

SUPPORTING INFORMATION

**DFT Study on the Iridium-Catalyzed Multi-alkylation of
Alcohol with Ammonia**

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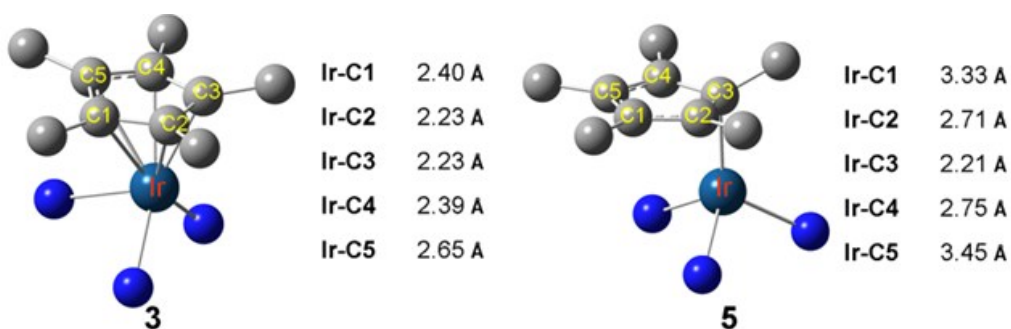


Figure S1. : ‘3’ and ‘5’ represent the precursor structures in triple and quintet state, respectively. The corresponding bond lengths were listed in the right. The hydrogen atoms have been omitted for clarity.

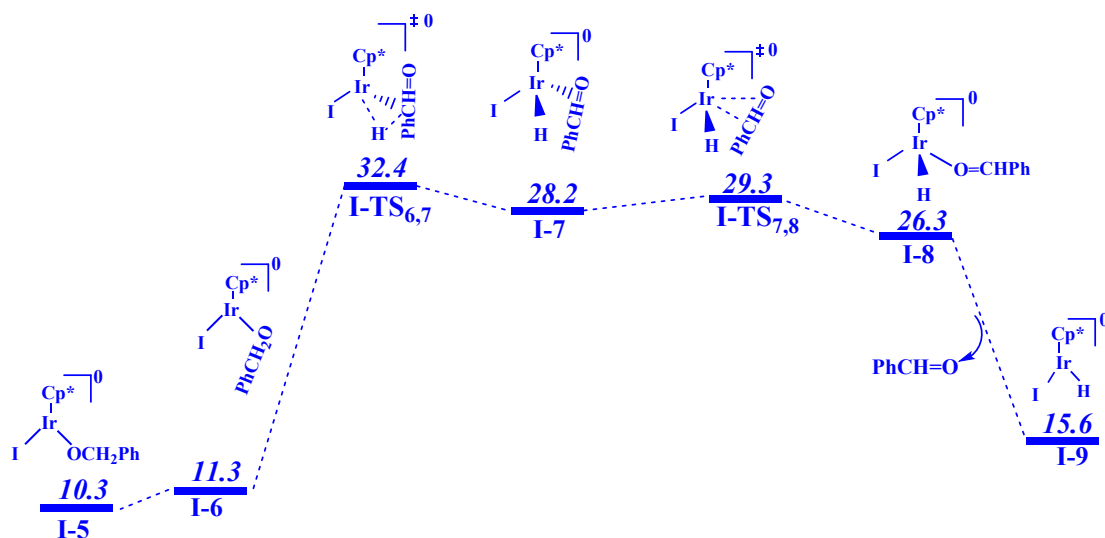


Figure S2. Relative free energy profile for the generation of free benzaldehyde catalyzed by catalyst **I-5** (italic numbers in kcal/mol).

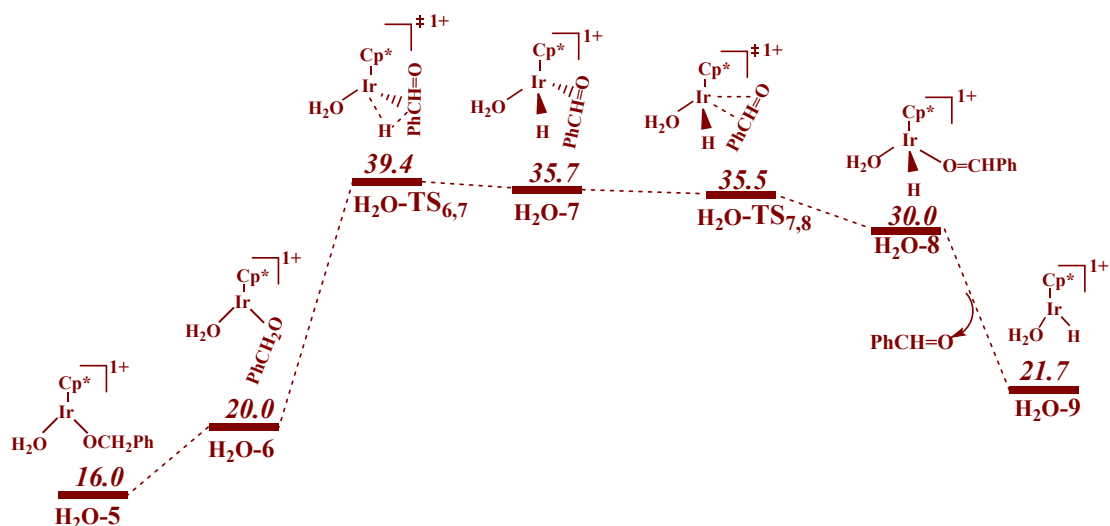


Figure S3. Relative free energy profile for the generation of free benzaldehyde catalyzed by catalyst H₂O-5 (italic numbers in kcal/mol).

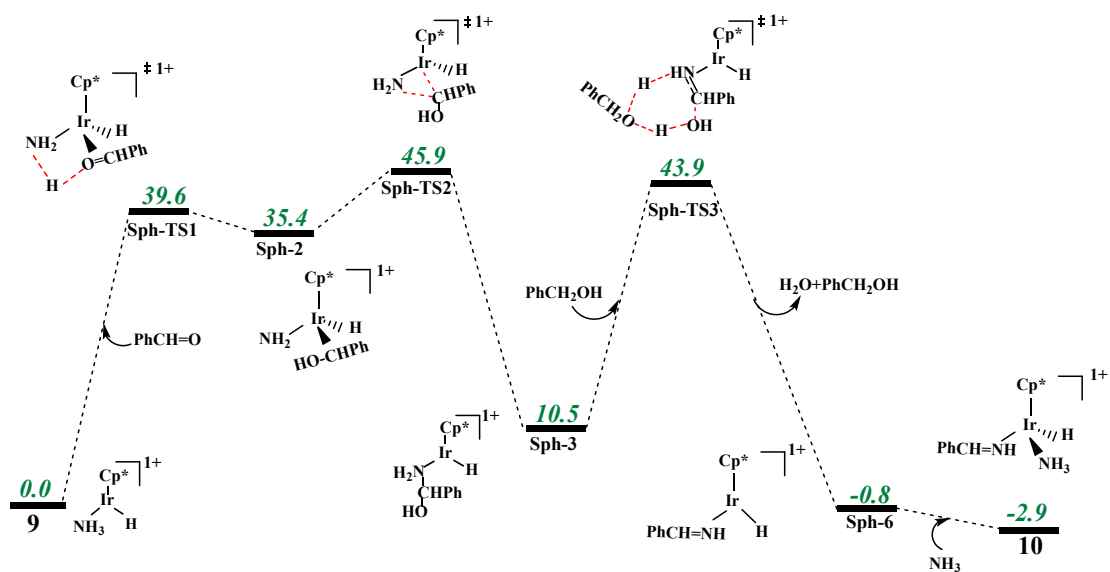


Figure S4. Relative free energy profile for the generation of imine PhCH=NH on the metal coordination sphere (italic numbers in kcal/mol).

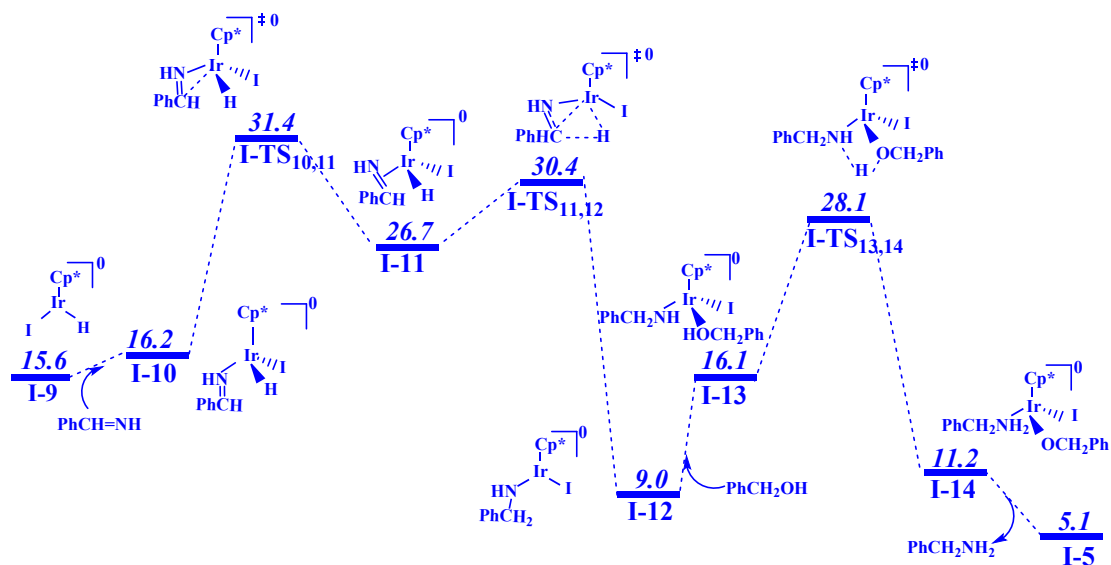


Figure S5. Relative free energy profile for the reduction of the PhCH=NH by the Ir-H reductant I-9 to afford first amine PhCH₂NH₂ (italic numbers in kcal/mol).

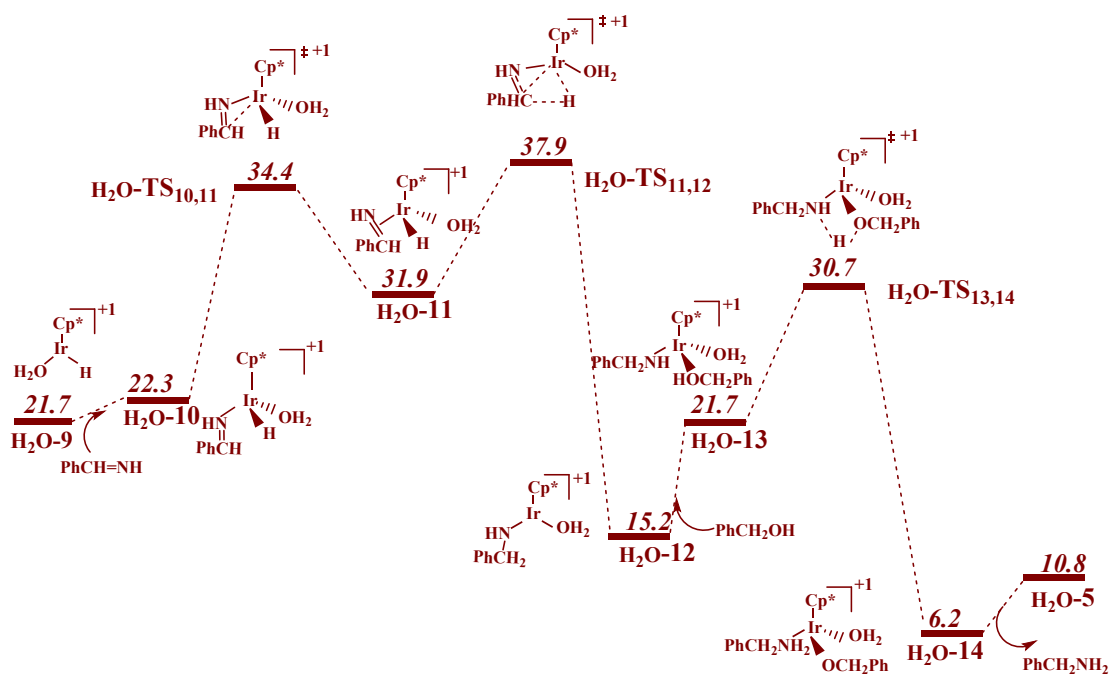


Figure S6. Relative free energy profile for the reduction of the PhCH=NH by the Ir-H reductant H₂O-9 to afford first amine PhCH₂NH₂ (italic numbers in kcal/mol).

As shown in Figure S8, transition state **I-TS_{11,12}** describes that free anion iodine I⁻ simultaneously H-bonds to one H atom of NH₃ ligand and two H atoms of Cp* ligand. Notice that the normal hydrogen transfer active barrier from intermediate **11** to transition state **TS_{11,12}** is 5.7 kcal/mol, whereas, the active barrier from **I-11** to **I-TS_{11,12}** affected by second coordination H-bonds is 1.3 kcal/mol. The analogous transition states **Cl-TS_{11,12}** and **Br-TS_{11,12}** were also located and the corresponding active barriers are 3.0 kcal/mol and 5.6 kcal/mol, respectively. These energies were recalculated by employing a series of the functionals M06-2X, M06-L, B3pw91, TPSS, and PBE which are usually used in transition-metal catalytic system. The corresponding free energies were comparatively listed in Table S1 and the same energy trends were found, where the energies of both M06-L and B3pw91 are very similar to M06. Therefore, counter anion I⁻ can more effectively facilitate the reduction hydrogen transfer by the second coordination sphere hydrogen-bonding interactions than halogen anion Cl⁻ and Br⁻, which is in consistent the experimental result.

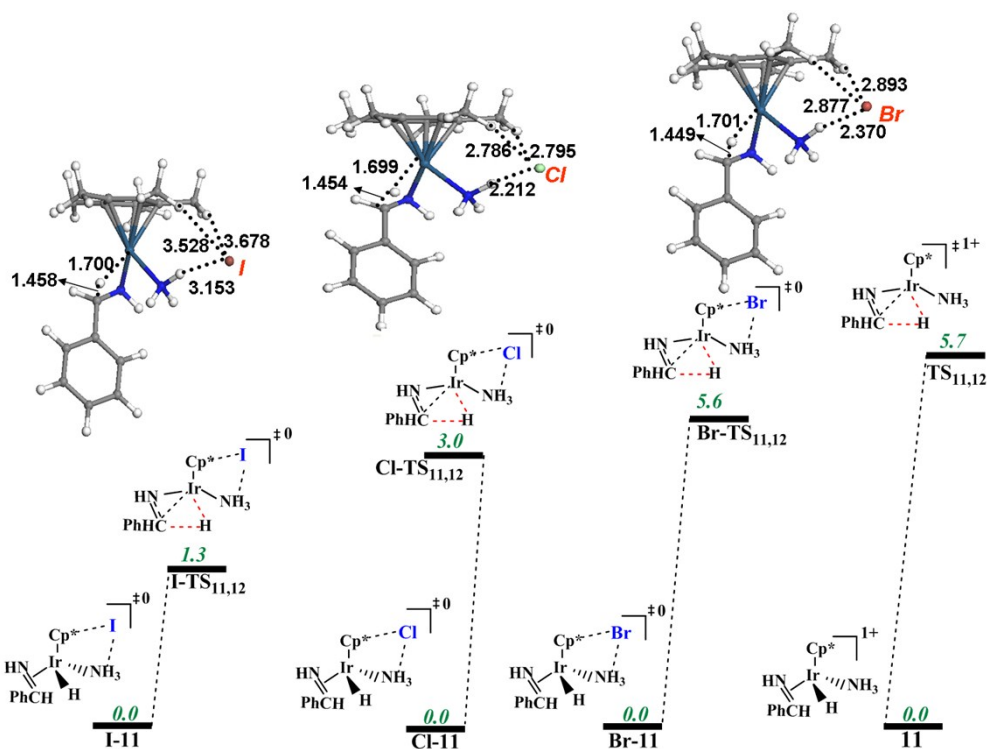


Figure S7. The free energies (italic numbers in kcal/mol) and the optimized transition states structures (bond length/Å) for PhCH=NH reduction hydrogen transfer affected by the second coordination H-bonding effects with counter anions I⁻, Cl⁻, and Br⁻.

