66144900	-1.10932900
BC-IN7i	$E = -955.15579323$	$\Delta H = 0.256003$	$\Delta G = 0.170588$
Ir	0.51627900	0.34821900	0.11624600
C	0.22129900	-1.65061900	-0.57199000
C	-0.14548600	-1.58384500	0.81434000
C	-1.21663200	-0.62013200	0.89363500
C	-1.63458600	-0.25462300	-0.46344000
C	-0.74963700	-0.87147600	-1.35549400
H	1.81680600	0.52057800	1.06966800
C	1.28126400	-2.50550100	-1.16736700
H	0.86195500	-3.46482300	-1.50191900
H	1.73866600	-2.02222300	-2.03785100
H	2.07731900	-2.71757900	-0.44694000
C	0.44680500	-2.35625200	1.93995200
H	-0.08678600	-3.30455900	2.08904800
H	1.50046300	-2.58740500	1.75336800
H	0.40134200	-1.79293900	2.87768800
C	-1.92705200	-0.19606500	2.12701000
H	-2.80382600	-0.83606100	2.29968300
H	-1.28110600	-0.26169800	3.00789400
H	-2.28028300	0.83758800	2.04612500
C	-2.73357900	0.69725600	-0.77291600
H	-3.71585200	0.23174700	-0.61657100
H	-2.68423900	1.58387900	-0.12920300
H	-2.68599300	1.04599000	-1.80914200
C	-0.68564700	-0.72632700	-2.83311300
H	-0.89541700	-1.68227500	-3.33082200
H	-1.40314200	0.01300700	-3.20068400
H	0.31285400	-0.40214400	-3.15224900
Cl	0.91269300	2.53438000	-0.66188500
PhCHO	$E = -345.44211679$	$\Delta H = 0.121004$	$\Delta G = 0.067875$
C	2.20617400	-0.24945500	-0.00000100
C	1.72803200	1.05754000	-0.00000100
C	0.35824900	1.28763800	0.00000000
C	-0.53015000	0.21136900	0.00000100
C	-0.04515500	-1.09954300	0.00000100
C	1.32140900	-1.32815600	0.00000000

H	3.27845600	-0.43151200	-0.00000200
H	2.42369300	1.89285900	-0.00000200
H	-0.03498300	2.30391000	0.00000000
H	-0.75935400	-1.91969700	0.00000200
H	1.70566300	-2.34513000	0.00000000
C	-1.97893600	0.46792000	0.00000300
H	-2.25124100	1.55064900	0.00000200
O	-2.83484000	-0.39083000	0.00000400

BC-TS9i $E = -1511.65907042$ $\Delta H = 0.477725$ $\Delta G = 0.351685$

Ir	0.85099800	-0.67499500	-0.56775400
C	0.44609200	-2.73781000	0.05193300
C	-0.43924500	-1.88022100	0.77698300
C	-1.26438800	-1.17512200	-0.17815200
C	-0.94460700	-1.67658900	-1.49641200
C	0.12381800	-2.60875500	-1.36893000
Cl	3.21420800	-0.93600700	-1.13424500
H	1.56973800	0.29446500	0.58350300
C	0.78740200	-3.38242400	-2.45332700
H	0.56759700	-4.45363300	-2.35508200
H	0.44831800	-3.06057600	-3.44297800
H	1.87621000	-3.25762400	-2.41928400
C	1.43690400	-3.69423900	0.61515600
H	1.80188600	-3.36413900	1.59338100
H	0.99390400	-4.69222100	0.73691800
H	2.30791900	-3.79095700	-0.04067300
C	-1.61390200	-1.22699400	-2.74648200
H	-2.63298700	-1.63317800	-2.80047800
H	-1.69233200	-0.13423400	-2.78429000
H	-1.07537000	-1.55638200	-3.64051000
C	-2.37038700	-0.22934600	0.12914200
H	-3.32843600	-0.76185800	0.20716200
H	-2.20561200	0.29870700	1.07457800
H	-2.47366100	0.52648400	-0.65724600
C	-0.50376500	-1.72664400	2.25649000
H	-1.24798000	-2.41284500	2.68189500
H	0.46113100	-1.94869800	2.72448700
H	-0.78843700	-0.70860600	2.54537100
C	1.75862800	0.80952500	-3.72556000
C	2.50283300	1.21649100	-4.82129700
C	3.19444000	2.42795600	-4.80056400
C	3.12287300	3.22841800	-3.66650700
C	2.37684000	2.82821200	-2.56205400
C	1.69467700	1.60442800	-2.57348300

