

Electronic Supplementary Information

Mechanism of Iridium-Catalysed Branched-Selective Hydroarylation of Vinyl Ethers: A Computational Study

Mei Zhang ^[a], Genping Huang^{[a,b]*}

^[a]Department of Chemistry, School of Science, Tianjin University, and ^[b]Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), Tianjin 300072, P.R. China.

E-mail: gphuang@tju.edu.cn

Web: <http://genpinghuang.weebly.com>

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2. Table of calculated energies and energy corrections

Stationary point	Single-point energy-B3LYP 6-311+G(2d,2p), lanl2tztz (a.u.)	Thermal correction to Gibbs free energy at 298.15 K (a.u.)	Solvation energy (toluene) (a.u.)	Optimization energy in gas phase 6-31G(d,p), lanl2dz (a.u.)	Dispersion correction (kcal/mol)
2a	-193.184555	0.058791	-193.121832	-193.119300	-6.1758
INT0	-1089.388873	0.389447	-1089.165555	-1089.107221	-86.4307
TS1	-896.171174	0.306560	-896.005460	-895.945662	-69.9675
INT1	-896.186433	0.308583	-896.026178	-895.965741	-69.3657
INT2	-896.183230	0.308077	-896.020897	-895.957799	-70.0642
TS3a	-1089.369154	0.390490	-1089.135807	-1089.079893	-90.6503
INT3a	-1089.377363	0.391025	-1089.143474	-1089.087899	-90.8670
TS2b	-1089.358228	0.389797	-1089.123643	-1089.068517	-92.2179
INT3b	-1089.373361	0.391555	-1089.138403	-1089.084312	-92.2475
TS3a	-1089.348427	0.392943	-1089.122663	-1089.065828	-87.8216
INT4a	-1089.375018	0.391734	-1089.154592	-1089.094073	-88.0946
INT5a	-1089.388320	0.391303	-1089.170643	-1089.111573	-85.1340
TS3b	-1089.348359	0.392697	-1089.121849	-1089.065394	-89.7652
INT4b	-1089.368617	0.391199	-1089.148556	-1089.087854	-90.6920
INT5b	-1089.392508	0.390376	-1089.173373	-1089.114449	-83.9508
TS4b	-1089.351456	0.391881	-1089.118567	-1089.065391	-92.3245
INT6b	-1089.377716	0.392253	-1089.155043	-1089.096426	-90.0980
TS4a	-1089.340633	0.392235	-1089.107291	-1089.053006	-91.8756
INT6a	-1089.379137	0.391881	-1089.156611	-1089.098237	-90.6762
TS5b	-1089.355214	0.389112	-1089.132852	-1089.073821	-88.1577
TS5a	-1089.351793	0.389009	-1089.129007	-1089.070285	-88.4013
3a	-672.685966	0.217276	-672.508866	-672.494628	-39.9333
4a	-672.686385	0.217711	-672.509130	-672.494380	-39.2153

3. Cartesian coordinates

INT0

Ir	3.04595200	2.30298200	8.89094700
C	1.71575100	0.68028300	9.51565500
H	2.17293000	-0.23443400	9.13991400
C	1.40753800	0.68638500	11.01195800
H	0.34226800	0.89184200	11.15485700
H	1.57352000	-0.31934800	11.40823000
C	2.26544600	1.69803600	11.80605200
H	1.72087900	2.04581600	12.69471300
H	3.15970000	1.19372800	12.18659400
C	2.71500800	2.88505400	10.97102600
H	3.61101600	3.38300500	11.34215100
C	1.85610100	3.66818200	10.16231300
H	2.17995700	4.68564000	9.95385700
C	0.35247200	3.43777100	10.05212900
H	-0.14768700	4.40231600	9.92520700
H	-0.01929600	3.02895900	10.99629500
C	-0.02224400	2.51230200	8.87529400
H	-0.16492400	3.11769600	7.97327300
H	-0.98650000	2.01939500	9.06304300
C	1.04141000	1.47623600	8.56877400
H	0.97754300	1.06760000	7.56069900
C	3.63352300	1.39013300	6.94175000
H	4.71375500	1.34848500	6.85092100
H	3.11953300	0.43498400	6.88302300
C	2.97891200	2.50162700	6.41190100
H	1.91233200	2.49150000	6.19384300
O	3.65639900	3.55110000	5.94484300
C	2.87119200	4.65255800	5.45479800
H	2.29557100	5.10603700	6.26815600
H	3.57955800	5.37508700	5.05220700
H	2.19650200	4.31872000	4.66034000
C	6.06459900	3.04421700	8.89708700
C	4.64672000	4.88227900	8.65960800
C	5.70877500	5.76640800	8.54762000
C	7.00632000	5.26063200	8.61525700
C	7.17561800	3.89337600	8.79224900
C	6.26818100	1.58493200	9.06882500
C	5.59838400	0.86166000	10.06994200
C	5.81322400	-0.51139300	10.21131200
C	6.69518700	-1.17576000	9.35844900
C	7.37621900	-0.46102400	8.36899700
C	7.17131800	0.91080600	8.22916600
H	3.62651400	5.23761300	8.60018100
H	5.51472000	6.82457800	8.41365700
H	7.86647200	5.91819600	8.54094600
H	8.16659100	3.46221500	8.87343400
H	4.96104300	1.38139800	10.77522500
H	5.30686400	-1.05644900	11.00205500
H	6.86262200	-2.24231300	9.47108800
H	8.06756600	-0.97174800	7.70610000
H	7.69396900	1.45808500	7.45000500
N	4.80019300	3.54920100	8.82894000

2a

C	-2.14850500	0.70701600	0.01773200
H	-1.79621400	-0.30558000	0.17135200
H	-3.21495800	0.84942500	-0.10694400
C	-1.34440500	1.77414800	-0.02528700
H	-1.72995700	2.77807500	-0.18174100
O	0.00594500	1.81906500	0.10616700
C	0.66655300	0.58086500	0.31915800
H	0.50089600	-0.10697700	-0.52008000
H	1.73047300	0.80835100	0.40055800
H	0.32143100	0.10091200	1.24404500

INT1

C	-3.09379400	1.90921200	-0.92339600
C	-0.83525300	1.43089000	-1.28042100
C	-0.71964300	2.47471800	-2.19020800
C	-1.83618000	3.27082700	-2.45109300
C	-3.03916700	2.98564800	-1.80772300
C	-4.31580500	1.47460300	-0.20470300
C	-4.60702600	0.08505700	-0.12778800
C	-5.76822000	-0.35078800	0.54047000
C	-6.61198200	0.57072500	1.14816800
C	-6.31732900	1.94106900	1.07658400
C	-5.18216900	2.39327000	0.40964600
H	0.01199400	0.80290200	-1.03361900
H	0.23085100	2.65813200	-2.67807600
H	-1.77307800	4.09547300	-3.15365300
H	-3.93275500	3.56827800	-2.00110500
H	-4.07748200	-0.61901500	-0.77901000
H	-6.00744300	-1.40948700	0.55823900
H	-7.50637100	0.23564400	1.66319800
H	-6.98003600	2.65913500	1.54961700
H	-4.95525600	3.45427600	0.37782200
N	-1.99515500	1.15404200	-0.65468300
Ir	-2.42792200	-0.17430900	0.93639000
C	-0.62382100	0.11354300	2.04271800
H	-0.17190400	1.05299300	1.72418100
C	-0.78645200	-0.03395600	3.55411400
H	-0.25515700	-0.92859800	3.89231100
H	-0.30158200	0.81151000	4.04982800
C	-2.27312100	-0.08519300	3.97203400
H	-2.39082500	-0.62048600	4.92433900
H	-2.63188600	0.93395100	4.14744300
C	-3.16405000	-0.70442100	2.91120100
H	-4.20181500	-0.37249100	2.94566300
C	-2.90472500	-1.90384700	2.21821800
H	-3.75872800	-2.39806300	1.75796900
C	-1.69716500	-2.79721500	2.47915800
H	-1.98755400	-3.84126900	2.33281500
H	-1.39757500	-2.71097800	3.52741500
C	-0.51653800	-2.45913900	1.54274100
H	-0.59912100	-3.04839800	0.62360400
H	0.43969200	-2.74390100	2.00358600
C	-0.48548100	-0.99615700	1.14397400
H	0.08747000	-0.81906500	0.23291900