Table S1. The single-point calculations (in kcal/mol) for four activation barriers (ΔG^\ddagger) in Figure 7 on the basis of various DFT functionals including M06, M06-2X, M06-L, B3PW91, TPSS, and PBE.

ΔG^\ddagger	M06	M06-2X	M06-L	B3pw91	TPSS	PBE
11 →TS _{11,12}	5.7	7.4	5.4	5.7	6.5	6.5
I-11 →I-TS _{11,1}	1.3	3.1	1.4	0.6	1.8	2.8
Cl-11 →Cl-TS _{11,1}	3.0	5.2	3.7	3.8	4.8	5.4
Br-11 →Br-TS _{11,1}	5.6	7.7	5.3	5.1	7.1	7.5

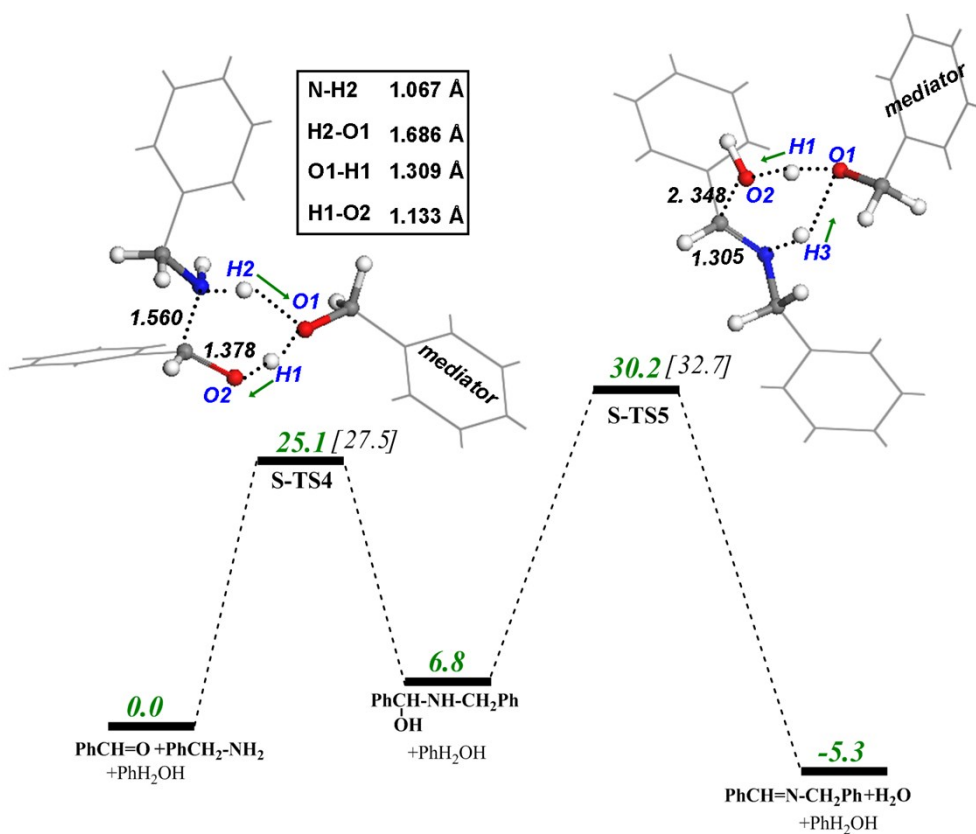


Figure S8. Relative free energy profile (italic numbers in kcal/mol) and optimized transition states structures (bond length/Å) for formation of dibenzylimine ($\text{PhCH=NCH}_2\text{Ph}$) from benzaldehyde (PhCH=O) with benzyl amine (PhCH_2NH_2) mediated by one benzyl alcohol molecule. When water is used as mediator, the corresponding free energy barriers are given in square bracket.

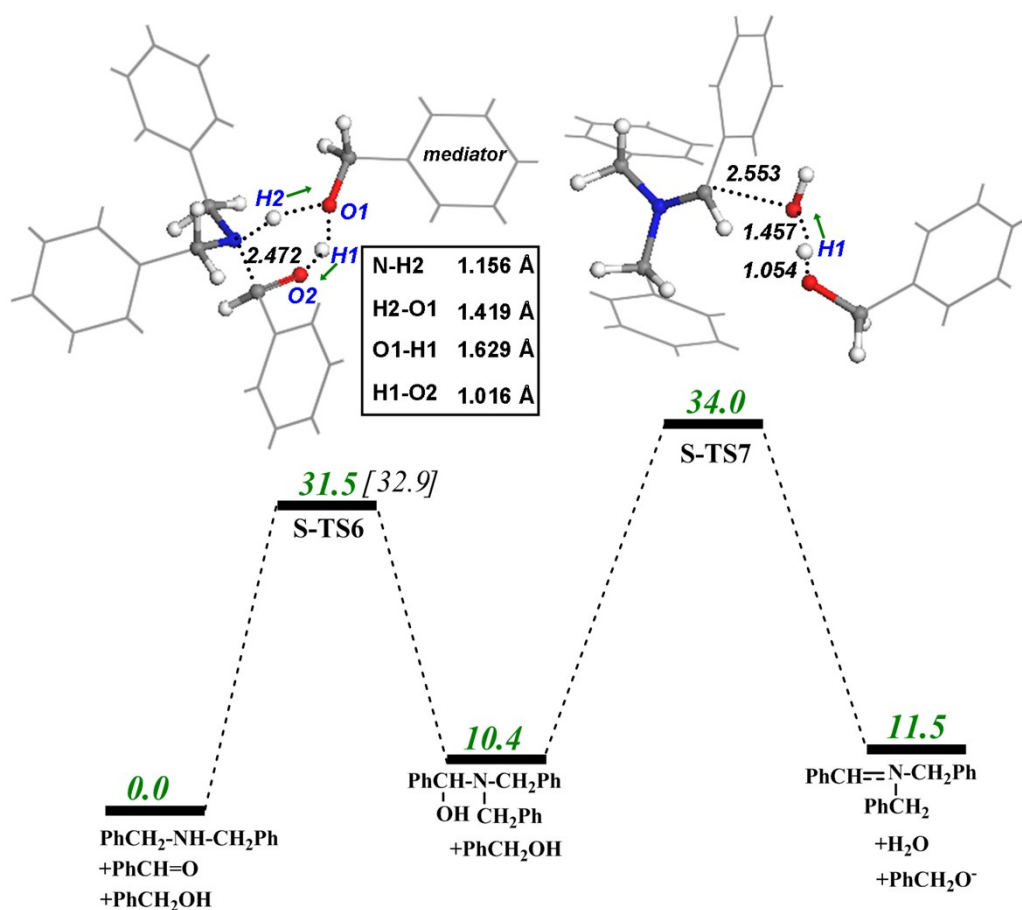
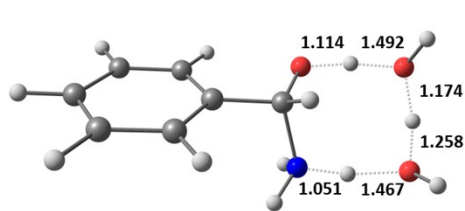
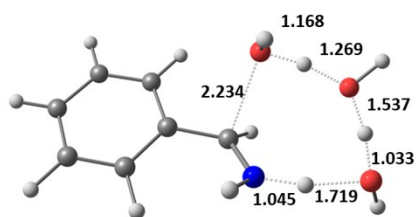


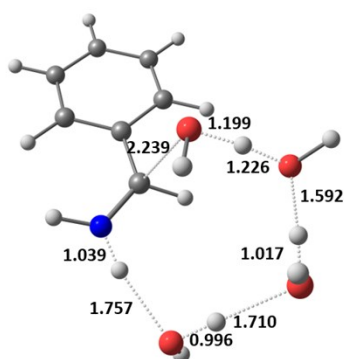
Figure S9. Relative free energy profile (italic numbers in kcal/mol) and optimized transition states structures (bond length/Å) for formation of $\text{PhCH}=\text{N}-(\text{CH}_2\text{Ph})\text{CH}_2\text{Ph}$.



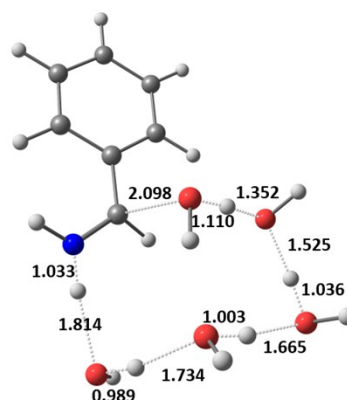
2-H₂O-S-TS1
 $\Delta G^\ddagger = 32.6$ kcal/mol



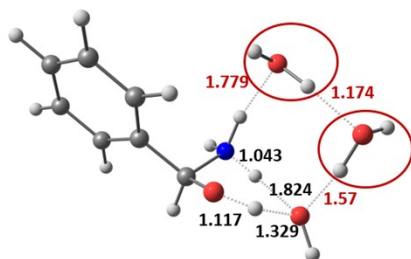
2-H₂O-S-TS2
 $\Delta G^\ddagger = 40.4$ kcal/mol



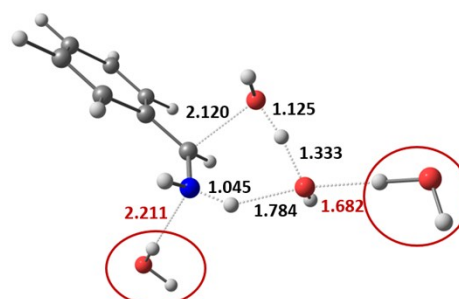
3-H₂O-S-TS2
 $\Delta G^\ddagger = 47.4$ kcal/mol



4-H₂O-S-TS2
 $\Delta G^\ddagger = 58.2$ kcal/mol

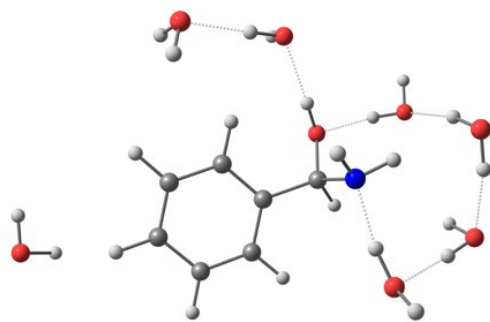


H-bond-S-TS1
 $\Delta G^\ddagger = 38.8$ kcal/mol

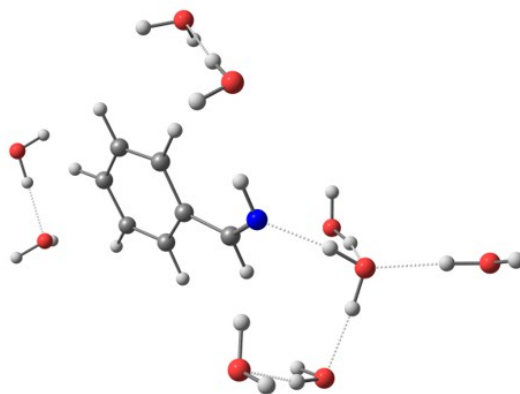


H-bond-S-TS2
 $\Delta G^\ddagger = 52.4$ kcal/mol

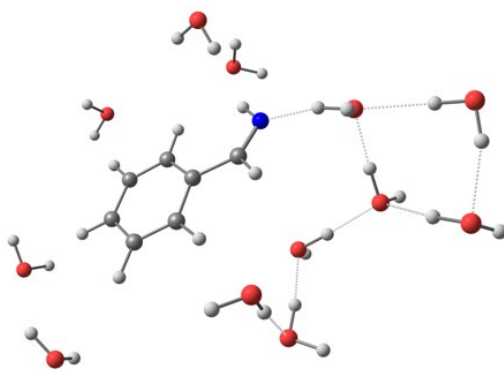
Figure S10. Both 2-H₂O-S-TS1 and 2-H₂O-S-TS2 involve two waters to assist the proton transfer. 3-H₂O-S-TS1 involve three waters to assist the proton transfer. 4-H₂O-S-TS1 involve four waters to assist the proton transfer. Both H-bond-S-TS1 and H-bond-S-TS2 involve one water to promote proton transfer and two more waters to H-bond to the transition state structures (see red font). (Bond length/Å).



Waters-1



Waters-2



Waters-3

Figure S11. **Waters-1:** the initial structure with seven waters were optimized to hemiaminal with water cluster. **Waters-2:** the initial structure with eight waters were optimized to imine with water cluster. **Waters-3:** the initial structure with eleven waters were optimized to imine with water cluster.

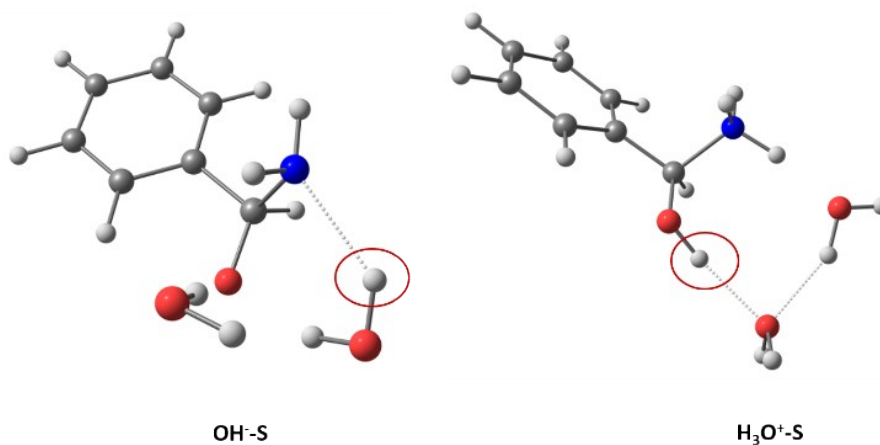
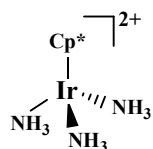


Figure S12. **OH-S** is the optimized stable structure by the adding of the OH^- where the hydrogen of ammonia is abstracted by OH^- . **H₃O⁺-S** is the optimized stable structure by the adding of the H_3O^+ where the proton of H_3O^+ transfers to O atom of aldehyde.