H	1.23180700	-0.14401700	-3.72709000
H	2.54986500	0.57848100	-5.70172700
H	3.77897200	2.74238600	-5.66196500
H	3.64498700	4.18307500	-3.63862300
H	2.29265000	3.48470300	-1.69642100
N	0.85253400	1.23898900	-1.51603600
C	-1.64913100	3.48876100	2.31493600
C	-0.58863300	2.77948700	2.87803600
C	0.33141200	2.13796200	2.05852900
C	0.20041200	2.19358100	0.66760900
C	-0.85626200	2.91322500	0.10947800
C	-1.77776800	3.55624600	0.93171000
H	-2.36975200	3.99133900	2.95622000
H	-0.47990200	2.72727500	3.95910600
H	1.15736100	1.57565900	2.49724200
H	-0.94274400	2.95966000	-0.97459400
H	-2.59804500	4.11565800	0.48691900
C	1.20697900	1.54246800	-0.22411400
H	2.24458600	1.88226700	-0.06169500

H ₂ O	$E = -76.42677925$	$\Delta H = 0.026518$	$\Delta G = -0.003089$
O	-1.07091100	-0.38426300	0.00000000
H	-0.11042800	-0.33613700	0.00000000
H	-1.34621400	0.53725300	0.00000000

BC-IN10i	$E = -1511.69230486$	$\Delta H = 0.483412$	$\Delta G = 0.356440$
Ir	0.76860700	-1.14551000	-0.24273100
C	0.03624600	-3.25906800	-0.22966700
C	-1.04048200	-2.33671600	-0.02084300
C	-1.14780600	-1.48990600	-1.19963500
C	-0.10633900	-1.86300700	-2.11064500
C	0.64796800	-2.93908200	-1.48439800
Cl	1.91160400	-1.39355900	1.89278100
H	2.72744200	0.81606400	1.17738200
C	1.81783400	-3.61644600	-2.10206700
H	1.49042000	-4.37622500	-2.82512100
H	2.44976300	-2.89759700	-2.63551200
H	2.43962300	-4.11069900	-1.34937200
C	0.49029300	-4.30792400	0.72201800
H	0.36610800	-3.98700000	1.76073700
H	-0.07901900	-5.23514000	0.57715300
H	1.55161400	-4.53873500	0.58401700
C	0.10083100	-1.37254000	-3.49802300
H	-0.35228600	-2.07045600	-4.21571400

H	-0.34686000	-0.38704300	-3.66013800
H	1.16626500	-1.29718900	-3.74147500
C	-2.21732200	-0.48176500	-1.42230300
H	-3.13855900	-0.97523700	-1.76096600
H	-2.45284200	0.05745500	-0.49729900
H	-1.93014700	0.25546400	-2.17867500
C	-1.94801500	-2.27917200	1.15704800
H	-2.89667300	-2.79249700	0.94818800
H	-1.49565300	-2.75109100	2.03476000
H	-2.18224600	-1.24204200	1.42592100
C	2.04047700	1.34076700	-2.77149900
C	1.74082300	2.02547500	-3.94479300
C	0.55893200	2.75487600	-4.04644900
C	-0.31327200	2.80593800	-2.96177100
C	-0.01365700	2.12610200	-1.78438900
C	1.16099500	1.37208800	-1.68412600
H	2.95683700	0.75678600	-2.68066200
H	2.43180500	1.98604200	-4.78464700
H	0.32204200	3.28947400	-4.96371600
H	-1.23223200	3.38546100	-3.02779500
H	-0.68467600	2.17201500	-0.92686200
N	1.48678700	0.65764600	-0.49735000
C	-0.21833400	4.47554100	2.25329400
C	0.74481200	4.84778100	1.32228700
C	1.56751700	3.88156900	0.74740600
C	1.43936900	2.53773200	1.09507500
C	0.46865300	2.17255800	2.03368000
C	-0.35263400	3.13403800	2.60992500
H	-0.86355200	5.22722100	2.70333700
H	0.85421900	5.89235000	1.03746100
H	2.31437400	4.17002800	0.00717700
H	0.36580600	1.12149500	2.30691300
H	-1.09830200	2.83852600	3.34562100
C	2.27971400	1.47613500	0.43060100
H	3.09796600	1.95642200	-0.13057800
B-TS12i	$E = -2376.06431632$	$\Delta H = 0.518886$	$\Delta G = 0.371346$
Ir	2.07611300	-1.46451300	-4.82923300
C	2.93168000	-2.99403100	-3.51687700
C	1.61817500	-3.40735400	-3.98890900
C	1.68784400	-3.52081900	-5.42499700
C	3.00377400	-3.10334100	-5.84595500
C	3.78145200	-2.82395600	-4.64429500
H	1.39729700	1.17560600	-6.36784700