TS1

C	-3.19919900	2.04038400	-0.85993500
C	-0.87016100	1.76792100	-0.81866900
C	-0.68675600	2.71058400	-1.81972100
C	-1.81275100	3.33230900	-2.36032500
C	-3.07085200	2.99370200	-1.87533400
C	-4.47340300	1.61539200	-0.26464300
C	-4.41709100	0.54308000	0.66522600
C	-5.61364100	0.08248500	1.23568700
C	-6.82907600	0.70589800	0.94760900
C	-6.86807200	1.78574600	0.06370700
C	-5.69532400	2.23854600	-0.54148700
H	-0.02104300	1.26559800	-0.37369300
H	0.31423700	2.94284600	-2.16400700
H	-1.71209900	4.07060200	-3.14929600
H	-3.95575200	3.46426300	-2.28523100
H	-3.52831200	-0.65207100	0.19712200
H	-5.60736200	-0.76550500	1.91288800
H	-7.74371200	0.34725600	1.40919500
H	-7.81148900	2.27236100	-0.16130000
H	-5.74639600	3.08591000	-1.21715300
N	-2.08806200	1.42947400	-0.34925500
Ir	-2.46559300	0.03554200	1.19500500
C	-0.36816400	-0.11973300	2.05499100
H	0.10209500	0.82689900	1.79061200

C	-0.41228200	-0.42097000	3.54975100
H	-0.01447500	-1.42036100	3.74073800
H	0.26047900	0.27196000	4.06309400
C	-1.83046800	-0.26847300	4.14589000
H	-1.91058400	-0.81515400	5.09618900
H	-2.00699600	0.78445000	4.39291300
C	-2.94349200	-0.71198300	3.21570900
H	-3.92014100	-0.30188900	3.46512400
C	-2.91687500	-1.83154700	2.37117200
H	-3.87763700	-2.18371700	2.00480700
C	-1.79673800	-2.86386200	2.30662000
H	-2.23869000	-3.84091400	2.09210800
H	-1.32869000	-2.95497600	3.28962500
C	-0.74098700	-2.55116500	1.22342800
H	-1.07663700	-2.94908400	0.26102400
H	0.20248300	-3.06665900	1.45456800
C	-0.47176000	-1.07529000	1.03918100
H	-0.08409100	-0.81673500	0.05595300
INT2			
C	-3.23677800	2.09524600	-0.84106500
C	-0.90681700	1.76534400	-0.85639500
C	-0.72084400	2.72199200	-1.84126400
C	-1.84439300	3.38560100	-2.34006000
C	-3.09992000	3.07083400	-1.83573500
C	-4.49840400	1.67100800	-0.22914600
C	-4.39913800	0.65150300	0.75432600
C	-5.58880800	0.18537000	1.32976900
C	-6.82782800	0.72921800	0.97680900
C	-6.90474800	1.74873600	0.02702500
C	-5.74063500	2.21767600	-0.57826800
H	-0.06540300	1.22799400	-0.43895300
H	0.27737600	2.93627400	-2.20434100
H	-1.74110000	4.14048300	-3.11297700
H	-3.97941600	3.57888100	-2.21096700
H	-2.80107500	-1.02217200	0.08783200
H	-5.57405900	-0.61443800	2.06392600
H	-7.73359900	0.35262100	1.44259600
H	-7.86575000	2.17181000	-0.24639700
H	-5.81403400	3.00601600	-1.32069900
N	-2.12513000	1.45245600	-0.36655000
Ir	-2.49603500	0.05226700	1.14717700
C	-0.29127700	-0.17368600	2.07470100
H	0.15929000	0.78345700	1.81525600
C	-0.41636900	-0.45702900	3.56440300
H	-0.07291700	-1.47157800	3.77720000
H	0.26404300	0.20974100	4.10207400
C	-1.84613200	-0.23867500	4.10774600
H	-1.95916500	-0.72368300	5.08804500
H	-2.00305800	0.83082100	4.29492700
C	-2.96056700	-0.71209800	3.19478700
H	-3.93216500	-0.28504200	3.43209800
C	-2.94914000	-1.83323200	2.36281600
H	-3.91463400	-2.16337800	1.98980200
C	-1.83640900	-2.87404900	2.29371300
H	-2.28915100	-3.84093400	2.05693300
H	-1.39267100	-2.98682800	3.28578100
C	-0.74373900	-2.57806200	1.23985400
H	-1.07101100	-2.95498300	0.26583200
H	0.16868100	-3.13875500	1.48658100
C	-0.40254200	-1.11358300	1.07162500
H	-0.01608900	-0.85602600	0.08806900
INT3a			
C	-3.65296000	2.88410600	2.07356200
C	-4.71496800	1.39294200	0.59420400
C	-5.86362200	2.16326500	0.54714200
C	-5.90092400	3.34557800	1.29267400
C	-4.79730500	3.69977900	2.05199100

C	-2.43737000	3.15335400	2.84043800
C	-1.39826000	2.19112300	2.75035300
C	-0.22025300	2.46740700	3.45475100
C	-0.07459600	3.62416000	4.22677800
C	-1.11272900	4.55370500	4.31334000
C	-2.29089100	4.31789900	3.61761900
H	-4.63176300	0.46696700	0.04111100
H	-6.70462200	1.84145700	-0.05608000
H	-6.78262800	3.97833600	1.28201100
H	-4.81420000	4.60904800	2.63911200
H	-2.52135700	-0.30995900	0.17375100
H	0.61973200	1.78213000	3.42071400
H	0.85485300	3.79875400	4.76154700
H	-1.00168400	5.45210400	4.91154500
H	-3.09153200	5.04800900	3.67905800
N	-3.63444700	1.73861900	1.33021400
Ir	-1.89530000	0.56273300	1.43004700
C	-0.00487000	-0.40739000	2.15250200
H	0.79408500	0.31223200	2.00208700
C	-0.12806600	-0.97902800	3.56583700
H	-0.01021400	-2.06596300	3.51276500
H	0.71558000	-0.61997600	4.16149900
C	-1.44389200	-0.60607200	4.28319400
H	-1.73127800	-1.39225500	4.99517600
H	-1.28816900	0.30033800	4.87129300
C	-2.60121900	-0.34580900	3.33840200
H	-3.37016800	0.31368500	3.73412600
C	-2.99101300	-1.21199500	2.29383900
H	-4.02231400	-1.13313600	1.96265300
C	-2.29984600	-2.54245700	2.00681900
H	-3.04311900	-3.24626300	1.62180500
H	-1.94985300	-2.96433000	2.95392400
C	-1.13712600	-2.43787000	0.99747500
H	-1.52466200	-2.60569500	-0.01140500
H	-0.39577500	-3.22881300	1.17983700
C	-0.43749000	-1.08982400	1.00500700
H	0.07572200	-0.84806700	0.07631500
C	-1.39746500	1.31952300	-1.08751800
C	-0.80919600	1.96266200	-0.00066200
H	0.23836800	1.74832600	0.18269700
H	-1.12476200	2.97927800	0.20613400
O	-2.43376600	1.83243300	-1.71698200
C	-3.03738500	1.02593200	-2.75094200
H	-3.51538400	0.14849800	-2.30471900
H	-3.78056900	1.65934300	-3.23165300
H	-2.28377300	0.71706900	-3.48074400
H	-0.96637700	0.41423400	-1.51272000
TS2a			
C	-3.60950300	2.95660400	2.10659700
C	-4.65395000	1.47491800	0.60483400
C	-5.80325700	2.24377500	0.55419300
C	-5.84807400	3.42118900	1.30766700
C	-4.75318600	3.77183500	2.08164700
C	-2.40475000	3.19944100	2.89272200
C	-1.37614600	2.22396900	2.80499600
C	-0.21256700	2.46291000	3.54469900
C	-0.06913200	3.60189600	4.34313700
C	-1.09186400	4.54806600	4.42351900
C	-2.25666700	4.34446800	3.69672600
H	-4.56536800	0.55230200	0.04613800
H	-6.63894600	1.92579500	-0.05816000
H	-6.73065500	4.05254600	1.29271000
H	-4.77710800	4.67569500	2.67701100
H	-2.27369700	0.00577000	-0.12261300
H	0.61770100	1.76817100	3.52129700
H	0.85040400	3.74812100	4.90268900
H	-0.97973700	5.43253800	5.04172400
H	-3.04945500	5.08336400	3.75363200