**Cartesian coordinates, atom numbers, and Gibbs free energies [in Hartree and
at the M06/BSII (SMD, water) level of theory] for the key structures involved in
this stud**

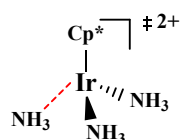


1

E=-663.7311814 (au)

C	1.35608300	-1.07135400	0.43590900
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C	1.32277800	-0.72066200	-0.97418000
C	1.22224900	0.70535200	-1.08611100
Ir	-0.54190900	-0.03732900	0.01505600
N	-1.89596500	-0.25174100	1.72152100
H	-2.82781100	0.12821100	1.55166800
H	-2.01665800	-1.23102900	1.98007300
N	-1.87947100	-1.46538200	-0.93566500
H	-2.34766600	-1.06919400	-1.75101600
H	-1.35047200	-2.27428500	-1.25973900
N	-1.99670400	1.46807800	-0.62864100
H	-2.20906500	2.11559500	0.12995500
H	-1.60808900	2.02023400	-1.39230900
H	-1.52061700	0.22721400	2.53952900
H	-2.60998600	-1.81487600	-0.31463900
H	-2.88452600	1.08428000	-0.95429200
C	1.44673900	0.27990400	2.67512500
H	2.50508300	0.32142000	2.96029200
H	0.96476000	1.18569800	3.04950100
H	1.00462300	-0.58582800	3.17356300

C	1.58537200	-2.44258900	0.99281400
H	1.09951500	-3.20605600	0.37991100
H	2.65811300	-2.67030700	1.02063300
H	1.20138600	-2.52751900	2.01212500
C	1.40104000	-1.69371400	-2.10634400
H	0.93248300	-1.30031200	-3.01075100
H	2.45311200	-1.90178800	-2.33630400
H	0.92835200	-2.64606800	-1.85189600
C	1.21536600	1.50089800	-2.35370600
H	0.62429600	2.41464200	-2.24860200
H	2.23827600	1.79814000	-2.61505300
H	0.81031000	0.92144300	-3.18634900
C	1.25390900	2.72460200	0.59813700
H	0.92965900	2.90917500	1.62455400
H	2.27377800	3.11412800	0.49207800
H	0.61117200	3.29691300	-0.07584700



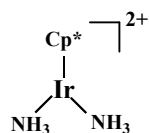
TS_{1,2}

E=-663.7091249(au)

C	0.83709600	1.52350700	-0.49077600
C	1.38235900	0.38068000	-1.14818700
C	1.70327400	-0.61642100	-0.12749300
C	0.87803800	1.27585000	0.95580200
C	1.43478200	-0.01581400	1.17821000
Ir	-0.40850300	-0.24960900	-0.03569800

N	-1.55018000	-1.03929500	-1.69575200
H	-1.58308100	-2.05940300	-1.69126100
H	-2.51178800	-0.70235900	-1.65000900
N	-3.30752000	0.84227000	0.29446000
H	-3.50138400	1.02264900	1.27694800
H	-3.46758900	1.71574400	-0.20198200
N	-1.46046000	-1.77618800	1.10721500
H	-1.55596700	-2.65182700	0.59289000
H	-0.98262700	-1.98827700	1.98229300
H	-1.16363600	-0.75444800	-2.59493700
H	-4.01735000	0.18676900	-0.02708100
H	-2.40032500	-1.45087400	1.33381500
C	1.60278100	0.21110200	-2.61593800
H	2.64196200	0.46517800	-2.85702600
H	1.43378400	-0.82224500	-2.92899400
H	0.95229700	0.86589700	-3.19909300
C	0.38821900	2.79964900	-1.12599300
H	-0.46568400	3.22761400	-0.59545100
H	1.20196500	3.53458000	-1.09406100
H	0.10899400	2.65186100	-2.17112700
C	0.45090400	2.25806600	1.99659200
H	0.24779100	1.77007000	2.95172300
H	1.25001900	2.99314500	2.15405600
H	-0.44293300	2.80436200	1.68530900
C	1.71164800	-0.66124800	2.49739500
H	1.57557600	-1.74450100	2.44782100
H	2.75199900	-0.47158100	2.78810400

H	1.06465900	-0.26397300	3.28223300
C	2.40282700	-1.91527900	-0.35824500
H	2.18226600	-2.32057200	-1.34799400
H	3.48714800	-1.75946500	-0.29128500
H	2.12419800	-2.65648600	0.39417000

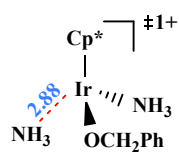


2

E=-607.1563039(au)

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C	0.88320600	-1.15680100	0.91419800
C	-0.25880400	-1.26925900	-1.11522500
C	1.06409300	-1.27127700	-0.49807800
Ir	0.00670100	0.60746500	-0.05372700
N	-1.44931700	2.23273900	-0.10889400
H	-1.32231100	2.85894900	0.68723800
H	-1.33490100	2.79485100	-0.95348400
N	1.57402200	2.15928600	-0.10923400
H	1.49330400	2.78665800	0.69155400
H	2.50351100	1.74317900	-0.09273500
H	-2.40873200	1.89015900	-0.08793700
H	1.49749800	2.73078900	-0.95124300
C	-1.17156000	-1.01740300	2.54052200
H	-1.24644000	-2.03266600	2.95076700
H	-0.56169000	-0.42546900	3.22667000

H	-2.17685300	-0.59329400	2.50489000
C	-2.73928200	-1.24300800	-0.26335000
H	-3.03645500	-0.78820600	-1.21107800
H	-3.06985500	-2.28842300	-0.27543700
H	-3.26847500	-0.73403400	0.54529100
C	-0.52593700	-1.41485800	-2.57335800
H	0.25874500	-0.94906900	-3.17351000
H	-0.54771000	-2.48354300	-2.82351700
H	-1.48980500	-0.98476700	-2.85214500
C	2.36122800	-1.40980600	-1.22671600
H	3.19090700	-0.99919500	-0.64766400
H	2.56983100	-2.47092400	-1.40845200
H	2.33021500	-0.90551300	-2.19550500
C	1.95616000	-1.14553600	1.95169400
H	1.66927300	-0.54474100	2.81767500
H	2.13346500	-2.17056500	2.29983000
H	2.89601400	-0.75853500	1.55256300



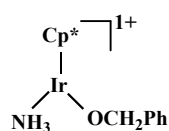
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C	-2.59726700	1.84165900	0.79696200
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C	-3.93882400	-0.00201400	0.23115100
C	-2.76383300	1.05792600	1.98287100
C	-3.65334100	-0.05577200	1.65313200

Ir	-4.72562700	1.78978800	1.33080100
N	-5.72686800	4.04977100	-0.19117900
H	-5.91329600	4.45067000	0.72717200
H	-4.89308800	4.51248600	-0.54519600
H	-4.51075800	3.12010500	4.42952700
H	-3.68278900	4.09168800	3.19405200
N	-6.88251500	1.55574500	1.17086000
H	-7.19352200	1.94603000	0.28381100
H	-7.26032300	0.61660900	1.26961800
H	-6.48553800	4.32452600	-0.81406000
H	-7.23640000	2.14675000	1.92737100
C	-3.34889200	1.63054200	-1.71580800
H	-2.47325800	1.23042800	-2.24177700
H	-4.24085800	1.28104900	-2.23893600
H	-3.31460000	2.71848300	-1.79685800
C	-1.72126000	3.04665600	0.64220700
H	-1.62468900	3.60061300	1.57851300
H	-0.71519200	2.74058600	0.33066500
H	-2.10538600	3.73007800	-0.11822900
C	-2.10618200	1.27701400	3.30888600
H	-2.76171500	0.99608100	4.13629600
H	-1.20188600	0.65996300	3.37602300
H	-1.80960600	2.31773200	3.44845700
C	-4.02008500	-1.17074900	2.58244600
H	-4.96917200	-1.63506000	2.30615700
H	-3.24847100	-1.95005600	2.54591300
H	-4.09703800	-0.82682300	3.61586000

C	-4.72887500	-1.01286200	-0.54487900
H	-5.24648600	-0.55858700	-1.39287600
H	-4.06340100	-1.78850300	-0.94173000
H	-5.47232700	-1.51339300	0.08020900
C	-4.67019500	3.80197400	3.58154100
O	-5.42594400	3.13273300	2.57170200
C	-5.42600800	5.02903000	4.03193700
C	-6.44705700	4.92265600	4.98568700
C	-5.14935200	6.28256000	3.47150900
C	-7.17857400	6.04625700	5.36961300
H	-6.66198400	3.95622700	5.43554900
C	-5.87841100	7.40983600	3.85439600
H	-4.34587800	6.38031300	2.74411700
C	-6.89568200	7.29186200	4.80319000
H	-7.96239100	5.95381200	6.11552500
H	-5.64765900	8.37847800	3.42098100
H	-7.46013900	8.16816700	5.10725200



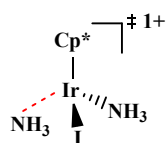
5

E=-896.7780979(au)

C	-1.68545300	1.12299300	1.19596500
C	-2.48259300	-0.10446000	1.14488100
C	-2.94744600	-0.29043900	-0.20223700
C	-1.61565600	1.64858600	-0.13011100
C	-2.36956300	0.75015100	-1.00847200

Ir	-0.71238200	-0.34999900	-0.11325900
H	1.77406500	1.60316600	0.02852400
H	1.86095000	0.75862300	1.58730500
N	-0.30261200	-2.30565000	-1.01093800
H	-0.89356900	-3.04130400	-0.62720500
H	-0.45719600	-2.28640200	-2.01805700
H	0.67310900	-2.55481100	-0.84956700
C	-2.84698200	-0.93653400	2.33112800
H	-3.73593700	-0.51549800	2.81827700
H	-3.07849900	-1.96466700	2.04473000
H	-2.04128700	-0.95294700	3.06898300
C	-1.11917200	1.73080800	2.43923400
H	-0.29276300	2.40852000	2.21539900
H	-1.89506100	2.30663300	2.95898500
H	-0.75982500	0.96377600	3.13020300
C	-0.95239300	2.91726200	-0.56135100
H	-0.49506500	2.81264100	-1.54870800
H	-1.69580300	3.72171400	-0.62426900
H	-0.18059000	3.22788200	0.14610700
C	-2.60525200	0.97078100	-2.46792200
H	-2.79459400	0.02989700	-2.98952000
H	-3.48317900	1.61453300	-2.60631800
H	-1.75278100	1.46364000	-2.94101800
C	-3.84519100	-1.38822900	-0.68210300
H	-3.73826700	-2.28859300	-0.07217900
H	-4.89255200	-1.06872100	-0.62212400
H	-3.63753200	-1.65125300	-1.72199100

C	2.04381600	0.65324200	0.50851700
O	1.25538900	-0.41609400	-0.01615000
C	3.50485700	0.34811500	0.25903700
C	4.20797500	-0.50498100	1.12201800
C	4.15850700	0.84905200	-0.87504000
C	5.53438200	-0.85169200	0.85771400
H	3.71110300	-0.89570300	2.00697000
C	5.48632400	0.50595300	-1.14268100
H	3.62393300	1.51438700	-1.54894600
C	6.17603000	-0.34764800	-0.27774800
H	6.06759100	-1.51239000	1.53555400
H	5.98118600	0.90335400	-2.02444000
H	7.20802600	-0.61601700	-0.48493300

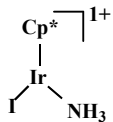


TS_{2,3}

E=-618.743097(au)

C	1.42829000	0.44208700	1.54952300
C	0.85523000	1.58519300	0.91707400
C	1.31281100	1.61233500	-0.47050100
C	2.29991300	-0.23038200	0.58588500
C	2.25635500	0.51792900	-0.64828000
Ir	0.27806700	-0.23731100	-0.21674700
N	0.02771300	-1.48283200	-2.01278600
H	-0.82103600	-1.24838200	-2.52549900
H	0.81615600	-1.41255300	-2.65335700

H	-0.05326300	-2.44994200	-1.70337200
C	-0.03751900	2.60054500	1.55147300
H	0.57272800	3.43707300	1.91437400
H	-0.76119300	3.00102300	0.83903200
H	-0.57976700	2.18484700	2.40254800
C	1.22240900	0.01489100	2.96642400
H	1.30474500	-1.06928800	3.07190700
H	1.99124100	0.47140500	3.60192900
H	0.24568300	0.32782200	3.34095100
C	3.17961400	-1.40015900	0.87962700
H	3.38540400	-1.98552400	-0.01905100
H	4.13835600	-1.03772900	1.27198200
H	2.73955800	-2.05703800	1.63282300
C	3.06386700	0.25284900	-1.87671100
H	2.52239000	0.54087700	-2.78099700
H	3.98625800	0.84500000	-1.83716900
H	3.34431700	-0.79987900	-1.95558500
C	1.01984200	2.69342800	-1.45806900
H	0.00736800	3.08244200	-1.32984800
H	1.72102000	3.52501600	-1.31238400
H	1.12905000	2.33759200	-2.48484900
I	-2.76326100	0.07270100	-0.01554700
N	-0.05004200	-3.04262300	0.76200600
H	-0.97320400	-3.36899400	1.03780300
H	0.51656300	-2.99291900	1.60507600
H	0.36069800	-3.76515700	0.17398600

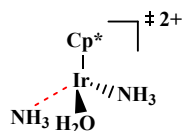


3

E=-562.1895602(au)

C	-1.16947300	1.63416400	-0.39174100
C	-0.90689800	1.38789300	0.98891000
C	-1.61864700	0.17094200	1.37596100
C	-2.07411500	0.59096500	-0.87250900
C	-2.38410500	-0.28485200	0.22988900
Ir	-0.23778600	-0.35225800	-0.18090200
N	0.07775800	-2.49642700	-0.37614200
H	0.71223300	-2.82914200	0.34914600
H	-0.79210900	-3.02231200	-0.30163600
H	0.50643100	-2.72555700	-1.27360700
C	-0.07632400	2.22171700	1.90838700
H	-0.73097100	2.90317200	2.46550700
H	0.45647600	1.60518200	2.63542000
H	0.65192700	2.82393200	1.36298300
C	-0.65909300	2.77287300	-1.21424200
H	-0.46781900	2.46262100	-2.24441000
H	-1.40629500	3.57530000	-1.24060200
H	0.26352500	3.18527500	-0.80155800
C	-2.64699700	0.52385800	-2.24810500
H	-2.99602500	-0.48132000	-2.49191500
H	-3.50409200	1.20622400	-2.31518500
H	-1.91695700	0.83587800	-2.99876700

C	-3.34987800	-1.42345600	0.21586100
H	-3.05401900	-2.20903200	0.91500600
H	-4.34034600	-1.06228800	0.51938000
H	-3.44406100	-1.85861000	-0.78127700
C	-1.67411600	-0.39985200	2.75371900
H	-0.73117300	-0.25119600	3.28460100
H	-2.46524400	0.10415900	3.32326400
H	-1.90093100	-1.46775600	2.73558400
I	2.68457600	-0.02568300	-0.05766600

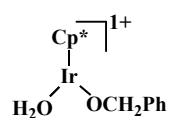


TS_{2,4}

E=-683.5756018 (au)

C	-2.37536600	1.67654400	0.85505100
C	-2.88859400	1.23488900	-0.40103600
C	-3.81334300	0.11933000	-0.15199200
C	-2.99234700	0.86115000	1.90732300
C	-3.84493300	-0.13460000	1.26135700
Ir	-4.59086900	1.89244200	0.88680100
N	-6.21967500	3.36524000	-1.19103200
H	-6.40224000	2.44274900	-1.58576900
H	-7.13369400	3.82155000	-1.14802000
H	-4.21777000	4.65013800	1.33772100
H	-5.41979200	4.21707100	0.38178100
N	-6.53619000	1.81721500	1.85585000
H	-7.31743800	1.76393900	1.19974800

H	-6.64103600	1.02598200	2.49141800
H	-5.70338900	3.86351100	-1.91799500
H	-6.67508600	2.66739300	2.40827300
C	-2.50266600	1.74298300	-1.75213200
H	-1.69792300	1.11282100	-2.15276700
H	-3.33079000	1.69378100	-2.46236400
H	-2.12804900	2.76728500	-1.71836900
C	-1.35594600	2.74652500	1.07947400
H	-1.49801000	3.25769500	2.03429400
H	-0.35895200	2.28824300	1.10602900
H	-1.35054000	3.48644600	0.27692100
C	-2.66190800	0.92337200	3.36014300
H	-3.47355900	0.54753400	3.98563600
H	-1.78365300	0.29004500	3.54791600
H	-2.40885900	1.93497200	3.68314200
C	-4.55027700	-1.26077800	1.94738600
H	-5.44288600	-1.58017100	1.40586700
H	-3.87388000	-2.12346400	1.99687900
H	-4.82596700	-1.01384200	2.97513600
C	-4.49632600	-0.68512500	-1.20888900
H	-4.73716600	-0.08863800	-2.09131000
H	-3.82007100	-1.48574900	-1.53713900
H	-5.40868500	-1.15957100	-0.84279600
O	-4.95632800	4.03065700	1.23071800