C	5.21517600	-2.43588900	-4.58165500
H	5.83576300	-3.32045600	-4.38275800
H	5.55808300	-1.98577600	-5.51721300
H	5.39498800	-1.71144300	-3.77955100
C	3.30947900	-2.73136700	-2.09961100
H	3.34963800	-1.64886300	-1.90633000
H	2.58317000	-3.16985700	-1.40809400
H	4.29217200	-3.16347500	-1.87587600
C	3.51357100	-3.09912300	-7.24339100
H	3.93818600	-4.07585800	-7.51280600
H	2.71070900	-2.87307700	-7.95414700
H	4.29113600	-2.34133500	-7.38050500
C	0.61725900	-4.01234300	-6.32765000
H	0.80320600	-5.06463800	-6.58225300
H	-0.37412200	-3.94347200	-5.87081900
H	0.59116800	-3.44319600	-7.26352100
C	0.48338900	-3.78760400	-3.10842500
H	0.62721100	-4.80195300	-2.71154100
H	0.40120800	-3.10311900	-2.25640100
H	-0.47027500	-3.76331200	-3.64387100
C	-1.50695600	-1.48504000	-6.66658800
C	-2.69223900	-2.21364700	-6.64565200
C	-3.30922800	-2.53048900	-5.43943100
C	-2.73067300	-2.09299200	-4.24959200
C	-1.54961800	-1.36187300	-4.26619700
C	-0.90723800	-1.05447300	-5.47530300
H	-1.04012800	-1.25019300	-7.62151500
H	-3.13673800	-2.53630100	-7.58557200
H	-4.23913700	-3.09438700	-5.42634700
H	-3.21087200	-2.30972500	-3.29679900
H	-1.11067500	-1.00606900	-3.33500800
N	0.30065500	-0.31086400	-5.43746500
C	-2.70369500	3.60582800	-6.55410800
C	-2.43812300	2.86708900	-7.70162000
C	-1.42850600	1.90744400	-7.69294900
C	-0.66888300	1.68006700	-6.54630100
C	-0.93522800	2.43418600	-5.39786800
C	-1.94812600	3.38572000	-5.40348900
H	-3.49572100	4.35213600	-6.55448300
H	-3.02198700	3.03160100	-8.60531200
H	-1.22610400	1.32293100	-8.59116700
H	-0.32135800	2.28379300	-4.50685700
H	-2.14631600	3.96636800	-4.50433200
C	0.44372500	0.66281100	-6.52785300

H	0.52968900	0.16951300	-7.51161400
Cl	3.59030800	0.34504100	-5.68037300
O	1.26823000	-0.08971300	-3.25752500
C	2.05773300	0.97191100	-2.84172200
O	1.66354700	2.11050700	-3.18231700
O	3.08991900	0.67665100	-2.20112300
K	4.18225900	2.61532200	-3.58852400
H	0.61369900	0.13732200	-4.15695700
PhCH ₂ NHPh	$E = -557.71010570$	$\Delta H = 0.245948$	$\Delta G = 0.171147$
H	-0.11788700	-0.83524300	0.91823500
H	0.28082100	-0.47012100	-1.67447300
C	-2.64561700	-0.64517400	1.12070600
C	-4.02503500	-0.60055700	1.00850500
C	-4.63146600	0.00517100	-0.09128500
C	-3.82493000	0.55814400	-1.07807300
C	-2.43743600	0.51365700	-0.98367200
C	-1.82533600	-0.08293700	0.12768000
H	-2.17807500	-1.11361700	1.98654900
H	-4.63619700	-1.04538100	1.79140600
H	-5.71439700	0.04032100	-0.17655100
H	-4.27785900	1.02936900	-1.94841200
H	-1.83319300	0.94404200	-1.77836600
N	-0.45068900	-0.11225300	0.29230100
C	4.55372400	-0.08437500	0.46627500
C	3.63937500	0.66385200	1.20381500
C	2.31420600	0.74563000	0.79513700
C	1.88361800	0.07901700	-0.35487100
C	2.80440500	-0.67164600	-1.08360500
C	4.13358200	-0.75138600	-0.67852400
H	5.59148200	-0.14711000	0.78552900
H	3.96185700	1.18891400	2.10025700
H	1.59524300	1.32850200	1.36882700
H	2.47383800	-1.20057600	-1.97671900
H	4.84044100	-1.34173200	-1.25725200
C	0.45145200	0.18471000	-0.80042000
H	0.25320300	1.21284800	-1.14235400
Ph-TS12i	$E = -1858.32971268$	$\Delta H = 0.627723$	$\Delta G = 0.479046$
Ir	0.95740000	-0.63552200	-0.97843500
C	0.43781900	-2.62711600	-1.69236600
C	-0.76129100	-1.79727900	-1.64212900
C	-0.57518700	-0.70342900	-2.54850700
C	0.76231100	-0.79578200	-3.09606500