N	-3.58280100	1.81990000	1.35233900
Ir	-1.84624200	0.66398100	1.44858900
C	0.03280200	-0.36188400	2.23662300
H	0.82322300	0.37702400	2.16012500
C	-0.17783700	-0.98947800	3.61291300
H	-0.06049600	-2.07323500	3.51819100
H	0.63086300	-0.65986600	4.27107400
C	-1.53169300	-0.64355700	4.27326300
H	-1.83770600	-1.44892700	4.95530600
H	-1.41014800	0.25005400	4.88937800
C	-2.64972300	-0.36913400	3.28745300
H	-3.43770200	0.27639100	3.66876200
C	-2.96925500	-1.17289400	2.17888200
H	-3.98321100	-1.08713800	1.79715100
C	-2.24613500	-2.47984100	1.85718400
H	-2.96069600	-3.17590200	1.40858700
H	-1.92363400	-2.94632500	2.79278300
C	-1.04949500	-2.30732200	0.89951300
H	-1.40294200	-2.39065900	-0.13315800
H	-0.32023700	-3.11867900	1.03664500
C	-0.33417900	-0.97622600	1.03912000
H	0.22039000	-0.66502300	0.15524500
C	-1.56139900	1.06486400	-1.01792200
C	-0.90298600	1.90652200	-0.04472200
H	0.17966700	1.81821700	0.00157300
H	-1.26050900	2.93218500	-0.01209600
O	-2.57251000	1.58620100	-1.72914800
C	-3.17464400	0.71187900	-2.69577500
H	-3.66530400	-0.13229600	-2.19566500
H	-3.91324100	1.30755700	-3.23011500
H	-2.42324400	0.33757300	-3.39894200
H	-0.99084500	0.27579100	-1.51339900
INT3b			
C	-3.66481600	2.80902300	2.02343100
C	-4.72658400	1.35693500	0.50521100
C	-5.86362500	2.14608100	0.45643000
C	-5.89747000	3.31155500	1.22640900
C	-4.79777000	3.63823900	2.00557900
C	-2.44458600	3.06213500	2.79698900
C	-1.38922800	2.12477300	2.65089400
C	-0.20749600	2.39184400	3.35761500
C	-0.07383000	3.50989900	4.18718000
C	-1.13320100	4.40922600	4.33424400
C	-2.31511800	4.18529100	3.63610300
H	-4.64403300	0.44523400	-0.07173500
H	-6.69674100	1.85044800	-0.17058200
H	-6.77049700	3.95622400	1.21591200
H	-4.80959400	4.54020500	2.60422500
H	-2.60752800	-0.43621300	0.18845300
H	0.64020400	1.71730700	3.28099000
H	0.85650000	3.67619300	4.72344400
H	-1.03945200	5.27166300	4.98632700
H	-3.13398900	4.88791200	3.75421000
N	-3.65393100	1.67337800	1.26616600
Ir	-1.93119600	0.46596400	1.36436300
C	-0.04370800	-0.53345800	2.01637500
H	0.77646100	0.14310500	1.79162600
C	-0.09560000	-1.05536700	3.45563700
H	-0.00976600	-2.14652600	3.43001300
H	0.79266500	-0.70420500	3.98791700
C	-1.35417700	-0.62760600	4.24189600
H	-1.62603300	-1.39442600	4.98093300
H	-1.13630300	0.27968000	4.80843400
C	-2.55474800	-0.34398400	3.36232400
H	-3.27144300	0.35976300	3.77857800
C	-3.03113100	-1.21344800	2.35727800
H	-4.07402300	-1.09725600	2.07637300
C	-2.42247800	-2.58821100	2.08735700

H	-3.21842200	-3.26244000	1.75926000
H	-2.05445500	-2.99588000	3.03415500
C	-1.30111000	-2.57792700	1.02704800
H	-1.73349200	-2.78990300	0.04560000
H	-0.57493700	-3.37885000	1.22563500
C	-0.56588000	-1.25371300	0.92678900
H	-0.10828100	-1.07748400	-0.04313700
C	-1.26209300	1.43130900	-0.62027500
C	-0.52621900	2.47903000	-0.07759500
H	0.48405800	2.32204200	0.30318600
H	-0.67455500	0.63357100	-1.05875200
O	-0.99157700	3.69744200	-0.03965900
C	-0.20585800	4.74181700	0.58734400
H	0.84678900	4.45225400	0.63489200
H	-0.32526800	5.62497200	-0.03961100
H	-0.60010500	4.92239500	1.58728400
H	-2.16279800	1.69923000	-1.16379400
TS2b			
C	-3.58183100	2.94101700	2.12578500
C	-4.63205800	1.49087500	0.59729800
C	-5.76618000	2.28082700	0.53470300
C	-5.80264400	3.45015700	1.30086100
C	-4.71354500	3.77276800	2.09454100
C	-2.38401900	3.16573700	2.93136300
C	-1.34974300	2.19710300	2.83159200
C	-0.20065000	2.42351400	3.60023200
C	-0.07137300	3.54308500	4.42842300
C	-1.09945400	4.48348800	4.51425200
C	-2.25335900	4.29096800	3.76610200
H	-4.55285900	0.57397900	0.02638000
H	-6.59520800	1.98435200	-0.09715600
H	-6.67334000	4.09758400	1.27874500
H	-4.73178700	4.67176200	2.69726800
H	-2.38308300	-0.05554000	0.01910200
H	0.63229300	1.73094800	3.57315500
H	0.83848500	3.67931400	5.00619900
H	-1.00229700	5.35261900	5.15646000
H	-3.05208900	5.02228600	3.83571500
N	-3.56498000	1.81028400	1.36401800
Ir	-1.83451900	0.63742700	1.45421200
C	0.03237500	-0.39934500	2.26343000
H	0.83341300	0.32916300	2.19754100
C	-0.19590600	-1.02613300	3.63743100
H	-0.07590900	-2.10981100	3.54369200
H	0.60332900	-0.69592300	4.30657300
C	-1.55940200	-0.68085500	4.27515700
H	-1.88612800	-1.49136700	4.94110500
H	-1.44603000	0.20549600	4.90276700
C	-2.65295200	-0.38821100	3.26599400
H	-3.44838600	0.25284100	3.63983700
C	-2.97360800	-1.20738900	2.16274200
H	-3.98494400	-1.12232400	1.77552700
C	-2.24871100	-2.51441700	1.85167900
H	-2.95837400	-3.21103900	1.39649500
H	-1.93599500	-2.97710300	2.79273600
C	-1.04407500	-2.33896200	0.90644300
H	-1.39161900	-2.41162400	-0.12925700
H	-0.31835900	-3.15394200	1.04065200
C	-0.32710600	-1.01030800	1.06085300
H	0.24461200	-0.70658000	0.18567500
C	-1.54137400	1.03769500	-0.85902600
C	-0.83835800	2.01634200	-0.10754600
H	0.23445100	1.90732000	0.04437200
H	-0.98238000	0.24412800	-1.33930800
O	-1.30960700	3.29243400	-0.14987300
C	-0.39064600	4.30595800	0.28225100
H	0.51147300	4.29447900	-0.34082500
H	-0.90672400	5.25629300	0.14852000