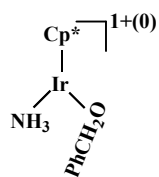


H₂O-5

E=-916.6509058(au)

C	-1.64974900	0.93524900	1.32089700
C	-2.53630100	-0.20297700	1.08458000
C	-2.97169600	-0.16387900	-0.28593100
C	-1.51408300	1.64514500	0.07222100
C	-2.31479200	0.94022000	-0.92738200
Ir	-0.73864900	-0.34454100	-0.13537400
H	1.72656100	1.42610400	0.51036000
H	1.90779000	0.23633800	1.81344500
H	-0.49687000	-2.05576200	-2.24641600
H	0.70743900	-2.22135800	-1.29785400
C	-2.97032700	-1.18511900	2.12356600
H	-3.83809200	-0.78997600	2.66680100
H	-3.25938800	-2.13920300	1.67756200
H	-2.17738400	-1.36872900	2.85255400
C	-1.08861000	1.34389400	2.64474400
H	-0.16841000	1.92040500	2.52809200
H	-1.81440800	1.97177800	3.17641200
H	-0.87555000	0.47587400	3.27339600
C	-0.78393100	2.92889800	-0.15194800
H	-0.32470500	2.95975800	-1.14322400
H	-1.48810100	3.76760400	-0.08320800
H	-0.00489200	3.08389900	0.59746400
C	-2.47361900	1.36241700	-2.35183500
H	-2.76584400	0.52395800	-2.98776800
H	-3.25375400	2.13036100	-2.42645700
H	-1.54757000	1.78910600	-2.74482300

C	-3.89456900	-1.14007500	-0.94633300
H	-3.86049800	-2.11774700	-0.45977400
H	-4.92827500	-0.77772800	-0.89349200
H	-3.64441100	-1.27452600	-2.00155000
C	2.03324200	0.39646100	0.73328600
O	1.21250600	-0.53112400	0.01681900
C	3.48476100	0.20955600	0.35172100
C	4.26251800	-0.78463400	0.96273900
C	4.06788300	1.00568400	-0.64392700
C	5.59386300	-0.97761000	0.58885400
H	3.82315800	-1.40344900	1.74156800
C	5.40017800	0.81766000	-1.01941000
H	3.47562700	1.78380000	-1.11973900
C	6.16577200	-0.17552500	-0.40317900
H	6.18668200	-1.74751800	1.07471900
H	5.84078200	1.44766500	-1.78704900
H	7.20333200	-0.32077900	-0.69020600
O	-0.26381900	-2.28167600	-1.33218800



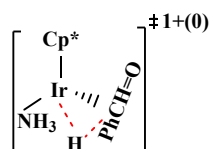
5

E=-896.7715878(au)

C	1.55602800	1.73538000	-0.01090400
C	2.32301900	0.90964400	-0.95148300
C	2.95650800	-0.14954400	-0.20918100
C	1.67601000	1.14554700	1.28255700

C	2.51487900	-0.05119200	1.15659900
Ir	0.73867400	-0.30475900	-0.09048300
N	0.49612300	-2.27983800	-0.98472300
H	1.40303500	-2.69651500	-1.18784000
H	-0.00811100	-2.91681600	-0.36754600
H	-0.02691700	-2.23741400	-1.85971100
C	2.52089300	1.21689700	-2.39998200
H	3.34016300	1.93811800	-2.51505100
H	2.78094400	0.32055200	-2.96708200
H	1.62371400	1.65906300	-2.83969500
C	0.83227800	2.99636700	-0.35700700
H	0.02409100	3.20069100	0.34859300
H	1.52889000	3.84330400	-0.32676600
H	0.40944100	2.95085400	-1.36362400
C	1.10162000	1.65983500	2.56313700
H	0.78709000	0.84172700	3.21629500
H	1.85958800	2.24168600	3.10210400
H	0.24280400	2.31056400	2.38582000
C	2.93518200	-0.92882500	2.29001200
H	3.20743100	-1.92776100	1.94248300
H	3.81142200	-0.49495100	2.78843400
H	2.14177600	-1.02383800	3.03523900
C	3.87983200	-1.18889000	-0.76401900
H	3.67642300	-1.38341100	-1.82008700
H	4.91993900	-0.85151800	-0.68171800
H	3.79333600	-2.13286500	-0.21953400
O	-1.25371600	-0.14419500	0.15141200

C	-2.20233700	-1.10388000	-0.30602600
H	-2.03174800	-1.35812400	-1.36296700
H	-2.13546100	-2.03845900	0.27138400
C	-3.59662000	-0.52859700	-0.16476600
C	-4.45126000	-0.93908200	0.86578400
C	-4.03819600	0.46569600	-1.05158200
C	-5.72251300	-0.37405900	1.00658700
H	-4.12102600	-1.70956200	1.55838600
C	-5.30394500	1.03588100	-0.91192100
H	-3.38571900	0.78881800	-1.85939400
C	-6.15055900	0.61590500	0.11945000
H	-6.37658800	-0.70656200	1.80782200
H	-5.63272800	1.80259200	-1.60800200
H	-7.13770400	1.05617300	0.22788000



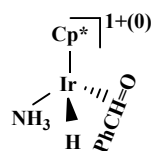
TS_{6,7}

E=-896.7453053(au)

C	-1.00186900	0.82145200	1.27855100
C	-1.37903400	-0.54498600	1.09948300
C	-1.64093800	-0.74934300	-0.32874700
C	-0.98925500	1.47319700	-0.01639500
C	-1.44481100	0.51094700	-0.99720700
Ir	0.46185000	-0.22944300	-0.13459400
N	1.31192100	-2.22613300	-0.11806900
H	0.58721700	-2.92090600	0.05668100

H	1.77114400	-2.47076300	-0.99369300
H	2.00983700	-2.30653000	0.62054600
C	-1.58888300	-1.57128900	2.16909100
H	-2.64657700	-1.60255600	2.45961500
H	-1.31483600	-2.57133000	1.82249400
H	-1.00274900	-1.34704100	3.06327900
C	-0.63691200	1.47964300	2.57023400
H	0.17748600	2.19587400	2.43461000
H	-1.50085400	2.03210900	2.96012500
H	-0.33727800	0.74971800	3.32479500
C	-0.73060400	2.92682800	-0.26597900
H	-0.34316000	3.09471700	-1.27380300
H	-1.66038700	3.50096300	-0.16725200
H	-0.01238800	3.33403200	0.44996600
C	-1.71762400	0.79790400	-2.44077600
H	-1.62362300	-0.10000600	-3.05509500
H	-2.74281100	1.17311600	-2.54930200
H	-1.04147700	1.55995200	-2.83434400
C	-2.19580900	-2.00176300	-0.93298500
H	-1.80944900	-2.89239700	-0.43070400
H	-3.28808300	-2.01311500	-0.83172600
H	-1.95472300	-2.07559700	-1.99572600
O	2.48261000	0.29239700	0.56269700
C	2.61835000	0.58977100	-0.71456700
H	2.40496600	1.62219200	-1.02022100
H	1.42897300	-0.05557800	-1.49296600
C	3.68997800	-0.06804700	-1.52773000

C	3.97304800	0.42403600	-2.81036200
C	4.44356000	-1.12996600	-1.01040400
C	4.99016500	-0.14810000	-3.57254800
H	3.39518400	1.25662200	-3.20437100
C	5.46489800	-1.69762600	-1.77346800
H	4.23927000	-1.49259100	-0.00835300
C	5.73714600	-1.21174600	-3.05541300
H	5.20517400	0.23729700	-4.56474000
H	6.05060400	-2.51646500	-1.36619200
H	6.53211400	-1.65551200	-3.64744500



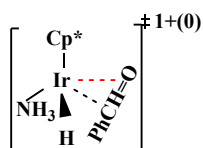
7

E=-896.7503022(au)

C	2.57460100	0.58860200	-0.81620300
C	2.78361400	-0.46947100	0.07722600
C	2.01572400	-0.19604800	1.30624400
C	1.67691600	1.55460700	-0.17541200
C	1.44789400	1.13834600	1.17750000
Ir	0.33230100	-0.29692200	-0.05305100
N	-0.18092000	-2.38349900	-0.08193200
H	0.65196100	-2.96646100	0.00114100
H	-0.81833900	-2.64019600	0.66891500
H	-0.63899100	-2.60230200	-0.96671500
C	3.60496500	-1.70130900	-0.13496100
H	4.53129600	-1.64358700	0.45012700

H	3.07152300	-2.59678500	0.20017600
H	3.87791700	-1.83515200	-1.18376700
C	3.11164400	0.74328500	-2.20359800
H	2.33569100	1.09402300	-2.89081100
H	3.91501300	1.49055900	-2.21952300
H	3.51655400	-0.19364200	-2.59117100
C	1.30436800	2.87722400	-0.77168900
H	0.47406700	3.34171100	-0.23607300
H	2.16034100	3.56213000	-0.72544200
H	1.02434500	2.77648500	-1.82409500
C	0.85717300	1.96214900	2.28134300
H	0.40159700	1.33431600	3.04978500
H	1.65017600	2.55324400	2.75616600
H	0.10007000	2.65622200	1.90977100
C	2.16879800	-0.97152200	2.58126700
H	2.19374900	-2.04801200	2.39108900
H	3.10913000	-0.70099600	3.07746700
H	1.35001900	-0.76615000	3.27439000
O	-0.84580300	-0.32731500	-1.89028600
C	-1.47662800	0.55347100	-1.16723500
H	-1.22920800	1.61242700	-1.31125700
H	-0.73804900	-0.28108800	1.09450300
C	-2.80590200	0.29565400	-0.56604900
C	-3.45675200	1.34880700	0.09660100
C	-3.43402200	-0.95737600	-0.65101400
C	-4.70052600	1.14601800	0.69266000
H	-2.97808200	2.32339300	0.15026100

C	-4.68065500	-1.15508800	-0.05993200
H	-2.94506900	-1.76869300	-1.18102900
C	-5.31360200	-0.10820000	0.61968300
H	-5.19169100	1.96421300	1.21111600
H	-5.16215700	-2.12630000	-0.12766800
H	-6.28185700	-0.26826800	1.08482300



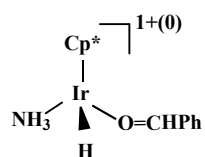
TS_{7,8}

E=-896.7498699(au)

C	-2.33222400	1.61905100	0.83643300
C	-2.81752400	1.16081200	-0.39774200
C	-3.71377900	0.01682600	-0.14251500
C	-2.87923500	0.76035200	1.89211800
C	-3.64035300	-0.28595800	1.28251600
Ir	-4.75072200	1.56695500	0.90396100
N	-5.95149600	2.54189000	-0.59695700
H	-5.40375100	2.74237700	-1.43351900
H	-6.75306200	1.98221600	-0.87963500
H	-6.30324400	3.42724300	-0.23289900
C	-2.52958700	1.70817800	-1.75935100
H	-1.78904600	1.07644000	-2.26589000
H	-3.42719400	1.71315100	-2.38533900
H	-2.13218800	2.72447100	-1.71635200
C	-1.43686400	2.79065100	1.09207600
H	-1.80616100	3.39451800	1.92651200

H	-0.42812400	2.45188400	1.35903200
H	-1.35323300	3.43462400	0.21413600
C	-2.51082700	0.87447800	3.33913900
H	-3.19385100	0.30785500	3.97530900
H	-1.49847200	0.48275800	3.50026800
H	-2.51390800	1.91692500	3.66997400
C	-4.18214200	-1.50963400	1.95626700
H	-5.07691300	-1.88068400	1.45233000
H	-3.42796900	-2.30605100	1.93288700
H	-4.43122100	-1.31518900	3.00179200
C	-4.25603600	-0.89326300	-1.20310200
H	-4.58012100	-0.33335200	-2.08410800
H	-3.48098100	-1.60057800	-1.52432700
H	-5.10640700	-1.47115500	-0.83354800
O	-5.21310800	3.55087300	1.97195500
C	-5.70613800	2.86117800	2.91825400
H	-5.03530000	2.44287700	3.68131900
H	-6.13534600	0.88226400	1.27869200
C	-7.14309600	2.77757700	3.20737900
C	-7.55706100	2.07698400	4.35260100
C	-8.09842000	3.41429300	2.39512100
C	-8.91091800	1.99811500	4.67363800
H	-6.81312500	1.59873300	4.98431900
C	-9.44851600	3.33306400	2.71948800
H	-7.77401400	3.96937800	1.52095400
C	-9.85691600	2.62314500	3.85613600
H	-9.22852400	1.45448300	5.55801500

H	-10.18726800	3.82268500	2.09226400
H	-10.91233400	2.56199200	4.10450600

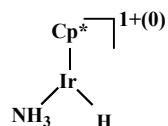


8

E=-896.7557096(au)

C	-1.23272700	0.97770000	1.47739300
C	-2.16385300	-0.07370800	1.51297300
C	-2.90091300	-0.07647500	0.23741900
C	-1.38600800	1.68947000	0.19861000
C	-2.48594100	1.09903000	-0.51026000
Ir	-0.88745500	-0.38027000	-0.44831200
N	-0.59330500	-2.54014800	-0.37120200
H	-0.99448200	-2.93498300	0.47894100
H	-1.01203000	-3.02719600	-1.16026000
H	0.40441500	-2.75382000	-0.37362200
C	-2.37835300	-1.07978100	2.59994000
H	-3.30983100	-0.86416000	3.13834100
H	-2.47302800	-2.09144500	2.19178300
H	-1.56304700	-1.07689200	3.32652000
C	-0.22920500	1.35617100	2.52072800
H	0.75874900	1.52198600	2.07852100
H	-0.52239300	2.29498000	3.00715500
H	-0.13418100	0.59157800	3.29466800
C	-0.69688900	2.97563300	-0.14631000
H	-0.67740000	3.14503900	-1.22563100

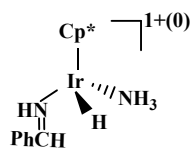
H	-1.21971200	3.82365900	0.31508200
H	0.33336300	2.99231600	0.22004300
C	-3.13976200	1.63926600	-1.74557900
H	-3.58905200	0.84423900	-2.34489000
H	-3.93800300	2.33756300	-1.46414100
H	-2.42815300	2.18135400	-2.37273900
C	-4.10655100	-0.92220700	-0.04547100
H	-3.97266600	-1.94264200	0.32423400
H	-4.99311000	-0.50413000	0.44858900
H	-4.31394800	-0.97379000	-1.11724900
O	1.34284800	-0.55392000	-0.50434300
C	2.16773300	0.37301600	-0.43333800
H	1.83055000	1.41258700	-0.53567400
H	-0.88004900	-0.59218500	-2.03293800
C	3.59062500	0.15714200	-0.21359400
C	4.43752200	1.27942200	-0.17038100
C	4.12132200	-1.13488200	-0.02847900
C	5.80174000	1.11274100	0.05520400
H	4.01728200	2.27132200	-0.31152100
C	5.48278200	-1.29366400	0.19747300
H	3.45990700	-1.99466100	-0.06034800
C	6.32206300	-0.17156600	0.23962700
H	6.45742100	1.97682800	0.08989000
H	5.89713400	-2.28620900	0.34365000
H	7.38514000	-0.30200800	0.41901900



E=-551.313373(au)