C	1.34938900	-2.03599900	-2.61426700
Cl	3.35823000	-0.33973300	-0.60933100
H	2.52589500	1.73790500	0.35812800
C	2.67189300	-2.57323800	-3.02488800
H	2.57072300	-3.10702900	-3.97933700
H	3.40828600	-1.77510100	-3.15644000
H	3.07699800	-3.27278800	-2.28751300
C	0.64794400	-3.87681000	-0.91342900
H	0.11494100	-3.84544600	0.04312600
H	0.28126700	-4.75035400	-1.46914800
H	1.70934400	-4.03801800	-0.69609700
C	1.35097500	0.12910500	-4.10166800
H	1.01604200	-0.11835400	-5.11837600
H	1.05984400	1.16499200	-3.89064900
H	2.44461900	0.08826400	-4.08568100
C	-1.57585000	0.31998700	-2.93667800
H	-2.02965500	0.03022300	-3.89449300
H	-2.37772400	0.42382300	-2.20002000
H	-1.11784200	1.30529300	-3.07360400
C	-1.97625500	-2.12030100	-0.84709000
H	-2.52285100	-2.95771900	-1.30091700
H	-1.70829300	-2.41261300	0.17508500
H	-2.65732300	-1.26594100	-0.78322400
C	-1.03616500	2.90534900	-0.82460000
C	-2.33960500	3.36530700	-0.98778000
C	-3.41106300	2.68683300	-0.41690400
C	-3.15878100	1.53817300	0.33202100
C	-1.85923900	1.07842400	0.50147800
C	-0.77166400	1.74490300	-0.08385100
H	-0.21657500	3.45707300	-1.28068200
H	-2.51553900	4.27043800	-1.56628700
H	-4.42699800	3.05484600	-0.53919200
H	-3.98073600	1.00338800	0.80554800
H	-1.66405900	0.18838600	1.09908100
N	0.53332700	1.23225800	0.11832400
C	1.04704600	5.20129400	3.27937700
C	1.47889800	5.58649900	2.01482100
C	1.62772900	4.63510700	1.00968400
C	1.35834400	3.28777400	1.25124400
C	0.92197100	2.91276000	2.52462700
C	0.76775900	3.86008800	3.52985800
H	0.92439500	5.94285900	4.06590300
H	1.69406200	6.63260400	1.80559100
H	1.95813500	4.94019500	0.01607700

H	0.69054100	1.86646900	2.72893800
H	0.42745000	3.54849600	4.51532100
C	1.57983700	2.25786400	0.17163500
H	1.71656900	2.75869900	-0.80253500
O	0.69903600	-0.87762300	1.27597200
C	1.74202800	-1.26602400	2.13813400
H	2.54545700	-0.50953600	2.14967000
H	2.20412700	-2.18327700	1.73855500
C	1.26814800	-1.51576900	3.54647500
C	-0.04593600	-1.28299600	3.94677500
C	2.18805400	-1.98379800	4.48950400
C	-0.43353700	-1.51455700	5.26533300
H	-0.76653700	-0.91689500	3.21819300
C	1.80290200	-2.21625000	5.80309900
H	3.21896200	-2.16562400	4.18299100
C	0.48654600	-1.98124300	6.19661800
H	-1.46307800	-1.32613000	5.56401900
H	2.53091200	-2.58213500	6.52440800
H	0.18286100	-2.16185200	7.22556500
H	0.61237200	0.21780600	1.08898900