H	-0.12348600	4.17500100	1.33389400
H	-2.42780100	1.37687500	-1.38781400
INT4a			
C	-3.19094900	3.07725500	1.25871500
C	-4.40321600	1.31502300	0.27645900
C	-5.51667400	2.11721800	0.08590100
C	-5.45822300	3.44858200	0.51218000
C	-4.29406900	3.92710900	1.09798700
C	-1.89438800	3.42260000	1.82699700
C	-0.92536900	2.38667100	1.85749800
C	0.34758000	2.67205200	2.35257100
C	0.65092600	3.95177200	2.83149100
C	-0.30719000	4.96720100	2.81723600
C	-1.57412200	4.70143500	2.31283200
H	-4.39224500	0.27498800	-0.03390400
H	-6.40364300	1.70728000	-0.38264300
H	-6.31312900	4.10439200	0.38337300
H	-4.23079000	4.95732100	1.42658600
H	0.85367800	2.44375200	-0.46902400
H	1.12393900	1.91871600	2.36655000
H	1.64800800	4.15048600	3.21341000
H	-0.06496400	5.95666800	3.18997200
H	-2.31780800	5.49203000	2.29338000
N	-3.27537400	1.77980400	0.85157900
Ir	-1.59387400	0.61179900	1.12761800
C	0.32150200	-0.49474600	1.93356300
H	1.15391900	0.08415800	1.54796500
C	0.27961200	-0.72287300	3.44019200
H	0.24069800	-1.79829500	3.63113400
H	1.23284700	-0.38399800	3.85698400
C	-0.85590000	0.00228700	4.20313700
H	-1.01070200	-0.48601600	5.17549000
H	-0.53906100	1.02414400	4.42851600
C	-2.17279300	0.08591800	3.47290700
H	-2.79339900	0.94100300	3.73318500
C	-2.73975700	-0.87930500	2.67660600
H	-3.77362400	-0.71822600	2.37384700
C	-2.18593100	-2.27462200	2.43547300
H	-3.02530200	-2.96895700	2.33348700
H	-1.62190100	-2.60935500	3.30815300
C	-1.31818600	-2.36788500	1.15999800
H	-1.97200500	-2.40323600	0.27733100
H	-0.77343100	-3.32321400	1.14011600
C	-0.31441700	-1.24931300	0.95923600
H	0.12246100	-1.18437100	-0.03431300
C	0.51134400	1.58599500	-1.06800900
C	-0.94128200	1.25854700	-0.75716700
H	-1.53190700	2.13707900	-1.04022500
H	-1.26776400	0.42875300	-1.41003100
O	1.35492100	0.46540700	-0.84047700
C	2.67820600	0.66796000	-1.31454200
H	3.15957800	1.52271600	-0.81716800
H	3.24535500	-0.23873800	-1.09460600
H	2.69147900	0.84379800	-2.39937700
H	0.58089500	1.88582900	-2.12795400
TS3a			
C	-3.15695200	3.04204100	1.22610200
C	-4.50770900	1.27203900	0.46911900
C	-5.59406700	2.11438900	0.28306000
C	-5.44974500	3.46866700	0.59716900
C	-4.22541900	3.93340200	1.06169400
C	-1.80648800	3.40080600	1.65909400
C	-0.77177400	2.45129900	1.41865900
C	0.53301400	2.77130500	1.81453500
C	0.80246200	3.96903600	2.47990900
C	-0.21876600	4.88563500	2.73995000
C	-1.51646300	4.59971400	2.32582200

H	-4.56377800	0.21242200	0.24841600
H	-6.52750500	1.71446700	-0.09550600
H	-6.28014700	4.15523300	0.46768000
H	-4.08427200	4.98515500	1.27970500
H	1.01779600	2.77411900	-0.77254100
H	1.34992500	2.10049700	1.58078400
H	1.82019300	4.18701900	2.78971800
H	-0.00524400	5.81470400	3.25759400
H	-2.31503600	5.30059900	2.54890000
N	-3.32558600	1.71972400	0.93909100
Ir	-1.64599700	0.49754900	1.23128800
C	0.24353000	-0.50525900	2.04147000
H	1.06785000	0.11802900	1.72144500
C	0.12886400	-0.76685300	3.53683000
H	0.08045000	-1.84439200	3.71453500
H	1.04729900	-0.42163600	4.02017500
C	-1.07635100	-0.05186700	4.18761800
H	-1.37379100	-0.56748100	5.11178500
H	-0.78157400	0.96006000	4.48173400
C	-2.27262800	0.06808100	3.26859000
H	-2.97669800	0.84704500	3.55930500
C	-2.77653300	-0.95593100	2.41882500
H	-3.82975900	-0.86460300	2.15628100
C	-2.22049700	-2.37723800	2.35173700
H	-3.04511000	-3.07136000	2.16577100
H	-1.80366000	-2.66384600	3.32102600
C	-1.17174300	-2.53028500	1.23192700
H	-1.68151800	-2.74043300	0.28554800
H	-0.51782800	-3.39448800	1.41874600
C	-0.31329900	-1.29593200	1.03393200
H	0.15162000	-1.19697900	0.05555700
C	0.58926300	1.79528100	-1.03381200
C	-0.81068900	1.66081100	-0.46488600
H	-1.44022200	2.46945500	-0.83472900
H	-1.26626500	0.71225700	-0.86454500
O	1.42271800	0.74637400	-0.58412400
C	2.69986700	0.75226700	-1.21439000
H	3.24082800	1.68776600	-1.01514500
H	3.26558200	-0.08446900	-0.80163200
H	2.60704900	0.62347800	-2.30146400
H	0.50136100	1.76692200	-2.13413600

INT4b

C	-3.52546100	2.98193600	1.31479700
C	-4.68282100	1.16653700	0.36202000
C	-5.86024100	1.89174700	0.27903200
C	-5.86230300	3.21202400	0.74310600
C	-4.69447700	3.75408100	1.26245700
C	-2.21973600	3.40194500	1.80689000
C	-1.18202300	2.43192800	1.75192000
C	0.09007000	2.79934600	2.19895300
C	0.33153200	4.08782600	2.68986700
C	-0.69127000	5.03600300	2.74663300
C	-1.96257500	4.68970800	2.30626300
H	-4.62327100	0.13824400	0.01940400
H	-6.74947100	1.43212200	-0.13614100
H	-6.76742000	3.80883100	0.69736600
H	-4.68027000	4.77490900	1.62429500
H	-2.78570700	2.55688300	-1.47048800
H	0.91621700	2.10115500	2.17193400
H	1.33138900	4.34625300	3.02623600
H	-0.49782100	6.03260600	3.12864600
H	-2.76042800	5.42453700	2.35049200
N	-3.54778800	1.69649900	0.86316900
Ir	-1.78632100	0.62968800	1.02126500
C	0.21402200	-0.33890300	1.76068800
H	0.98967600	0.28806100	1.33389900
C	0.26282400	-0.53472000	3.27319900
H	0.34092200	-1.60532100	3.48087400