C	-1.54040000	-0.49309300	0.32266900
C	-1.38367700	0.60494800	-0.58982600
C	-0.53549700	1.63431500	0.03695900
C	-0.61811000	-0.24007400	1.41735000
C	-0.08404200	1.12663600	1.26278800
Ir	0.49318400	-0.45397300	-0.38752900
N	2.65515200	-0.46862600	-0.79480900
H	2.80905900	-0.52244800	-1.80264500
H	3.15210400	0.34991500	-0.44790400
H	3.09064700	-1.29430600	-0.38637100
C	-2.10692000	0.78903200	-1.88479900
H	-3.00360800	1.40137900	-1.72486400
H	-1.48212500	1.30500100	-2.61885500
H	-2.42348200	-0.16723100	-2.30678600
C	-2.49931700	-1.63739400	0.19849400
H	-2.11910700	-2.53408700	0.69330100
H	-3.45779000	-1.37774000	0.66453100
H	-2.69274900	-1.88448700	-0.84800800
C	-0.47513700	-1.07396800	2.64984600
H	0.52423200	-0.98136200	3.08228100
H	-1.19905600	-0.74382600	3.40646700
H	-0.66650500	-2.12873400	2.44003400
C	0.79963100	1.79914700	2.26286600
H	1.34852200	2.63535600	1.82490800
H	0.19187100	2.19106200	3.08848700

H	1.51907200	1.09829800	2.69523400
C	-0.24513600	2.97299400	-0.56313700
H	-0.06550300	2.89983300	-1.63941000
H	-1.10363700	3.64195200	-0.42225300
H	0.62460800	3.44379900	-0.09978200
H	0.52386200	-1.99135200	-0.87423300



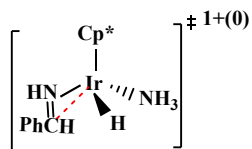
10

E=-876.8857589(au)

C	-2.95958000	-0.26265600	0.17153100
C	-2.62177400	0.45941900	-1.02763400
C	-1.70812200	1.51695200	-0.66136100
C	-2.36616200	0.45514100	1.30704300
C	-1.61641400	1.53925400	0.80301000
Ir	-0.77447500	-0.43416100	-0.18473900
N	-0.29138800	-2.26519900	0.88720800
H	-0.59200600	-3.09641800	0.38285600
H	0.70798400	-2.36697700	1.06549100
H	-0.76047000	-2.27427600	1.79285500
C	-3.16852300	0.20045000	-2.39924500
H	-4.07944000	0.79289700	-2.55184700
H	-2.45490900	0.48159100	-3.17683400
H	-3.42978900	-0.85128500	-2.53625800
C	-3.96691000	-1.36828100	0.28982900
H	-3.71599200	-2.05204200	1.10550600

H	-4.96540800	-0.96153500	0.49584500
H	-4.02912200	-1.95099500	-0.63266900
C	-2.55853900	0.06444000	2.73957300
H	-1.82110500	0.53720200	3.39198400
H	-3.55608400	0.36413700	3.08494100
H	-2.48722200	-1.02017000	2.87090700
C	-0.83642700	2.55407100	1.58066700
H	0.14912300	2.72867900	1.13614400
H	-1.36206300	3.51723400	1.58262800
H	-0.69289700	2.24743100	2.61912900
C	-1.18988500	2.59468400	-1.56790200
H	-1.07934800	2.23515600	-2.59400200
H	-1.87862300	3.44918500	-1.58570700
H	-0.21697500	2.96440300	-1.23238900
H	-0.45575100	-1.31680800	-1.47824300
C	2.31987400	-0.67846900	-0.35812900
H	2.17386300	-1.69988400	-0.70833700
N	1.25713800	0.02350700	-0.14714100
H	1.43924900	0.98025200	0.16011700
C	3.70726700	-0.25301800	-0.16925100
C	4.71847200	-1.18823800	-0.45672400
C	4.07145500	1.02530900	0.29802000
C	6.06093500	-0.85728400	-0.28292000
H	4.44182400	-2.17607400	-0.81416400
C	5.41284600	1.35188900	0.46865700
H	3.31280000	1.76625600	0.53243300
C	6.41072200	0.41310700	0.18005500

H	6.83141200	-1.58885000	-0.50569800
H	5.68403600	2.33901800	0.83012500
H	7.45580100	0.67350000	0.31828300

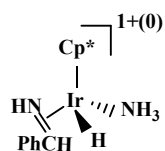


TS_{10,11}

E=-876.8661455(au)

C	0.84507000	1.84383000	0.39685300
C	1.42319200	1.22243500	-0.78884300
C	1.90686000	-0.06522500	-0.39416200
C	1.17584900	0.98854700	1.55147700
C	1.80165500	-0.17011400	1.06979600
Ir	-0.32310300	0.11225300	-0.08196800
N	-2.19532900	0.44596100	0.94271600
H	-2.70350400	-0.43806300	0.95665200
H	-2.04595800	0.74564600	1.90603200
H	-2.77874000	1.14598600	0.48997600
C	1.57329900	1.86113000	-2.13608200
H	2.52128800	2.41216600	-2.17783300
H	1.58403200	1.11653900	-2.93529500
H	0.76740800	2.57035100	-2.33700000
C	0.35487100	3.25624900	0.50182100
H	-0.39774500	3.35795200	1.28852500
H	1.18573500	3.93004200	0.74741100
H	-0.08508100	3.59650800	-0.43876800
C	0.84479700	1.33847500	2.96821800

H	0.97802300	0.48830100	3.64031000
H	1.49301400	2.15144500	3.31830600
H	-0.18765400	1.69183300	3.06180200
C	2.27451300	-1.35305600	1.85574800
H	1.97098400	-2.29202300	1.38206300
H	3.37044600	-1.36193000	1.91000200
H	1.88856400	-1.34423300	2.87720300
C	2.64402000	-1.03991700	-1.26150100
H	2.32652200	-0.96860200	-2.30407900
H	3.72238800	-0.83738100	-1.22478100
H	2.49264400	-2.06891600	-0.92551500
H	-1.17700900	0.51524600	-1.36392300
C	-0.84280300	-2.46656500	-1.03843300
H	0.12122200	-2.95236500	-1.21797700
N	-1.20975900	-2.14197900	0.17633200
H	-0.48500100	-2.44583000	0.82996100
C	-1.70527800	-2.36147100	-2.22165900
C	-1.17419700	-2.75203400	-3.46233700
C	-3.04324800	-1.93075000	-2.15112400
C	-1.95415100	-2.69263200	-4.61722900
H	-0.14573000	-3.09952800	-3.51471400
C	-3.81946300	-1.87501500	-3.30401600
H	-3.46409900	-1.64404000	-1.19283800
C	-3.27663000	-2.25151300	-4.54011700
H	-1.53238300	-2.99264700	-5.57166300
H	-4.85137800	-1.54198500	-3.24518200
H	-3.88758900	-2.20632300	-5.43683400

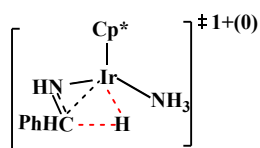


11

E=-876.871778(au)

C	2.14139900	-0.15401700	1.25970900
C	1.66980400	1.20435000	1.05043700
C	1.75087000	1.46917100	-0.35997200
C	2.67112100	-0.63963800	-0.02086100
C	2.43645900	0.34510700	-1.00139700
Ir	0.32631600	-0.23018600	0.04265100
N	-0.33217800	-2.27309300	0.19154400
H	-1.01929100	-2.42592400	0.92652600
H	-0.75994000	-2.53844100	-0.69525700
H	0.45610400	-2.89563100	0.36593400
C	1.26809700	2.17727900	2.11731900
H	2.14663300	2.74724200	2.44402500
H	0.52434400	2.88922000	1.75286800
H	0.85728100	1.66705400	2.99094300
C	2.38180500	-0.81265800	2.58515700
H	2.29425400	-1.89993300	2.51273900
H	3.39297000	-0.58414300	2.94446400
H	1.67211700	-0.46286000	3.33843300
C	3.34462600	-1.96276800	-0.20084300
H	3.41364900	-2.24545400	-1.25319000
H	4.36260600	-1.92184200	0.20630800
H	2.81707700	-2.75621000	0.33735300
C	2.81492100	0.30356500	-2.44792600

H	2.01689000	0.69951400	-3.08372800
H	3.70128400	0.92709800	-2.62029900
H	3.04933400	-0.71043200	-2.77800600
C	1.42649200	2.76152700	-1.04431900
H	0.72366500	3.35888500	-0.45998400
H	2.34027900	3.35334500	-1.17979300
H	0.99595300	2.59236800	-2.03556300
H	-0.74612600	-0.01335300	1.18309500
C	-1.50197900	0.59796700	-1.13463700
H	-1.29454500	1.66009000	-1.27910200
N	-0.83914400	-0.32949100	-1.85134200
H	-0.17352100	0.13694700	-2.47115000
C	-2.82181900	0.30313900	-0.52589800
C	-3.49860100	1.32812800	0.15473800
C	-3.44016400	-0.95192400	-0.65202600
C	-4.75350100	1.09892400	0.71813300
H	-3.03359300	2.30693500	0.24208000
C	-4.69502000	-1.17911100	-0.08871200
H	-2.94084800	-1.74165300	-1.20333900
C	-5.35487500	-0.15754200	0.60194400
H	-5.26410800	1.90095700	1.24313100
H	-5.16382600	-2.15317300	-0.19627900
H	-6.33353400	-0.33716900	1.03715200

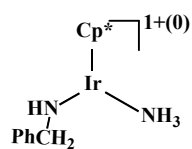


TS_{11,12}

E=-876.8608919(au)

C	-1.39445500	0.74296900	-0.94273900
C	-0.77665000	1.57961800	0.07021100
C	-0.85263600	0.87613500	1.33662600
C	-1.74294800	-0.50679000	-0.33746800
C	-1.40049600	-0.42121800	1.08915300
Ir	0.45439500	-0.27924900	-0.12492200
N	1.01732400	-2.37617500	-0.06514700
H	1.85391800	-2.60496700	-0.60135700
H	1.17767400	-2.68051800	0.89438100
H	0.25564100	-2.94156400	-0.43812600
C	-0.33760700	3.00079100	-0.11225500
H	-1.17663900	3.68675400	0.05946800
H	0.45465600	3.26476300	0.59279000
H	0.03403000	3.17853300	-1.12431500
C	-1.63685100	1.13876400	-2.36600400
H	-1.66406400	0.27077500	-3.02829700
H	-2.60387300	1.65104900	-2.44561000
H	-0.86978200	1.82652800	-2.72928500
C	-2.47207000	-1.64663300	-0.98020500
H	-2.13808100	-2.61032000	-0.58406800
H	-3.54911900	-1.56840800	-0.78578000
H	-2.32618200	-1.65459500	-2.06304500
C	-1.71573100	-1.47105200	2.10952700
H	-1.06352200	-1.39452200	2.98262100
H	-2.75186600	-1.36195700	2.45417200
H	-1.61326500	-2.47652900	1.69297800

C	-0.44114900	1.43226400	2.66314600
H	0.41910700	2.09970600	2.57003300
H	-1.26584900	2.01621100	3.09094100
H	-0.19038600	0.64145300	3.37363000
H	1.44639500	-0.26682200	-1.51104600
C	2.63788800	0.27390600	-0.87266000
H	2.51009600	1.30040500	-1.21344800
N	2.50503900	0.11386200	0.49408700
H	2.92866000	-0.77110600	0.77773600
C	3.62788100	-0.48032400	-1.71761000
C	3.91120000	0.01716500	-2.99915100
C	4.28679300	-1.63667100	-1.27549700
C	4.82748700	-0.63043400	-3.82623600
H	3.40854000	0.91784700	-3.34285500
C	5.20570000	-2.28403300	-2.10428600
H	4.09828300	-2.03633600	-0.28255700
C	5.47639000	-1.78579400	-3.38068200
H	5.03759100	-0.23304800	-4.81476700
H	5.71159200	-3.17705000	-1.74966800
H	6.19147200	-2.29149100	-4.02265900



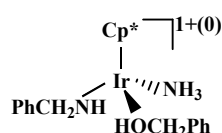
12

E=-876.8980341(au)

C	1.38127300	0.17145500	1.70058400
C	0.65735200	1.27739900	1.07312700

C	1.41181000	1.69161000	-0.07220200
C	2.59848900	-0.04189600	0.96393900
C	2.61343100	0.85970600	-0.14735200
Ir	0.76604000	-0.39373000	-0.34460000
N	1.13086800	-2.47263600	-0.91974000
H	0.83639400	-2.68705400	-1.87239000
H	2.12315800	-2.69368000	-0.85033900
H	0.63693300	-3.11470800	-0.30048500
C	-0.57169300	1.93133900	1.62291000
H	-0.28863600	2.66713300	2.38611800
H	-1.13093900	2.45583100	0.84529500
H	-1.23674800	1.20435200	2.09501500
C	0.99221400	-0.49700300	2.98107800
H	1.39217600	-1.51164100	3.04461600
H	1.38773300	0.07168500	3.83290200
H	-0.09357200	-0.54708500	3.09314200
C	3.65105000	-1.05803600	1.28725600
H	4.17381200	-1.39552200	0.38881300
H	4.39996500	-0.62491800	1.96155800
H	3.22560100	-1.93251500	1.78555500
C	3.70642400	1.01676500	-1.15707600
H	3.31143700	1.32103400	-2.12949800
H	4.41356200	1.78952000	-0.82901700
H	4.26705800	0.08856900	-1.29039500
C	1.10384800	2.84131400	-0.97908500
H	0.03532200	3.06802600	-0.99030000
H	1.63351700	3.73916700	-0.63685900

H	1.42465100	2.63928200	-2.00432700
C	-1.95287500	0.32129800	-1.55895900
H	-2.27837600	0.27523800	-2.60964300
H	-1.58694300	1.33850900	-1.39619200
N	-0.85163200	-0.60916800	-1.36373200
H	-1.05829100	-1.52110900	-1.76568200
C	-3.17603200	0.09353100	-0.67789300
C	-4.01939300	1.17624300	-0.38745300
C	-3.51503400	-1.17139400	-0.18010200
C	-5.17316100	1.00138700	0.37906900
H	-3.76814200	2.16423100	-0.76660200
C	-4.66744500	-1.34871500	0.59133400
H	-2.87593100	-2.02387800	-0.39153300
C	-5.50094200	-0.26423200	0.87367000
H	-5.81178100	1.85356200	0.59477400
H	-4.91268700	-2.33649800	0.97193500
H	-6.39490800	-0.40234300	1.47497000



13

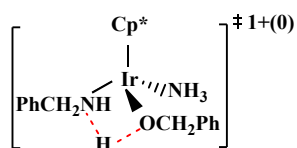
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C	-3.87728500	0.28396700	-0.23407500
C	-3.17538000	1.12665700	1.83863400
C	-3.89160100	0.06746300	1.21317900

Ir	-4.92018000	1.95543700	0.62750200
N	-6.00463500	3.02178700	-0.84703800
H	-6.94485800	3.16375400	-0.47390100
H	-5.32102900	3.43763900	3.63556300
H	-3.97924700	4.36723500	2.93527600
N	-6.92340700	1.44638800	1.34223300
H	-7.53839900	1.17335600	0.57680300
H	-6.91213400	0.68189500	2.01564200
H	-7.33635400	2.26163300	1.79604800
C	-2.58660200	1.96636000	-1.81247400
H	-1.54567100	1.65217400	-1.96069600
H	-3.17276900	1.55792000	-2.63717900
H	-2.61287600	3.05727500	-1.87210000
C	-1.84254000	3.22846400	0.98973300
H	-2.04215800	3.71110000	1.94897300
H	-0.78618500	2.93080400	0.98491700
H	-1.98458000	3.96425300	0.19511100
C	-2.88964200	1.27672900	3.30078000
H	-3.64038200	0.76922700	3.91141300
H	-1.91327100	0.83752900	3.54223000
H	-2.85910100	2.32703700	3.59983500
C	-4.53714400	-1.09626400	1.89719900
H	-5.44425200	-1.41267200	1.37566800
H	-3.84793100	-1.94963400	1.90498300
H	-4.79441300	-0.86496000	2.93363400
C	-4.36041200	-0.69300500	-1.26175400
H	-4.58660400	-0.19771000	-2.20895000