B-TS2i $E = -2165.00088985$ $\Delta H = 0.418609$ $\Delta G = 0.290039$

Ir	-0.14834500	-0.74250900	0.44130900
C	-0.64743500	-2.72770100	1.07274500
C	-1.83690500	-2.06278200	0.60636100
C	-1.63896400	-1.68180900	-0.77463100
C	-0.32507600	-2.15785300	-1.17088500
C	0.28976200	-2.79792100	-0.04141400
Cl	1.83011500	-0.30304400	1.86608800
O	-1.11095800	1.08306600	1.07732900
C	-0.80439000	1.56854900	2.33470100
O	-0.19062200	2.66102200	2.36402200
O	-1.14395800	0.85849500	3.30852600
K	1.13049900	1.55847500	4.31548800
O	0.31821800	1.09182100	-0.71790700
C	1.59820500	1.67160100	-0.80135900
H	2.35167700	0.87790700	-0.92951800
H	1.84875900	2.18268600	0.14323800
C	1.70200400	2.64585800	-1.94544100
C	0.57120600	3.18698600	-2.55487500
C	2.96431000	3.04873400	-2.38835000
C	0.70048900	4.11295000	-3.58680500
H	-0.41297500	2.87197500	-2.21642900
C	3.09515300	3.97488400	-3.41635500

H	3.85368800	2.62621900	-1.91887500
C	1.96026800	4.51171200	-4.02020000
H	-0.19157800	4.52738900	-4.05287100
H	4.08589000	4.27673900	-3.75076100
H	2.05973100	5.23605700	-4.82586200
H	-0.35926400	1.47817100	0.12588700
C	1.62579000	-3.44979000	-0.02231000
H	1.54219700	-4.51711800	-0.26649900
H	2.30326200	-2.98916500	-0.74918200
H	2.10005600	-3.36331600	0.95989700
C	0.29540100	-1.97289800	-2.50914200
H	0.14852900	-2.86931900	-3.12553900
H	-0.14277900	-1.12299000	-3.04089200
H	1.37312500	-1.79395900	-2.42766100
C	-2.61906000	-0.96323800	-1.63152300
H	-3.25686900	-1.66536000	-2.18446300
H	-3.26882000	-0.32153000	-1.02726600
H	-2.11498900	-0.32007500	-2.36041600
C	-3.04913300	-1.76938600	1.41241000
H	-3.84254800	-2.48896400	1.16980700
H	-2.84359000	-1.83224500	2.48421700
H	-3.42750000	-0.76256400	1.20956600
C	-0.44904400	-3.28729700	2.43749000
H	-0.98996800	-4.23613300	2.55149400
H	0.60797500	-3.47728700	2.64522000
H	-0.81407700	-2.59190400	3.20131800

S3. The energetic span model

The energetic span model offers a direct method to calculate the turnover frequency (TOF) of a catalytic cycle based on a theoretically obtained energy profile.¹ The TOF in s⁻¹ is given by eq 1:²

$$\text{TOF} = \frac{e^{-\Delta G_{\text{rx}}} - 1}{\sum_{i,j=1}^N e^{T_i - I_j - \delta G'_{i,j}}} \quad (1)$$

$$\delta G'_{i,j} = \begin{cases} \Delta G_{\text{rx}} & \text{if } i > j \\ 0 & \text{if } i \leq j \end{cases}$$

where I_j and T_i are the free energies of the j th intermediate and the i th transition state, respectively, and ΔG_{rx} is the reaction free energy. All these energies are dimensionless quantities expressed in $k_b T$ units, i.e.,

$$I_j = G(I_j)/k_b T, \quad T_i = G(T_i)/k_b T, \quad \Delta G_{\text{rx}} = [G(\text{Products}) - G(\text{Reactants})]/k_b T.$$

Eq 1 can be used to calculate the TOF only when both the transition state theory and the steady state regime are applicable to the studied catalytic system.

The degree of TOF control (X_i) specifies the sensitivity of the TOF to a change in the energy of a specific state of the cycle and can be expressed as follows:²

$$X_{T_i} = \frac{\sum_j e^{T_i - I_j - \delta G'_{ij}}}{\sum_{ij} e^{T_i - I_j - \delta G'_{ij}}} \quad (2)$$

$$X_{I_j} = \frac{\sum_i e^{T_i - I_j - \delta G'_{ij}}}{\sum_{ij} e^{T_i - I_j - \delta G'_{ij}}}$$

In a catalytic cycle, the intermediate with the highest X_i is called the TOF-determining intermediate (TDI) while the transition states with the highest X_T and the second highest X_T are called the TOF-determining transition state (TDTS) and the second TOF-determining transition state (STDTS), respectively.