H	1.19592800	-0.09569400	3.63866100
C	-0.90254700	0.08578900	4.08669200
H	-0.97137700	-0.42154000	5.05909700
H	-0.66558600	1.12885800	4.31019900
C	-2.25260200	0.05943500	3.41361600
H	-2.92006400	0.87697900	3.67788800
C	-2.77472500	-0.95965800	2.66099500
H	-3.82489300	-0.88088800	2.38313500
C	-2.11850000	-2.30939000	2.42635800
H	-2.89973200	-3.07395500	2.37675200
H	-1.49465900	-2.57286600	3.28279100
C	-1.29790100	-2.36679700	1.12057400
H	-1.98012800	-2.48623100	0.26787000
H	-0.66999400	-3.27002700	1.10481600
C	-0.40601500	-1.17302600	0.84188500
H	-0.03458300	-1.10792300	-0.17709800
C	-1.70109000	2.46230100	-1.55015300
C	-1.23027200	1.14320500	-0.94759600
H	-1.44614600	2.49285500	-2.61582900
O	0.09817100	0.81327300	-1.28051100
C	1.07052300	1.85505500	-1.29766300
H	1.10228100	2.39765200	-0.34524600
H	2.03144500	1.36674000	-1.46985000
H	0.89262800	2.57057600	-2.10772600
H	-1.25048500	3.33193100	-1.06623000
H	-1.83092500	0.32018000	-1.39863100
TS3b			
C	-3.50276900	2.93700700	1.29457300
C	-4.79642700	1.08144700	0.65408800
C	-5.94387500	1.85392800	0.54501500
C	-5.86061800	3.21638900	0.84265400
C	-4.63456500	3.75850800	1.20982800
C	-2.14517000	3.39319300	1.60562400
C	-1.06882900	2.50753100	1.31184600
C	0.23077800	2.92083200	1.62066600
C	0.47124700	4.15229300	2.23535200
C	-0.58877400	5.01018100	2.53512700
C	-1.89039700	4.62751400	2.22102600
H	-4.80322500	0.01959600	0.44060400
H	-6.87594200	1.39392300	0.23803500
H	-6.73882800	3.85030100	0.77430500
H	-4.54356900	4.81916300	1.41025800
H	-2.65497000	2.77926300	-1.20564200
H	1.07153300	2.28516200	1.36882100
H	1.48985400	4.44185900	2.47616100
H	-0.40417300	5.96630800	3.01333400
H	-2.71509700	5.28010600	2.49063400
N	-3.61119200	1.60296300	1.03159100
Ir	-1.85169400	0.47375300	1.24209600
C	0.10825600	-0.39244400	1.97589400
H	0.87829800	0.29968500	1.65826300
C	0.05754800	-0.69554400	3.46802100
H	0.09612000	-1.77728400	3.62077500
H	0.95961700	-0.29162100	3.93649400
C	-1.18405100	-0.08843300	4.15725700
H	-1.42798200	-0.64601300	5.07264500
H	-0.95680200	0.93513300	4.47102300
C	-2.39907900	-0.02885800	3.25364600
H	-3.15712500	0.67880200	3.58970900
C	-2.85222800	-1.07975000	2.39482700
H	-3.91878800	-1.07125000	2.17467000
C	-2.19824300	-2.45864000	2.30367200
H	-2.97241300	-3.20879900	2.11786900
H	-1.75007400	-2.72622400	3.26490900
C	-1.15505100	-2.52012300	1.17091100
H	-1.65894600	-2.76459600	0.23001400
H	-0.42640400	-3.32565300	1.34302700
C	-0.41434600	-1.21235000	0.96939400

H	0.01109400	-1.07111600	-0.02272200
C	-1.58888900	2.67805600	-1.40737000
C	-0.98896800	1.57617200	-0.55179000
H	-1.47960500	2.40840700	-2.46433600
O	0.33005200	1.25574900	-0.76052200
C	1.19308300	2.17052000	-1.45606400
H	1.24676900	3.13833600	-0.94920600
H	2.17607400	1.69939200	-1.44625400
H	0.87235200	2.31022300	-2.49221300
H	-1.11272000	3.64628300	-1.24442800
H	-1.59384600	0.63247900	-0.75953600

INT5a

C	-2.98059100	3.06594200	1.08647200
C	-4.62691000	1.42162600	0.84513500
C	-5.57394000	2.37444900	0.48484300
C	-5.19892200	3.71815000	0.44414000
C	-3.88348000	4.07121300	0.75077300
C	-1.54762000	3.26986900	1.45251600
C	-0.50364900	2.68214400	0.67033900
C	0.82497800	2.89038700	1.10713100
C	1.11261800	3.65813500	2.22925300
C	0.08133300	4.25953300	2.96145500
C	-1.23779300	4.05898800	2.57863300
H	-4.87255700	0.36752700	0.90552700
H	-6.58473000	2.06412900	0.24559000
H	-5.92037400	4.48176700	0.17151800
H	-3.55315300	5.10366300	0.72188900
H	0.95389400	2.87084200	-1.72424700
H	1.63035300	2.43973100	0.53985900
H	2.14628900	3.80465300	2.52704500
H	0.30806200	4.87205700	3.82814500
H	-2.04796800	4.50270400	3.14937800
N	-3.36070300	1.76453700	1.14210400
Ir	-1.71236300	0.64317800	1.83863500
C	-0.04998800	0.00110200	3.12090000
H	0.54110900	0.90005600	3.29006300
C	-0.52883800	-0.72121300	4.37660100
H	-0.26503600	-1.78054600	4.31458000
H	0.00956400	-0.32580100	5.24262200
C	-2.04831700	-0.54810400	4.59792300
H	-2.45583600	-1.38525600	5.18241300
H	-2.23114100	0.35526000	5.18909200
C	-2.81609300	-0.40152400	3.29851700
H	-3.79092000	0.07331800	3.42270900
C	-2.65205900	-1.23298800	2.13333400
H	-3.52036000	-1.32211600	1.47985000
C	-1.70414000	-2.43280900	2.07486400
H	-2.14000200	-3.20150600	1.43055500
H	-1.62330700	-2.88346400	3.06866000
C	-0.31183400	-2.04145400	1.53069600
H	-0.31206500	-2.13555700	0.44021900
H	0.45773300	-2.73429100	1.89842400
C	0.07158500	-0.61088400	1.85816000
H	0.75418600	-0.15222000	1.14317800
C	0.40770500	1.91699800	-1.63706000
C	-0.79247400	2.06141100	-0.70486700
H	-1.54565600	2.67822400	-1.20921100
H	-1.24134100	1.05933500	-0.61921900
O	1.25615100	0.89478000	-1.14353400
C	2.34829600	0.61428900	-2.01153500
H	2.99227200	1.49461700	-2.14713200
H	2.92879500	-0.18578200	-1.54929900
H	1.99656600	0.28053800	-2.99763200
H	0.04222900	1.65495600	-2.64178700