H	-3.59342300	-1.45356000	-1.45612300
H	-5.26345800	-1.20852000	-0.92459500
C	-5.06921600	4.27270300	2.97917700
O	-5.57376600	3.92812400	1.66653700
H	-5.22231700	4.58783900	1.00027000
C	-6.17395300	2.44039200	-2.19015100
H	-5.18467400	2.33465800	-2.64524200
H	-6.61846100	1.43410600	-2.15758100
O	-4.72854500	5.25463400	-0.46172800
H	-5.25124700	4.39819300	-0.77180800
H	-5.33854700	5.98831100	-0.62707500
C	-7.03530100	3.32433500	-3.07562300
C	-8.30856200	2.91005100	-3.48723000
C	-6.57750400	4.58798400	-3.48389900
C	-9.10681800	3.73156500	-4.28985200
H	-8.67676100	1.93403200	-3.17956000
C	-7.37064100	5.41070200	-4.28436600
H	-5.59553300	4.92802300	-3.16519500
C	-8.63982000	4.98457700	-4.69042800
H	-10.09106700	3.39184500	-4.60040600
H	-6.99901200	6.38362000	-4.59431800
H	-9.25701800	5.62475200	-5.31439100
C	-5.69452000	5.55366200	3.47916600
C	-6.70118500	5.52880800	4.45279800
C	-5.28275000	6.79056700	2.95896700
C	-7.28801900	6.71591300	4.89935500
H	-7.02225100	4.57577400	4.86574100

C	-5.87207500	7.97651600	3.39787000
H	-4.50153100	6.81870500	2.20314100
C	-6.87558100	7.94144400	4.37140400
H	-8.06475500	6.68324200	5.65802100
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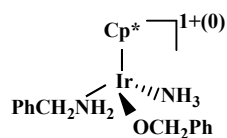
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C	-3.22549800	1.08247300	1.86954300
C	-3.95481300	0.05551200	1.19961000
Ir	-4.90495600	1.98369300	0.63598500
N	-5.99489100	3.05660100	-0.86058200
H	-6.96471000	3.10289400	-0.54432900
H	-5.14042900	3.50413200	3.64527300
H	-3.89072500	4.45784700	2.81790300
N	-6.91789400	1.49538800	1.33197500
H	-7.52636300	1.19093100	0.57305300
H	-6.91360100	0.75896800	2.03593800

H	-7.33103700	2.32969400	1.74999600
C	-2.49325500	1.95569100	-1.74678700
H	-1.46898300	1.58380700	-1.87720800
H	-3.08105700	1.59801000	-2.59349300
H	-2.45412800	3.04707600	-1.78380200
C	-1.76687800	3.12872100	1.09815400
H	-1.96888700	3.60614800	2.05934200
H	-0.72773900	2.77605500	1.11810300
H	-1.84587900	3.88261700	0.31157100
C	-2.97964600	1.19366700	3.34265100
H	-3.76391000	0.69670100	3.91858000
H	-2.02461500	0.72014400	3.60350800
H	-2.92809300	2.23647600	3.66454900
C	-4.66534200	-1.09216300	1.84473400
H	-5.53458600	-1.40397200	1.26037800
H	-3.98824900	-1.95233200	1.91402400
H	-4.99657900	-0.84678100	2.85676000
C	-4.36409700	-0.64735500	-1.30097400
H	-4.53683400	-0.12963900	-2.24698700
H	-3.61537900	-1.42968600	-1.47937600
H	-5.29535900	-1.13856800	-1.00716100
C	-4.97016800	4.32368600	2.94427400

O	-5.55693900	3.92473400	1.68398000
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C	-6.02943700	2.55875200	-2.25076100
H	-5.01792300	2.63126700	-2.66029300
H	-6.32159400	1.50162000	-2.29163700
O	-5.00087400	5.30876300	-0.39743200
H	-5.48000400	4.31510500	-0.73772100
H	-5.70095700	5.96950000	-0.50340200
C	-6.98422200	3.36290300	-3.11447300
C	-8.16692800	2.78715100	-3.59682600
C	-6.71148900	4.70373300	-3.43211600
C	-9.05769200	3.52721300	-4.38027300
H	-8.38942000	1.74944400	-3.35948900
C	-7.59849400	5.44551300	-4.21329800
H	-5.80365500	5.16763400	-3.05551700
C	-8.77531100	4.85870100	-4.69050500
H	-9.96932500	3.06315700	-4.74635600
H	-7.37225300	6.48097000	-4.45252100
H	-9.46485900	5.43618000	-5.29964000
C	-5.60631800	5.59725300	3.45134700
C	-6.59376200	5.55980600	4.44449300
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C	-7.19616900	6.73803100	4.89351200
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C	-5.83289600	8.01579300	3.35821900
H	-4.46644400	6.87627300	2.14179400
C	-6.81749600	7.96793200	4.35002700
H	-7.95758200	6.69563600	5.66710400
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H	-7.28435300	8.88469700	4.69843300



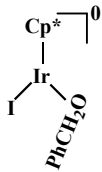
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C	-3.26151100	1.11587400	1.90716300
C	-3.85149200	0.08998200	1.07503700
Ir	-4.87535800	2.01574600	0.69651300
N	-6.01114400	3.03036700	-0.87765300
H	-6.83377700	3.42589600	-0.41895100
H	-5.50692600	3.29915100	3.60538300
H	-4.07375400	4.16095700	3.02696700
N	-6.86308200	1.45189100	1.38209200
H	-7.50197300	1.22028600	0.62210500
H	-6.84829400	0.66204500	2.02491800

H	-7.23229400	2.26745100	1.87255300
C	-2.44289500	2.40560300	-1.56329000
H	-1.48290700	1.97764800	-1.87807900
H	-3.14380200	2.28851200	-2.39420100
H	-2.29207600	3.47214300	-1.38486200
C	-1.84185800	3.28465600	1.43412100
H	-1.98860300	3.52649300	2.48822700
H	-0.77869000	3.05399600	1.29180100
H	-2.07208100	4.17178800	0.83986100
C	-3.11509000	1.06557800	3.39734800
H	-3.94753800	0.53160400	3.86244300
H	-2.19011200	0.54397100	3.67449600
H	-3.07205700	2.06778000	3.83013200
C	-4.51802000	-1.15626800	1.56767000
H	-5.26979800	-1.51509900	0.86069400
H	-3.77115400	-1.95000100	1.69213400
H	-4.99915500	-1.00148400	2.53686700
C	-3.99462400	-0.40456700	-1.49033800
H	-4.09579400	0.19253800	-2.39901000
H	-3.19363100	-1.13424200	-1.66487200
H	-4.92280600	-0.96217500	-1.34072200
C	-5.16931600	4.10274600	2.93216500
O	-5.55575800	3.83947600	1.59184900
H	-4.75299900	4.88473800	0.54585500
C	-6.44505800	2.29289700	-2.09638900
H	-5.54641000	1.93520300	-2.60169700
H	-7.02091100	1.42314000	-1.76852500

O	-4.28581300	5.41394900	-0.16173900
H	-5.44087600	3.83984200	-1.14003000
H	-4.79211300	6.23680000	-0.20862200
C	-7.26528000	3.16235100	-3.02449700
C	-8.64651100	3.30683900	-2.82879700
C	-6.65110100	3.86806600	-4.06855900
C	-9.39793800	4.14240100	-3.65728200
H	-9.13339400	2.75826700	-2.02588100
C	-7.40096900	4.70317800	-4.89983500
H	-5.58194700	3.75781400	-4.23223500
C	-8.77596300	4.84314700	-4.69455100
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H	-6.91300700	5.24078400	-5.70781600
H	-9.36063200	5.49086200	-5.34139800
C	-5.76441100	5.41797400	3.40427200
C	-6.79332600	5.44718000	4.35407200
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C	-6.86265300	7.86542600	4.26084700
H	-8.13313100	6.66569400	5.52453800
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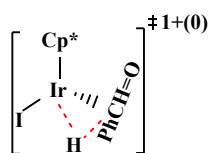


I-5

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C	1.09850300	-2.35553800	-0.45844000
C	2.07829600	-1.50433200	-1.12458800
Ir	0.61491800	-0.29626400	-0.04865500
C	2.73294200	-0.60772200	2.48433200
H	3.51479600	-1.27431300	2.87012800
H	3.15648100	0.39582800	2.40662300
H	1.92377500	-0.58635900	3.21800300
C	0.44359900	-2.79518900	2.04345500
H	-0.52669100	-3.14943400	1.68870200
H	1.01401600	-3.66616100	2.39003900
H	0.28072800	-2.13986000	2.90235900
C	0.21917400	-3.36817200	-1.11848200
H	-0.08481400	-3.04324000	-2.11659100
H	0.75860700	-4.31748900	-1.22476300
H	-0.68077800	-3.55848700	-0.52948300
C	2.34192700	-1.48089400	-2.59495700
H	2.73315700	-0.51354500	-2.91719500
H	3.08814900	-2.24585000	-2.84540800
H	1.43748700	-1.69858300	-3.16747000

C	3.97722500	0.13100700	-0.37149200
H	4.04597900	0.91263500	0.38776000
H	4.91323000	-0.44113800	-0.34786600
H	3.90612000	0.61041100	-1.35035400
O	-1.40046600	-0.33451500	-0.13107600
C	-2.24562700	0.80797800	-0.22497300
H	-2.02779500	1.53233600	0.57069900
H	-2.10447700	1.32846500	-1.18339600
C	-3.68910700	0.36338900	-0.10454700
C	-4.45376500	0.07414200	-1.24295500
C	-4.27320300	0.19204000	1.15918500
C	-5.77257100	-0.37201800	-1.12402700
H	-4.01397000	0.20822400	-2.22855500
C	-5.58996600	-0.25493200	1.28384900
H	-3.69197100	0.42053600	2.04971900
C	-6.34330600	-0.53852500	0.14057900
H	-6.35467400	-0.58587500	-2.01617600
H	-6.03027100	-0.37634900	2.26972200
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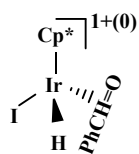
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C	-2.06519700	-1.87457000	0.23035000
C	-2.10963400	-0.96762300	1.36437800
Ir	-0.58521000	-0.29107100	-0.08725500
C	-3.24031300	1.32451000	-1.44146000
H	-4.33433900	1.38212500	-1.37351300
H	-2.83903100	2.29489100	-1.13988800
H	-2.98031700	1.15962400	-2.48982900
C	-2.63399600	-1.71010800	-2.32005900
H	-1.90479200	-2.50288200	-2.50320300
H	-3.63371700	-2.14967000	-2.42665000
H	-2.51961900	-0.94740500	-3.09330200
C	-1.82494800	-3.34893200	0.30338500
H	-1.13965200	-3.60079500	1.11620900
H	-2.77115200	-3.87201000	0.49226900
H	-1.41095500	-3.73678100	-0.63037000
C	-1.89398400	-1.33204500	2.80048900
H	-1.47357800	-0.49687400	3.36544400
H	-2.85213700	-1.59944300	3.26322100
H	-1.22295500	-2.18750600	2.90111800
C	-2.76937000	1.53199000	1.71033200
H	-2.61720400	2.45525400	1.14912800
H	-3.81632700	1.50703800	2.03894300
H	-2.14004900	1.56301500	2.60216100
O	0.90964500	-0.74167100	-1.61283300
C	1.47426000	-1.36069200	-0.59888900
H	1.17414100	-2.39881000	-0.40549500

H	0.82694000	-0.73052800	0.72621100
C	2.89998400	-1.09301800	-0.24481600
C	3.53011900	-1.91055500	0.70519100
C	3.63891100	-0.10860900	-0.91351500
C	4.88356300	-1.74075300	0.99008600
H	2.95612000	-2.68265100	1.21190400
C	4.99734500	0.05089500	-0.63549000
H	3.15099300	0.50929100	-1.65944400
C	5.62053900	-0.76069400	0.31683900
H	5.36569700	-2.37700800	1.72629900
H	5.57203300	0.80441000	-1.16592300
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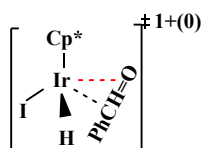
I-7

E=-851.7786128(au)

C	-2.60249600	-1.05402600	-0.85243500
C	-2.83402800	-0.12725600	0.16730000
C	-2.02479500	-0.50721100	1.34372200
C	-1.64255200	-2.04040400	-0.34989100
C	-1.40207800	-1.78629400	1.05125000
Ir	-0.36464300	-0.22276900	-0.02476400
C	-3.74468000	1.05609300	0.13390100
H	-4.68431000	0.81097300	0.64612800
H	-3.30731100	1.91125600	0.65525700

H	-3.98928100	1.35842400	-0.88651100
C	-3.16706100	-1.06573600	-2.23794200
H	-2.38432300	-1.24722500	-2.98100500
H	-3.90542500	-1.87029800	-2.34517700
H	-3.66095000	-0.12288700	-2.48186800
C	-1.24078300	-3.26367900	-1.11205000
H	-0.41416200	-3.79058600	-0.63233500
H	-2.09245600	-3.95324600	-1.16877800
H	-0.95298400	-3.01650900	-2.13796900
C	-0.76694200	-2.72670400	2.02883500
H	-0.36751300	-2.19387400	2.89422700
H	-1.51579000	-3.44302000	2.38971200
H	0.04596300	-3.29520200	1.57096400
C	-2.19225200	0.09302800	2.70806700
H	-2.27692000	1.18131900	2.65804300
H	-3.10552500	-0.29274000	3.17867100
H	-1.34959000	-0.15420200	3.35759600
O	0.88218300	-0.25440600	-1.91862400
C	1.45512000	-1.11809400	-1.14321800
H	1.18262700	-2.17605300	-1.24189100
H	0.72297600	-0.24367300	1.10574600
C	2.78868900	-0.88349800	-0.53563900
C	3.40030900	-1.93201400	0.16965300
C	3.46343400	0.34004300	-0.67244100
C	4.65350800	-1.75371800	0.75382800
H	2.88488900	-2.88502100	0.26131800
C	4.71783400	0.51477600	-0.09006500

H	3.00210900	1.14510300	-1.23453400
C	5.31332900	-0.52725900	0.62933900
H	5.11649600	-2.56875800	1.30232200
H	5.23482800	1.46407000	-0.19677500
H	6.28915500	-0.38578600	1.08472000
I	0.10377800	2.71034200	-0.00934600

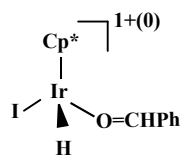


I-TS_{7,8}

E=-851.775776(au)

C	-2.60331400	-1.15562500	-0.90603000
C	-2.92590500	-0.12735600	-0.02526700
C	-2.18595300	-0.35030100	1.23948400
C	-1.66585800	-2.06421600	-0.22444900
C	-1.54509000	-1.65293900	1.15103400
Ir	-0.43901100	-0.21951500	0.00318400
C	-3.83782900	1.03337200	-0.26172200
H	-4.79269800	0.86980900	0.25460100
H	-3.41521900	1.96114700	0.13432300
H	-4.05254900	1.17716400	-1.32295300
C	-3.05173100	-1.33850000	-2.32212100
H	-2.20435900	-1.55532900	-2.98041800
H	-3.74223000	-2.18779200	-2.40000300
H	-3.56452800	-0.45352400	-2.70480400
C	-1.19936300	-3.36205000	-0.80826600
H	-0.37561100	-3.79122100	-0.23400200