On the basis of eqs (1) and (2), M. À. Carvajal' group designs a Fortran program (see **S4**),³ with which one can easily compute the TOF and identify the TDI, the TDTS and the STDTS.

References

1. S. Kozuch and S. Shaik, *Acc. Chem. Res.*, 2011, **44**, 101-110.
2. (a) C. Amatore and A. Jutand, *J. Organomet. Chem.*, 1999, **576**, 254-278; (b) S. Kozuch and S. Shaik, *J. Am. Chem. Soc.*, 2006, **128**, 3355-3365; (c) S. Kozuch and S. Shaik, *J. Phys. Chem. A*, 2008, **112**, 6032-6041.
3. M. À Carvajal, S. Kozuch and S. Shaik, *Organometallics*, 2009, **28**, 3656-3665.

S4. Fortran program for TOF and X_i calculations

```
! TOF PROGRAM
! Reads a .ene input file and delivers the TOF and the
! degree of TOF control of each intermediate and TS.
! The input file must be in the following syntax:
!
! TEMPERATURE
! FIRST INTERMEDIATE (space) FIRST TS
! SECOND INTERMEDIATE (space) SECOND TS
! ...
! N INTERMEDIATE (space) N TS
! FINAL INTERMEDIATE
!
! All the energies must be in kcal/mol, and temperature in Kelvin.
!
!
program TOF
```

```

implicit none
REAL,PARAMETER::kbh=20836643994,kbcal=0.001987207
REAL,allocatable::i(:),ts(:),xi(:),xts(:)
REAL::temp,ktemp,dummy,dg,delta,m=0.,tof,de,maxtsr,tsd
INTEGER::step=-1,a,b,maxts,maxi
CHARACTER::namefile*250
WRITE(*,*)'Name of the input file?'
READ(*,*)namefile
OPEN(1,FILE=TRIM(namefile)//'.ene')
OPEN(2,FILE=TRIM(namefile)//'.tof')
READ(1,*)dummy
do
    READ(1,*,END=10)dummy
    step=step+1
END do
10 ALLOCATE(i(0:step),ts(step),xi(step),xts(step))
xts=0.
xi=0.
REWIND(1)
READ(1,*)temp
ktemp=kbcal*temp
do a=0,step-1
    READ(1,*)i(a),ts(a+1)
    i(a)=i(a)/ktemp
    ts(a+1)=ts(a+1)/ktemp
end do
READ(1,*)i(step)
i(step)=i(step)/ktemp
dg=i(step)-i(0)
delta=EXP(-dg)-1
do a=1,step
    maxtsr=0.
    do b=1,step
        IF(a>b)then
            de=EXP(ts(a)-i(b)-dg)
        else
            de=EXP(ts(a)-i(b))
        END if
        xts(a)=xts(a)+de
        xi(b)=xi(b)+de
        m=m+de
    end do
end do
tof=kbh*temp*delta/m

```

```

xi=xi/m
xts=xts/m
WRITE(*,40)tof
WRITE(2,40)tof
40 FORMAT(/,' TOF=',e9.2,' 1/s',/)
WRITE(2,45)temp
45 FORMAT(' Temperature=',f7.2)
WRITE(2,*)"  Ei    Ets   Xi    Xts"
WRITE(2,50) i(0)*ktemp,ts(1)*ktemp,xi(step),xts(1)
do a=2,step
    WRITE(2,50) i(a-1)*ktemp,ts(a)*ktemp,xi(a-1),xts(a)
end do
WRITE(2,60)i(step)*ktemp
50 FORMAT(f6.2,f6.2,f6.2,f6.2)
60 FORMAT(F6.2)
end program

```

Input and Output examples:

File: test.ene

```

298.15
0 25.2
-6.3 20.8
5.1 18.5
-15.3

```

File: test.tof

TOF= 0.80E-07 1/s

Temperature= 298.15

Ei	Ets	Xi	Xts
0.00	25.20	0.04	0.04
-6.30	20.80	0.96	0.94
5.10	18.50	0.00	0.02
-15.30			