INT5b

C	-3.25625900	2.74070700	0.98213100
C	-4.99261900	1.34242900	1.69520500

C	-5.91279600	2.02486100	0.90763500
C	-5.47169000	3.09444400	0.12738800
C	-4.12486300	3.45799000	0.16324200
C	-1.80612500	3.02593900	1.20509000
C	-0.83646000	3.07481300	0.17630600
C	0.48189400	3.38452400	0.52471300
C	0.86139200	3.65102600	1.84588400
C	-0.08230000	3.59204800	2.86344900
C	-1.41280700	3.25906400	2.55579300
H	-5.28472700	0.49977900	2.31056700
H	-6.95310400	1.72001200	0.91011200
H	-6.16939900	3.64620800	-0.49429200
H	-3.75464700	4.29637700	-0.41501700
H	-1.82044700	4.77654500	-1.78361100
H	1.23132800	3.39129400	-0.25955300
H	1.89281900	3.90475400	2.06909300
H	0.19114500	3.81263200	3.89031700
H	-2.17846200	3.37246500	3.32243300
N	-3.69428300	1.69364000	1.72858400
Ir	-1.98965700	0.83202700	2.62155800
C	-0.35061600	0.15072900	3.93038500
H	-0.00295400	1.03148300	4.46690400
C	-0.74815800	-1.03264300	4.80584200
H	-0.22289300	-1.93154100	4.47098000
H	-0.40968200	-0.84885000	5.82939000
C	-2.27559800	-1.25989700	4.80634900
H	-2.51396100	-2.30666900	5.04177600
H	-2.73284800	-0.65691100	5.59771900
C	-2.92767500	-0.85836700	3.49668800
H	-3.99881400	-0.67364800	3.59386200
C	-2.45622200	-1.21287000	2.19075800
H	-3.20146200	-1.22610100	1.39550500
C	-1.22643000	-2.07825500	1.92564600
H	-1.39335800	-2.66646700	1.01895500
H	-1.10564500	-2.80058700	2.73813200
C	0.05078000	-1.22515900	1.75078000
H	0.14223600	-0.92474600	0.70216700
H	0.94695400	-1.81638000	1.98466800
C	0.02909800	0.04653300	2.57729300
H	0.65383200	0.84784700	2.18190200
C	-1.11619900	4.02489100	-2.15357200
C	-1.14440300	2.75954800	-1.28074100
H	-1.38695100	3.79836300	-3.18790300
O	-0.16374700	1.80569600	-1.67636300
C	-0.40453300	1.18268500	-2.93097100
H	-0.29720500	1.87682400	-3.77365200
H	0.34273000	0.39364300	-3.03345600
H	-1.40735300	0.73171500	-2.96946600
H	-0.11653800	4.46874500	-2.14782200
H	-2.14231900	2.29956900	-1.35120900
TS4b			
C	-4.11551700	2.38584500	1.18140400
C	-4.77680700	0.63688300	-0.23159300
C	-5.95705200	1.28521200	-0.56471400
C	-6.21851400	2.53536500	-0.00205600
C	-5.28864700	3.08564500	0.87049800
C	-3.07763900	2.88747500	2.09584100
C	-1.77237000	2.33718500	1.98376500
C	-0.79714900	2.80093600	2.88278500
C	-1.08892600	3.74311600	3.87137800
C	-2.38456200	4.25480600	3.97787400
C	-3.37500000	3.82875300	3.09222500
H	-4.52719100	-0.33081500	-0.64601700
H	-6.64744400	0.81662800	-1.25663200
H	-7.12715400	3.07515200	-0.24809000
H	-5.45485400	4.06561600	1.30146300
H	-2.51553900	-0.96122800	0.12468900
H	0.22389800	2.43394900	2.80318400

H	-0.31208100	4.07861800	4.55191900
H	-2.62471300	4.98193900	4.74710400
H	-4.38620100	4.20713700	3.20676800
N	-3.87453000	1.16587500	0.62410500
Ir	-2.07521800	0.18517600	1.13520900
C	-0.15254900	-0.45702300	2.05404700
H	0.60153900	0.25039400	1.71344400
C	-0.22445500	-0.66163400	3.56987700
H	-0.03054100	-1.71702500	3.78543800
H	0.59942000	-0.11135500	4.03377500
C	-1.55492000	-0.21299100	4.21863300
H	-1.75346200	-0.81020400	5.11985500
H	-1.45952000	0.82046200	4.55765800
C	-2.75324600	-0.28746200	3.29215700
H	-3.55451100	0.41304700	3.51438700
C	-3.07512300	-1.38885400	2.49971500
H	-4.09627100	-1.45018000	2.13274600
C	-2.29253100	-2.69839200	2.51568000
H	-2.98977000	-3.52281500	2.34112700
H	-1.89241900	-2.85399800	3.52201400
C	-1.15748700	-2.77621100	1.46859600
H	-1.54703500	-3.20872900	0.54271100
H	-0.36715400	-3.45646300	1.81601000
C	-0.53875000	-1.43540100	1.12166300
H	-0.06201500	-1.40716400	0.14513300
C	-0.95132100	2.40676500	0.08373700
C	-1.21233600	1.12263300	-0.55579100
H	-1.90407300	1.20654800	-1.39359400
H	-0.29039400	0.62160000	-0.85654700
O	-1.53832600	3.47561300	-0.46516000
C	-1.13823500	4.77380100	0.00643300
H	-1.52221800	5.48747800	-0.72157500
H	-1.57228500	4.97128700	0.98998600
H	-0.04691600	4.84566000	0.05471600
H	0.04417900	2.57466400	0.49376100
INT6b			
C	-3.81708200	2.48521600	1.18451100
C	-4.63673600	0.82228900	-0.24161900
C	-5.76778700	1.57162200	-0.53594800
C	-5.93414300	2.81123700	0.08210700
C	-4.94763800	3.26934700	0.95155200
C	-2.71446200	2.90588200	2.09575200
C	-1.37387000	3.02008400	1.64018800
C	-0.39672100	3.44642500	2.55186700
C	-0.71618600	3.75933000	3.87187300
C	-2.04093300	3.66901600	4.30902700
C	-3.03010600	3.24928300	3.42357000
H	-4.47039300	-0.15393400	-0.68039000
H	-6.50220100	1.18107700	-1.23099500
H	-6.81314000	3.41528200	-0.11835800
H	-5.02738800	4.23720400	1.43338400
H	-2.29021500	-0.84410200	0.09718100
H	0.62618900	3.56661000	2.20429000
H	0.06016800	4.09845500	4.55082400
H	-2.30211000	3.93359700	5.32871000
H	-4.06208100	3.18116900	3.75619000
N	-3.69262000	1.26158500	0.61471000
Ir	-2.03293300	0.15859400	1.23905000
C	-0.27664400	-0.55766700	2.43915000
H	0.46935000	0.21724400	2.27240600
C	-0.62657100	-0.82401400	3.90177500
H	-0.49298700	-1.88795400	4.11280600
H	0.10295500	-0.30164000	4.52729200
C	-2.04422800	-0.36101400	4.31735700
H	-2.34722900	-0.88390900	5.23530900
H	-2.01034600	0.70163200	4.57753700
C	-3.11064300	-0.53977200	3.25447500
H	-3.95199900	0.14708200	3.32201300