H	-2.02181200	-4.08934300	-0.81173700
H	-0.87135800	-3.23656700	-1.84418800
C	-1.00609800	-2.46493400	2.28944200
H	-0.62362600	-1.82707700	3.08924800
H	-1.80837300	-3.08544100	2.70858900
H	-0.20189000	-3.13003200	1.96628600
C	-2.45659600	0.40414800	2.50710900
H	-2.55108300	1.47694600	2.32144500
H	-3.39617500	0.05849900	2.95747600
H	-1.65851400	0.25379500	3.23791300
O	1.08570500	-0.30760800	-1.87601800
C	1.72803200	-1.14800400	-1.19059300
H	1.39478400	-2.19567400	-1.16449000
H	0.73988400	-0.32259000	1.04265100
C	3.02944800	-0.88483400	-0.55865400
C	3.64969700	-1.92585300	0.15230700
C	3.66457300	0.36467100	-0.66403400
C	4.88029700	-1.71557500	0.77072400
H	3.15794100	-2.89273100	0.22109700
C	4.89631400	0.56918500	-0.04882600
H	3.18804800	1.16017500	-1.22699200
C	5.50194300	-0.46702000	0.67300900
H	5.35433000	-2.51936400	1.32556000
H	5.38848800	1.53381500	-0.12723600
H	6.46030400	-0.30086000	1.15621600
I	0.10337800	2.64480600	-0.02782100

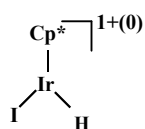


I-8

E=-851.7802119(au)

C	0.76499800	-1.90941400	1.37534100
C	1.82983900	-1.03029700	1.59669200
C	2.62245600	-0.94386500	0.35244100
C	0.85773300	-2.41082300	-0.00920800
C	2.09727500	-1.91386100	-0.57923600
Ir	0.70670300	-0.30615700	-0.44068900
C	2.14326600	-0.26575300	2.84346300
H	3.00332600	-0.71525600	3.35620100
H	2.40703700	0.77175000	2.61904200
H	1.30246700	-0.26318200	3.54061800
C	-0.34216400	-2.27169300	2.31260900
H	-1.31888100	-2.18426100	1.82400400
H	-0.24015400	-3.31471800	2.63730200
H	-0.34688700	-1.63928700	3.20294000
C	0.04039200	-3.54190200	-0.55444400
H	0.04879500	-3.55205100	-1.64703000
H	0.44781400	-4.50081800	-0.20710300
H	-0.99860300	-3.48868500	-0.21878500
C	2.75890500	-2.40478700	-1.83064400
H	3.38318800	-1.63134500	-2.28372200
H	3.40274600	-3.26145800	-1.59436400
H	2.02599500	-2.73208200	-2.57173200

C	3.94610100	-0.24891400	0.24096800
H	3.94517800	0.70412700	0.77527000
H	4.73769300	-0.87315300	0.67596000
H	4.20753300	-0.05427400	-0.80189400
O	-1.47522000	0.20780200	-0.47162500
C	-2.42133300	-0.59695000	-0.48693400
H	-2.23304500	-1.65815700	-0.69575300
H	0.78516700	-0.06012200	-2.02263400
C	-3.80112000	-0.20712000	-0.23075600
C	-4.79258600	-1.20447500	-0.25004600
C	-4.14802000	1.12808700	0.05474300
C	-6.11858200	-0.87144400	0.01606100
H	-4.51426100	-2.23161600	-0.46904300
C	-5.47295100	1.45367500	0.31678900
H	-3.37479900	1.88922300	0.06915500
C	-6.45664700	0.45500700	0.29920600
H	-6.88584500	-1.63888000	0.00479500
H	-5.74655600	2.48040600	0.53860800
H	-7.49008300	0.71532800	0.50816300
I	1.12815900	2.82749800	-0.04407900

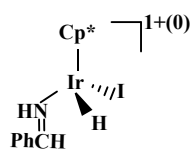


I-9

E=-506.3455846(au)

C	-1.46792300	1.49891800	-0.49612000
C	-1.27237700	1.39776800	0.88455100

C	-1.64949700	0.03150100	1.29253400
C	-1.99551800	0.21084800	-0.98866300
C	-2.24998800	-0.64125400	0.15264600
Ir	-0.14784100	-0.46037800	-0.13673700
C	-0.74427700	2.43885200	1.81884200
H	-1.56557700	2.86197100	2.41149400
H	-0.02461700	2.01388000	2.52397200
H	-0.25862600	3.25819600	1.28492900
C	-1.18978300	2.67154300	-1.38020100
H	-0.67999000	2.36653700	-2.29892000
H	-2.13331700	3.14614600	-1.67846000
H	-0.57775400	3.42486800	-0.88031500
C	-2.44809100	-0.03439400	-2.39337100
H	-2.50806400	-1.10331200	-2.61059100
H	-3.44384400	0.39942000	-2.55244800
H	-1.76713600	0.42524400	-3.11472100
C	-3.02990900	-1.91924200	0.17031500
H	-2.68429400	-2.58656900	0.96356800
H	-4.09257600	-1.71040600	0.34603600
H	-2.94554900	-2.44962000	-0.78120400
C	-1.69739100	-0.44239800	2.71097500
H	-0.84472600	-0.06946600	3.28438400
H	-2.61164100	-0.07678000	3.19678900
H	-1.70165700	-1.53336900	2.76700600
H	0.09535400	-2.03228300	-0.37995700
I	2.74710000	-0.04072000	-0.04871500

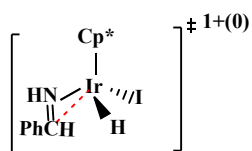


I-10

E=-831.9086103(au)

C	2.88950900	-0.45133900	0.05891600
C	2.46392000	-1.41081400	-0.91157000
C	1.46557700	-2.25792000	-0.27162800
C	2.29066600	-0.80653200	1.35592000
C	1.44139800	-1.90726600	1.15718700
Ir	0.67755000	-0.24724400	-0.35046500
C	3.00664500	-1.58754900	-2.29746400
H	3.83620800	-2.30588000	-2.27918300
H	2.24831800	-1.97533800	-2.98136300
H	3.38779100	-0.64852000	-2.70508000
C	3.97256700	0.56961900	-0.12048300
H	3.80567300	1.44624600	0.50982300
H	4.94416000	0.14126400	0.15904200
H	4.04321800	0.90465700	-1.15800800
C	2.58581900	-0.10314500	2.64386400
H	1.83920300	-0.32961400	3.40845000
H	3.56538900	-0.41272000	3.03052300
H	2.61942900	0.98144300	2.50879900
C	0.62109400	-2.62359800	2.18428900
H	-0.36809900	-2.88693200	1.79555900
H	1.11082200	-3.56196500	2.47381900
H	0.48653000	-2.02421900	3.08742400

C	0.86722300	-3.50241900	-0.85649800
H	0.74201700	-3.41218300	-1.93838600
H	1.51614700	-4.36703100	-0.66440900
H	-0.11072100	-3.71994500	-0.41845400
H	0.29490100	0.10673600	-1.85735600
C	-2.40070400	0.07045500	-0.54942500
H	-2.20335500	0.82356800	-1.30976200
N	-1.37100400	-0.50440100	-0.02586000
H	-1.59048200	-1.20975800	0.67837100
C	-3.80699600	-0.17498900	-0.23141100
C	-4.76750200	0.58552300	-0.92379800
C	-4.23877500	-1.11616900	0.72415600
C	-6.12665100	0.41229300	-0.67065100
H	-4.43737200	1.31301300	-1.66008400
C	-5.59702400	-1.28708700	0.97204500
H	-3.52042900	-1.71530700	1.27626400
C	-6.54397700	-0.52488500	0.27713600
H	-6.85734200	1.00577800	-1.21140200
H	-5.92157800	-2.01439900	1.70986700
H	-7.60243000	-0.66226600	0.47695700
I	0.50681100	2.71296000	0.16965800



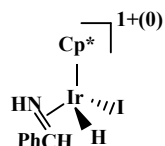
I-TS_{10,11}

E=-831.8846258(au)

C	-2.14311600	-0.45377500	1.19696400
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C	-1.31516100	-1.63980300	1.32780900
C	-1.24854600	-2.25263400	0.02455900
C	-2.74279100	-0.47163600	-0.15250100
C	-2.18734500	-1.54400700	-0.85970600
Ir	-0.35175800	-0.21087200	0.02243900
C	-0.73437000	-2.18337500	2.60038700
H	-1.44173400	-2.87430300	3.07732700
H	0.19602300	-2.72545000	2.41661400
H	-0.51634800	-1.38236100	3.30939000
C	-2.61331700	0.42769400	2.31568800
H	-2.76048000	1.45256600	1.96901100
H	-3.56411300	0.05910100	2.72359200
H	-1.88431200	0.45878200	3.12825700
C	-3.74319900	0.53380200	-0.63130800
H	-3.95570300	0.42250000	-1.69681100
H	-4.68876400	0.41987400	-0.08637500
H	-3.37914400	1.55242400	-0.46423300
C	-2.45948700	-1.93630100	-2.28176700
H	-1.53814800	-2.20192200	-2.81214600
H	-3.11245500	-2.81728000	-2.32767400
H	-2.94384200	-1.13183600	-2.83888600
C	-0.61541700	-3.57663500	-0.29409000
H	0.24944700	-3.77015900	0.34430500
H	-1.33236600	-4.39489000	-0.14145000
H	-0.28419300	-3.62942100	-1.33526400
H	0.85051500	0.04103700	1.00022300
C	1.85496500	-1.00698300	-1.40740100

H	1.86307100	-2.05253600	-1.74491400
N	0.94083100	-0.17209200	-1.83538300
H	0.33733400	-0.62005800	-2.52338500
C	3.03170000	-0.61821100	-0.62656600
C	3.93734300	-1.61721800	-0.23497700
C	3.31054000	0.72769600	-0.32287600
C	5.09479400	-1.28674000	0.46802800
H	3.73021600	-2.65586500	-0.48302500
C	4.46775000	1.05208900	0.37475900
H	2.60540800	1.49408100	-0.62659300
C	5.35998300	0.04897000	0.77450900
H	5.78788500	-2.06591600	0.77110500
H	4.67788400	2.09089000	0.61112200
H	6.26222200	0.31129400	1.31979600
I	-0.34310900	2.57063400	-0.11507800



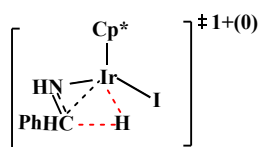
I-11

E=-831.8951173(au)

C	-2.17391900	-0.27408000	1.24689200
C	-1.57053200	-1.58443200	1.20490800
C	-1.66013000	-2.04198500	-0.16845800
C	-2.80630300	-0.02911400	-0.05986400
C	-2.48821600	-1.09258000	-0.91919700
Ir	-0.34171000	-0.27390100	-0.02778900
C	-1.08605100	-2.38325900	2.37647900

H	-1.91777400	-2.96750900	2.78984300
H	-0.29752800	-3.08198600	2.08897900
H	-0.70259100	-1.73844500	3.17010700
C	-2.44118900	0.54108200	2.47624500
H	-2.45415600	1.61029700	2.25118300
H	-3.42019800	0.27906500	2.89739900
H	-1.68716600	0.36364600	3.24636900
C	-3.65092300	1.16309800	-0.37141600
H	-3.79352000	1.29139400	-1.44635100
H	-4.64050500	1.04086000	0.08720900
H	-3.21675100	2.08018000	0.03493800
C	-2.89957100	-1.28013700	-2.34551800
H	-2.08231600	-1.69512400	-2.94359700
H	-3.73535300	-1.98847300	-2.41012300
H	-3.21869900	-0.34179400	-2.80383100
C	-1.27784500	-3.40018400	-0.66779100
H	-0.48638200	-3.84612800	-0.06226500
H	-2.14997300	-4.06476100	-0.62244400
H	-0.94547900	-3.36765600	-1.70907800
H	0.74571500	-0.24435500	1.11348400
C	1.43396000	-1.30211000	-1.03119900
H	1.20549400	-2.36903500	-1.01598700
N	0.81698100	-0.49179300	-1.91899500
H	0.13700300	-1.04088200	-2.44997200
C	2.77067100	-0.97213500	-0.47678100
C	3.39295700	-1.89672000	0.37790000
C	3.45744400	0.20314200	-0.81997800

C	4.66180400	-1.64334200	0.89774100
H	2.87441700	-2.81729400	0.63472800
C	4.72762000	0.45421200	-0.30158500
H	2.99717100	0.90969400	-1.50145300
C	5.33290300	-0.46378200	0.56241400
H	5.12844300	-2.36714900	1.55975800
H	5.24989600	1.36582400	-0.57791800
H	6.32295600	-0.26605300	0.96281400
I	0.15743400	2.71325500	0.00743800



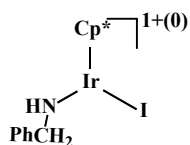
I-TS_{11,12}

E=-831.8863781(au)

C	-2.12576200	-1.18663300	1.29594000
C	-2.01845200	-1.92044600	0.03719200
C	-2.42200300	-1.03473900	-1.03160700
C	-2.51932100	0.14776000	1.00435200
C	-2.66785900	0.26230500	-0.45432700
Ir	-0.57828400	-0.25037600	-0.08265700
C	-1.72638300	-3.38426100	-0.10849400
H	-2.64959800	-3.97458600	-0.04312000
H	-1.26169600	-3.59952300	-1.07400700
H	-1.05390900	-3.74099100	0.67631800
C	-1.88942200	-1.77009100	2.65747600
H	-1.60058200	-1.00169700	3.37732900
H	-2.80173200	-2.25431100	3.02846000

H	-1.09993500	-2.52542900	2.63970300
C	-2.81751200	1.24120600	1.98393700
H	-2.40326700	2.19345100	1.64507300
H	-3.90171700	1.35954900	2.10717200
H	-2.38866000	1.02717400	2.96520700
C	-3.19461500	1.47213700	-1.16431200
H	-2.91484800	1.46994800	-2.21974500
H	-4.29041000	1.50146300	-1.10128700
H	-2.79999600	2.38887000	-0.72219600
C	-2.50732600	-1.41227900	-2.47893300
H	-1.59037300	-1.91259100	-2.80324400
H	-3.35371100	-2.08830800	-2.65103600
H	-2.64481900	-0.53292700	-3.11069500
H	0.99567800	-0.72315000	0.63486600
C	1.54173000	-1.25928600	-0.43894100
H	1.32992900	-2.31650700	-0.26013100
N	0.84644100	-0.76133000	-1.55655600
H	1.30744500	0.08477500	-1.89333000
C	3.00012100	-0.96487100	-0.17748100
C	3.76905700	-1.94577100	0.46426400
C	3.61619100	0.22841700	-0.57487800
C	5.12771600	-1.74383700	0.70355400
H	3.30009600	-2.87858200	0.76941400
C	4.97568500	0.42948100	-0.33729300
H	3.03268700	1.00971900	-1.04920900
C	5.73503500	-0.55290400	0.30146900
H	5.71071800	-2.51603400	1.19722600

H	5.44066200	1.36045700	-0.64818700
H	6.79343400	-0.39112500	0.48459900
I	0.45634200	2.32134900	0.09848600

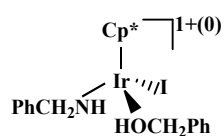


I-12

E=-831.9245004(au)

C	-0.94069600	-1.29739200	1.64232100
C	0.04900800	-2.01055900	0.84090300
C	-0.59205100	-2.39664500	-0.39672300
C	-2.18952000	-1.30733300	0.92799000
C	-1.97893400	-1.93672400	-0.33744000
Ir	-0.51908200	-0.23697800	-0.24944800
C	1.41602200	-2.40713500	1.30115200
H	1.35011800	-3.32508100	1.89915800
H	2.08441400	-2.60210900	0.46006000
H	1.86668900	-1.63402700	1.92793200
C	-0.72111800	-0.78550300	3.03113800
H	-1.38638500	0.04963600	3.26127400
H	-0.91968300	-1.58135000	3.76082900
H	0.30968100	-0.45268400	3.17602400
C	-3.48524000	-0.73768000	1.41758500
H	-4.09700800	-0.35884200	0.59562500
H	-4.06415000	-1.51604300	1.93053600
H	-3.32657900	0.07711800	2.12707400
C	-3.01166800	-2.18635100	-1.39067400