C	-3.24684700	-1.61246700	2.40155200
H	-4.16883800	-1.67310000	1.82819800
C	-2.38539600	-2.86526700	2.42482200
H	-3.00416900	-3.71480000	2.12119000
H	-2.08210900	-3.07085100	3.45428000
C	-1.14312800	-2.81601700	1.49959600
H	-1.43125000	-3.12156500	0.48843600
H	-0.40320400	-3.55569300	1.83607500
C	-0.47026800	-1.46250400	1.39354400
H	0.14785700	-1.33640100	0.50718300
C	-0.98549500	2.75553200	0.17454800
C	-0.85854600	1.24906400	-0.10722700
H	-1.14262600	1.07224600	-1.14835000
H	0.19016200	0.95140500	0.00597100
O	-1.93768200	3.30231600	-0.72558300
C	-1.87585500	4.71768200	-0.84646500
H	-2.60534600	5.00187000	-1.60688400
H	-2.12438200	5.22682000	0.09567700
H	-0.87778000	5.04487400	-1.16911700
H	-0.01230300	3.24392100	0.00169400
TS4a			
C	-4.37604700	2.40007700	1.42891700
C	-4.94798800	0.68932700	-0.07025300
C	-6.18829900	1.25273300	-0.32275200
C	-6.52563200	2.44620000	0.31898900
C	-5.61281900	3.01852600	1.19302900
C	-3.35767600	2.92391300	2.34501200
C	-2.03926100	2.41261300	2.22749600
C	-1.06661600	2.87466700	3.12727700
C	-1.38043800	3.79915200	4.12289600
C	-2.68284700	4.29514700	4.23198400
C	-3.66529600	3.85559100	3.34830900
H	-4.63690300	-0.22659400	-0.55319000
H	-6.86525100	0.76809000	-1.01681800
H	-7.48139100	2.92518900	0.13289600
H	-5.84256500	3.95482200	1.68653400
H	-2.53173000	-0.69751100	0.02527200
H	-0.03997600	2.53057300	3.03861300
H	-0.60950400	4.13669000	4.80900900
H	-2.93168100	5.01720100	5.00264500
H	-4.68077700	4.22110900	3.46290200
N	-4.05759500	1.24146200	0.78338700
Ir	-2.15783600	0.39167400	1.13980900
C	-0.16783500	-0.19087300	1.98388100
H	0.52269100	0.60706200	1.71707600
C	-0.20336100	-0.55806700	3.47043200
H	0.05777500	-1.61602500	3.57041100
H	0.59306200	-0.00961700	3.98174200
C	-1.54715000	-0.26158800	4.17263000
H	-1.69527400	-0.95051500	5.01635700
H	-1.51417500	0.74069300	4.60488900
C	-2.74886100	-0.33039000	3.25418000
H	-3.59517300	0.28554900	3.54748300
C	-2.99661900	-1.35797100	2.33725500
H	-4.02037700	-1.45775500	1.98662400
C	-2.13099000	-2.61118400	2.21991400
H	-2.77549400	-3.45571000	1.96025200
H	-1.71809500	-2.84377000	3.20586000
C	-0.99876100	-2.50718800	1.17246700
H	-1.35884800	-2.87860300	0.20913600
H	-0.15795200	-3.15565200	1.45639400
C	-0.48205900	-1.09729600	0.95730100
H	-0.01643700	-0.93298500	-0.01118800
C	-1.23579400	2.54132400	0.37996100
C	-1.41389300	1.50327500	-0.59781600
H	-0.50919800	1.00309000	-0.94796500
H	-0.22436400	2.68964200	0.73684300
O	-2.32072000	1.77875500	-1.60004800

C	-2.38190100	0.79341100	-2.62295100
H	-3.08730700	1.15827100	-3.37003900
H	-1.40084300	0.65050800	-3.09483100
H	-2.72772700	-0.17108100	-2.22435400
H	-1.79512200	3.45403600	0.20342100
INT6a			
C	-4.33375700	2.46441100	1.41644900
C	-5.11619700	0.84652900	-0.08360100
C	-6.32793000	1.50976600	-0.22927200
C	-6.54687100	2.68424900	0.49061900
C	-5.53552100	3.16647300	1.31956400
C	-3.18565500	2.91601300	2.24913000
C	-1.90983600	3.13568700	1.65866900
C	-0.86601600	3.57055900	2.49473200
C	-1.06710100	3.80670000	3.85210000
C	-2.33487100	3.62179000	4.41510600
C	-3.38473000	3.17873000	3.61661800
H	-4.89926100	-0.07027600	-0.61709900
H	-7.08031100	1.10691000	-0.89762900
H	-7.48399900	3.22337600	0.39757600
H	-5.65444100	4.09056900	1.87406500
H	-2.65286700	-0.68358000	0.01682200
H	0.10667900	3.76996100	2.05331100
H	-0.24506500	4.15996100	4.46697300
H	-2.50254400	3.82717100	5.46758600
H	-4.37081000	3.03006700	4.04716500
N	-4.14785100	1.30493300	0.73436600
Ir	-2.32984300	0.34943300	1.11837600
C	-0.36203500	-0.19558600	2.04650600
H	0.27935900	0.64696300	1.79433400
C	-0.46122600	-0.51230300	3.53811000
H	-0.16313400	-1.55135400	3.70076100
H	0.28089500	0.09541700	4.06380800
C	-1.84626900	-0.23873800	4.17503400
H	-1.93214800	-0.80208200	5.11485800
H	-1.90562500	0.81719000	4.45561300
C	-3.03705300	-0.54471800	3.28928900
H	-3.92972300	0.04425000	3.49049000
C	-3.16994600	-1.61172200	2.43863300
H	-4.14557700	-1.76541000	1.98357800
C	-2.16680600	-2.74177800	2.28637800
H	-2.71546000	-3.66122500	2.06096900
H	-1.67645500	-2.91574300	3.24711300
C	-1.10697900	-2.52810200	1.17684100
H	-1.52041700	-2.84548700	0.21389300
H	-0.24504900	-3.18418700	1.36301700
C	-0.61099300	-1.10590300	1.01612900
H	-0.13588100	-0.90589700	0.05825000
C	-1.69981800	3.04339100	0.15253000
C	-1.49525700	1.60175200	-0.34920200
H	-0.42000700	1.36978300	-0.42348300
H	-0.85340800	3.67574500	-0.13502700
O	-2.07726700	1.52466900	-1.62889800
C	-1.61687800	0.46121700	-2.43866100
H	-2.07253900	0.58524000	-3.42265200
H	-0.52262100	0.48109700	-2.54734600
H	-1.91143100	-0.51959500	-2.03167800
H	-2.57738300	3.44468100	-0.36353400
TS5a			
C	-4.40208400	2.44163000	1.56187300
C	-5.25847800	0.68285500	0.27408700
C	-6.49838100	1.29986800	0.17089800
C	-6.69350400	2.52631100	0.80663900
C	-5.63300900	3.10031800	1.50372300
C	-3.22129400	3.00855300	2.26460900
C	-1.99660100	3.20132700	1.57680300
C	-0.91017100	3.72185000	2.29326500

C	-1.01612100	4.04284000	3.64643000
C	-2.23146600	3.86876300	4.31174000
C	-3.32871300	3.35927300	3.61954900
H	-5.05561500	-0.27300900	-0.19413400
H	-7.28940800	0.82209800	-0.39579100
H	-7.65111600	3.03361000	0.74881400
H	-5.73602200	4.06499400	1.98770900
H	-2.24010100	0.20698600	-0.32827200
H	0.02404300	3.90869100	1.77021500
H	-0.15922700	4.45040900	4.17376500
H	-2.32720900	4.13476800	5.35957500
H	-4.27585900	3.21828000	4.13246200
N	-4.23644300	1.23167800	0.96365600
Ir	-2.38456500	0.25125200	1.26194300
C	-0.45131400	-0.36199700	2.12193200
H	0.24265100	0.45179200	1.91524400
C	-0.56792900	-0.74789400	3.59661000
H	-0.34923400	-1.81353000	3.70743000
H	0.21177000	-0.22340400	4.15601500
C	-1.94198900	-0.40505700	4.21865100
H	-2.12320100	-1.03189300	5.10352200
H	-1.92276300	0.62811500	4.57962400
C	-3.10487400	-0.52381400	3.25044300
H	-3.97920300	0.07195100	3.50779800
C	-3.29739600	-1.55144600	2.31781000
H	-4.29342600	-1.63838500	1.88747200
C	-2.41664400	-2.78613300	2.19259100
H	-3.04599400	-3.63727500	1.91635000
H	-1.99323500	-3.02596600	3.17137100
C	-1.29932600	-2.62574000	1.13987300
H	-1.69272800	-2.88983900	0.15301400
H	-0.48232900	-3.33284400	1.34218500
C	-0.74519400	-1.21902600	1.04673500
H	-0.23049700	-1.01521500	0.10989300
C	-1.87641600	2.98423000	0.07696300
C	-1.38211000	1.61204400	-0.38007900
H	-0.34095200	1.41119300	-0.09975800
H	-1.18134600	3.72278500	-0.34216700
O	-1.54256900	1.58883300	-1.76092700
C	-0.90639800	0.51783900	-2.44211700
H	-1.03442900	0.70167500	-3.50919100
H	0.16555200	0.47209200	-2.20594900
H	-1.37509900	-0.44456800	-2.18476100
H	-2.83697500	3.16294400	-0.41401700
TS5b			
C	-3.66299800	2.65525800	1.18255300
C	-4.50206600	0.88703600	-0.09469500
C	-5.63862200	1.60560800	-0.43809100
C	-5.80203800	2.88855100	0.08392700
C	-4.80368700	3.41282200	0.89901400
C	-2.56043000	3.20171500	2.01957200
C	-1.23441900	3.30272900	1.53637400
C	-0.26111800	3.86164900	2.37148400
C	-0.56814800	4.30025800	3.66031400
C	-1.87780800	4.20622600	4.13100700
C	-2.86666200	3.66897200	3.30814500
H	-4.33698100	-0.11780700	-0.46443500
H	-6.37724500	1.15943700	-1.09413300
H	-6.68454800	3.47483400	-0.15138600
H	-4.87866300	4.41673000	1.30112100
H	-1.52058500	0.18361100	-0.23169500
H	0.75370800	3.97224600	1.99738200
H	0.20816700	4.73153000	4.28464400
H	-2.13212600	4.55803300	5.12569200
H	-3.88999700	3.60066900	3.66649600
N	-3.54470500	1.38780000	0.71447100
Ir	-1.89215700	0.21344400	1.32081200
C	-0.24078100	-0.68730700	2.48365400

H	0.58020900	0.02682000	2.44453500
C	-0.68558300	-1.07412200	3.89347500
H	-0.64044700	-2.16087300	4.00340800
H	0.03758100	-0.67162700	4.60827700
C	-2.09201000	-0.54572200	4.26379400
H	-2.51329500	-1.13810100	5.08838200
H	-2.00233900	0.47693100	4.64485400
C	-3.06922100	-0.51231000	3.10202800
H	-3.89009000	0.19484500	3.21372500
C	-3.22034400	-1.49608500	2.12334500
H	-4.11863400	-1.44083900	1.51254000
C	-2.48472300	-2.82564900	2.09628400
H	-3.15318900	-3.58477100	1.67955800
H	-2.26887400	-3.13939000	3.12055100
C	-1.19132900	-2.78363200	1.25378900
H	-1.44060700	-2.95689200	0.20212100
H	-0.52158100	-3.60411100	1.54794600
C	-0.44574400	-1.46772800	1.33375800
H	0.24536800	-1.30808800	0.50752000
C	-0.82425000	2.85045200	0.13008600
C	-0.48455000	1.35646200	0.03942600
H	-0.30657500	1.14058000	-1.02009900
H	0.45231700	1.14227700	0.55764800
O	-1.79323100	3.14134000	-0.86087200
C	-1.85409900	4.51723400	-1.22194300
H	-2.59793600	4.60104100	-2.01571100
H	-2.15520300	5.15126400	-0.37711800
H	-0.88476800	4.87033000	-1.59976300
H	0.10915200	3.38547700	-0.11927200
3a			
C	-4.02033600	1.82200700	0.03163600
C	-2.15700700	3.15397100	0.30797500
C	-2.86840200	4.32699900	0.05925300
C	-4.22769600	4.21520500	-0.23227700
C	-4.81030300	2.95180200	-0.25063800
C	-4.63599100	0.46407300	0.06559700
C	-4.03957000	-0.67985700	-0.51276800
C	-4.71935100	-1.90346300	-0.43965300
C	-5.95317200	-2.01882600	0.19593400
C	-6.53988000	-0.89366000	0.77515500
C	-5.88431600	0.33115400	0.70135200
H	-1.09163000	3.19398800	0.52980500
H	-2.36999600	5.29070200	0.08579500
H	-4.82329800	5.09712600	-0.45090800
H	-5.85923900	2.82956000	-0.49805000
H	-4.27057700	-2.76830700	-0.91570900
H	-6.45325300	-2.98240700	0.23758100
H	-7.49696100	-0.96806800	1.28333700
H	-6.33077000	1.20527400	1.16639800
N	-2.70469400	1.93381500	0.29853000
C	-2.69459200	-0.65891300	-1.22552800
H	-2.48005000	0.35840400	-1.57591700
C	-1.56080500	-1.10866400	-0.29230100
H	-1.74799500	-2.12631400	0.06427200
H	-0.59474500	-1.09402700	-0.80752200
H	-1.50103100	-0.43175500	0.56182500
O	-2.81313500	-1.52615100	-2.36119600
C	-1.81860600	-1.33758200	-3.34331200
H	-0.81235600	-1.61266400	-2.99432600
H	-2.07814400	-1.98239600	-4.18727900
H	-1.78549100	-0.29378200	-3.69490900
4a			
C	-4.09544700	2.00354400	0.02519900
C	-2.38349700	3.53836500	0.21457100
C	-3.24435900	4.62624800	0.07362900
C	-4.60082900	4.36310600	-0.11491200
C	-5.03178800	3.04030500	-0.14342600

C	-4.54198300	0.58092600	0.04943800
C	-3.85925400	-0.45841200	-0.62647800
C	-4.36864400	-1.76167400	-0.53045100
C	-5.51469100	-2.05302000	0.20593700
C	-6.18939300	-1.02690100	0.86733500
C	-5.70302500	0.27402700	0.78220300
H	-1.31548200	3.69855500	0.35502300
H	-2.86064600	5.64102500	0.10317000
H	-5.31106300	5.17467900	-0.24653300
H	-6.07657800	2.80217800	-0.31163900
H	-3.84010900	-2.55836900	-1.04427900
H	-5.87807200	-3.07535700	0.26209500
H	-7.08157900	-1.23680500	1.45027600
H	-6.21245100	1.07080900	1.31658900
N	-2.78357700	2.26245000	0.19385500
C	-2.61766300	-0.23513300	-1.46732800
H	-2.56086300	0.79939900	-1.81013800
C	-1.31144900	-0.55759800	-0.73642300
H	-0.45416200	-0.22122800	-1.34561100
H	-1.27740700	-0.01376200	0.21781300
H	-2.66694000	-0.87429700	-2.35691300
O	-1.23755000	-1.95919200	-0.52806700
C	-0.11815700	-2.33883100	0.23908400
H	-0.13242600	-1.88084600	1.24092900
H	-0.14864600	-3.42616900	0.34827800
H	0.82995300	-2.05972900	-0.24963700