H	-2.56922400	-2.19378800	-2.38984800
H	-3.48408600	-3.16405500	-1.22948500
H	-3.79894100	-1.42937000	-1.37005600
C	-0.01718100	-3.27169500	-1.46534500
H	1.07302700	-3.20940800	-1.49253300
H	-0.28683900	-4.31809400	-1.27342100
H	-0.40271100	-3.00605300	-2.45302000
C	2.22768900	-0.05659600	-1.62919300
H	2.49322700	0.29470100	-2.63861000
H	2.11574100	-1.14119800	-1.70298200
N	0.95275800	0.52833800	-1.24327200
H	0.93444700	1.53409700	-1.38762300
C	3.39756200	0.25229900	-0.70113100
C	4.41342800	-0.69860200	-0.52715800
C	3.51455500	1.48383900	-0.04154500
C	5.51989500	-0.42794400	0.28172900
H	4.33655800	-1.65906100	-1.03155400
C	4.61780500	1.75617200	0.77156900
H	2.74017100	2.23627600	-0.16104000
C	5.62500500	0.80173400	0.93657500
H	6.29386800	-1.18027000	0.40648800
H	4.69033400	2.71585700	1.27600300
H	6.48114000	1.01328900	1.57071700
I	-1.62643700	2.46709700	-0.10040900



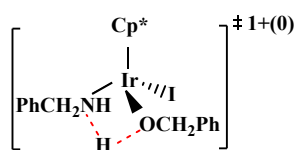
I-13

E=-1178.565974(au)

C	-1.31460700	-0.38211500	-2.26643700
C	-2.51807700	0.35294500	-1.95070800
C	-3.29717300	-0.46669500	-1.02457000
C	-1.38334200	-1.66854800	-1.57259400
C	-2.61718700	-1.72734600	-0.85503200
Ir	-1.35889500	0.06618600	-0.14989200
N	-0.34051400	1.66323500	0.28725500
H	-0.16106200	1.84853700	1.27206700
H	2.70054800	-0.28374700	-1.62325400
H	3.63877800	0.60361800	-0.40806400
C	-2.96124600	1.64720100	-2.55478500
H	-3.59107300	1.45049700	-3.43181100
H	-3.55121200	2.23686700	-1.84854400
H	-2.11188100	2.25019800	-2.88292000
C	-0.27000200	-0.00202100	-3.26706200
H	0.70775600	-0.40701300	-2.99316900
H	-0.53535200	-0.40699500	-4.25203200
H	-0.17974700	1.08223700	-3.36707000
C	-0.35590400	-2.75074700	-1.68001300
H	-0.47572600	-3.49435000	-0.88944700
H	-0.45031700	-3.26533000	-2.64462000
H	0.65725100	-2.34563500	-1.61676900
C	-3.12239700	-2.88202800	-0.04655300
H	-3.70765100	-2.54511200	0.81190900
H	-3.77379000	-3.51151900	-0.66564500

H	-2.30758400	-3.50891100	0.32202500
C	-4.64714100	-0.11132800	-0.48610800
H	-4.74115500	0.96658100	-0.33186900
H	-5.42847300	-0.41620800	-1.19442600
H	-4.84338400	-0.61307500	0.46409000
C	3.07196900	-0.31966500	-0.59062000
O	1.98486200	-0.42245600	0.34064600
H	1.36595300	0.32269200	0.19760900
C	-0.09805600	2.85677100	-0.52930700
H	-0.14558400	2.57420300	-1.58366800
H	-0.89502200	3.59714400	-0.35930600
C	1.24213900	3.50156000	-0.23383900
C	1.39387400	4.35066500	0.87227400
C	2.35769200	3.24711900	-1.04416000
C	2.63166600	4.92727200	1.16578300
H	0.53315900	4.56662600	1.50114600
C	3.59693100	3.82545300	-0.75626700
H	2.25121300	2.59921200	-1.91057700
C	3.73709300	4.66577600	0.35129500
H	2.73174200	5.58603400	2.02383500
H	4.44947800	3.62449000	-1.39909600
H	4.69886500	5.11861600	0.57444200
C	3.97219500	-1.51833700	-0.41175600
C	4.00424600	-2.54725800	-1.36118800
C	4.76660200	-1.63538400	0.73888200
C	4.81534900	-3.67000000	-1.17009800
H	3.39226900	-2.46708400	-2.25627300

C	5.57373200	-2.75623700	0.93539000
H	4.75171700	-0.84167600	1.48162000
C	5.60030100	-3.77732500	-0.02033000
H	4.83141100	-4.45878700	-1.91691200
H	6.18499600	-2.83301900	1.83023700
H	6.23010300	-4.64927100	0.13140000
I	-1.24827400	-0.65467000	2.64750300



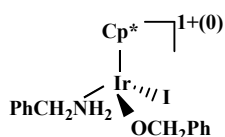
I-TS_{13,14}

E=-1178.544535(au)

C	-1.72393800	-0.14305900	-2.33280400
C	-2.23554300	1.07693500	-1.74756800
C	-3.11444000	0.71999000	-0.65831900
C	-2.36524000	-1.25595200	-1.63729200
C	-3.22311200	-0.73847900	-0.62784700
Ir	-1.12219500	-0.01840200	-0.20732400
N	0.64459900	1.09058900	0.11811700
H	0.60028400	1.54636100	1.02784800
H	0.68456000	-3.03731700	-0.83730700
H	1.31257400	-1.65373300	-1.74448100
C	-1.99742700	2.46757200	-2.24963000
H	-2.79518300	2.74968900	-2.94862400
H	-1.99840900	3.19282100	-1.43287000
H	-1.04650900	2.55367300	-2.77849200
C	-0.89243600	-0.24846000	-3.57637500

H	-0.28284700	-1.15554300	-3.57687200
H	-1.52981700	-0.27938100	-4.47007000
H	-0.21747400	0.60449700	-3.68147300
C	-2.18172800	-2.70403600	-1.97669900
H	-2.31837000	-3.34172000	-1.10091700
H	-2.91613200	-3.00901300	-2.73305700
H	-1.18862500	-2.89982000	-2.38665900
C	-4.12981900	-1.52298700	0.27082500
H	-4.18905200	-1.07190100	1.26312800
H	-5.14212200	-1.56251500	-0.15220800
H	-3.77861900	-2.54925600	0.39890700
C	-3.94890000	1.66613000	0.15033400
H	-3.48208600	2.65099600	0.21798300
H	-4.93683700	1.78843800	-0.31275900
H	-4.08546100	1.29765200	1.16848500
C	1.29889600	-2.13191900	-0.75268900
O	0.68404100	-1.29621700	0.21934700
H	1.09437900	-0.27478600	0.23374200
C	1.17612900	2.03201000	-0.87173600
H	1.25966400	1.50186600	-1.82962500
H	0.50054400	2.88325300	-1.03705800
C	2.53608800	2.57332700	-0.46581300
C	2.69494400	3.92240600	-0.12886200
C	3.65392600	1.72857800	-0.40111900
C	3.93978900	4.42264500	0.26095900
H	1.83521500	4.58754200	-0.17162400
C	4.89765700	2.22361800	-0.01254600

H	3.54852400	0.67579500	-0.65062700
C	5.04467900	3.57350300	0.31955600
H	4.04369200	5.47283300	0.51967300
H	5.75331300	1.55564500	0.03220300
H	6.01408000	3.95856700	0.62320700
C	2.71173600	-2.50453000	-0.34677300
C	3.01546100	-2.77795400	0.99399600
C	3.72525800	-2.60437300	-1.30716300
C	4.30840900	-3.14939800	1.36110000
H	2.23517900	-2.67882400	1.74199200
C	5.01909100	-2.98261300	-0.94059300
H	3.50256400	-2.38430500	-2.34922600
C	5.31318100	-3.25636900	0.39559300
H	4.53361000	-3.35352500	2.40419700
H	5.79608900	-3.05437500	-1.69668400
H	6.31983000	-3.54477200	0.68490100
I	-1.39317000	0.01253300	2.57821700



I-14

E=-1178.574148(au)

C	1.38228600	-2.62964000	-1.47650800
C	0.29899800	-2.98828300	-0.59090100
C	0.75833100	-2.80136800	0.75270200
C	2.56611300	-2.33832100	-0.66258200
C	2.17537000	-2.42651100	0.70771900

Ir	0.97033500	-0.87556800	-0.29129300
N	-0.86817400	0.27043500	-0.66710600
H	-1.58821400	0.02747900	0.01868000
H	3.44354100	0.65305000	0.79536300
H	3.59491400	1.08316100	-0.91889300
C	-1.06053900	-3.46906100	-0.99284700
H	-1.10372100	-4.56269800	-0.91947600
H	-1.84032100	-3.06338600	-0.34300700
H	-1.29459400	-3.19979900	-2.02464800
C	1.36316700	-2.70051500	-2.96927100
H	2.05643200	-1.97920600	-3.40855400
H	1.66966600	-3.70207600	-3.29704400
H	0.36433200	-2.50772200	-3.36748900
C	3.93504000	-2.06141900	-1.19649500
H	4.55929500	-1.55094900	-0.46033500
H	4.42665500	-3.00649000	-1.45855200
H	3.89519800	-1.44863800	-2.10107200
C	3.05233400	-2.22950200	1.90165600
H	2.49131900	-1.81659700	2.74373400
H	3.46818900	-3.19352500	2.22058200
H	3.88748900	-1.56103200	1.68022900
C	-0.02399400	-3.07126700	1.99699700
H	-1.09207800	-2.90493500	1.84106500
H	0.11494000	-4.11638600	2.30212700
H	0.30620000	-2.43662100	2.82242700
C	3.02687600	1.28551800	0.00004400
O	1.64611200	0.98171900	-0.20803900

H	-0.61939200	1.24709200	-0.49828600
C	-1.44242200	0.14667700	-2.04175600
H	-0.65586600	0.42193900	-2.74767800
H	-1.68627600	-0.90509300	-2.19690600
C	-2.66614100	1.01190200	-2.24463900
C	-2.53108500	2.35518500	-2.62387900
C	-3.95127500	0.49272700	-2.03508800
C	-3.65696000	3.16441700	-2.78765600
H	-1.53864400	2.76526300	-2.79567100
C	-5.07921200	1.29956600	-2.19997800
H	-4.06713600	-0.54819300	-1.74412200
C	-4.93406800	2.63723500	-2.57637100
H	-3.53869600	4.20237800	-3.08528400
H	-6.06924900	0.88311600	-2.03801000
H	-5.81108200	3.26446100	-2.70765200
C	3.16967800	2.74234000	0.38371000
C	3.05496700	3.13526600	1.72516300
C	3.36304300	3.72839300	-0.59351600
C	3.13252300	4.48257400	2.08347800
H	2.91122400	2.37824200	2.49261400
C	3.44228200	5.07761900	-0.23960300
H	3.45776200	3.43487500	-1.63637600
C	3.32562400	5.45727000	1.10026900
H	3.04600300	4.77157200	3.12718000
H	3.59714300	5.83104800	-1.00687200
H	3.38884100	6.50578500	1.37717800
I	-3.35447100	0.01699900	2.52027200

S-TS1

E=-478.4010187 (au)

C	-1.97991700	-1.49370300	-0.31297600
H	-1.01649700	-2.02622800	-0.33494300
O	-1.84971200	-0.13190900	-0.13656800
N	-2.52273000	-1.71038200	-1.74314900
H	-2.39206000	-2.67166300	-2.06259900
H	-3.51847300	-1.48113100	-1.77929300
H	-1.94702900	-0.96564800	-2.31774800
O	-1.12125400	0.33406800	-2.40070700
H	-1.41919400	0.22219000	-1.13029000
C	-2.89878700	-2.15253300	0.69409700
C	-2.64988700	-3.46189200	1.12064200
C	-4.01819700	-1.47036100	1.18722900
C	-3.51013500	-4.08552700	2.02687900
H	-1.77710100	-3.99046900	0.74568200
C	-4.87876900	-2.09323800	2.09158800
H	-4.20375700	-0.45046500	0.86622000
C	-4.62719000	-3.40229700	2.51252800
H	-3.30567600	-5.10007900	2.35585000
H	-5.74414300	-1.55710100	2.47014400
H	-5.29581200	-3.88475700	3.21934900
H	-0.20532300	0.02344700	-2.45305100

S-TS2

E=-478.3853634 (au)

C	-1.25787700	-1.50606500	-0.53180000
H	-0.27454600	-1.95142600	-0.55797200
O	0.01313500	-0.74109100	1.42342300
H	-0.76085100	-0.25743700	1.74564600
N	-2.17914200	-2.18920000	0.09169200
H	-3.12597500	-1.83332000	0.17136600
H	-1.79993900	-2.82490700	0.83329000
O	-0.58065700	-3.04567300	2.05268500
H	-0.26824600	-1.98825500	1.81443500
C	-1.48892700	-0.33882100	-1.36808400
C	-0.39726300	0.16662000	-2.09742100
C	-2.74423400	0.28903100	-1.47650800
C	-0.55700400	1.27435700	-2.92449000
H	0.57184400	-0.31405200	-2.00441600
C	-2.89904500	1.39440200	-2.30598300
H	-3.59780900	-0.07932700	-0.91627400
C	-1.80792800	1.88776600	-3.03022700
H	0.28898700	1.65918400	-3.48455300
H	-3.86866200	1.87448600	-2.38894000
H	-1.93457000	2.75194600	-3.67506300
H	0.07663400	-3.58740400	1.59287100

Sol-TS3

E=-748.5959627(au)

C	1.58701000	1.41414100	-0.53289600
H	1.25533600	1.45235400	-1.58767100
O	1.86052000	2.50050000	0.07244800

C	-0.77734200	0.05307900	-0.82670100
H	-0.90605600	0.55504300	-1.80235500
H	-0.20234300	-0.86594300	-1.03788500
O	-0.07681300	0.86071600	0.08940800
H	0.26675300	3.58495100	0.03263300
H	-0.68892600	2.27094300	0.15300000
C	2.39399200	0.17961400	-0.22899400
C	2.54184100	-0.83058700	-1.18748600
C	3.02865400	0.04022400	1.01324600
C	3.29941300	-1.97096800	-0.90536700
H	2.07262500	-0.71615700	-2.16134000
C	3.78149900	-1.09715700	1.29788400
H	2.92687700	0.83439800	1.74662700
C	3.91728600	-2.10786800	0.33907200
H	3.41079300	-2.74695700	-1.65724100
H	4.26681600	-1.19799400	2.26460800
H	4.50711500	-2.99253900	0.56066600
H	-1.27844300	3.71981700	-0.65199800
N	-0.73903200	3.36303300	0.13646700
H	-1.10583600	3.75238100	1.00463900
C	-2.14751500	-0.35284700	-0.31072800
C	-3.18173600	-0.64003500	-1.21260400
C	-2.39828500	-0.48353200	1.06133200
C	-4.43462700	-1.05394900	-0.75670400
H	-3.00315500	-0.53405100	-2.28023300
C	-3.65242400	-0.89277000	1.52085100
H	-1.60613800	-0.25545000	1.76727000

C	-4.67528700	-1.18073700	0.61412000
H	-5.22483400	-1.26863000	-1.47078800
H	-3.83063900	-0.98626000	2.58863200
H	-5.65124100	-1.49651500	0.97116700

Sol-TS4

E= -1018.479688 (au)

C	-3.33713400	1.25293800	0.94923300
H	-2.61473600	0.47131900	1.18971400
H	-4.20857900	1.13739400	1.59744900
N	-2.72188400	2.57281100	1.29984800
C	-3.74055500	5.86341000	0.81315200
H	-2.64712300	5.86642500	0.64315300
H	-4.18659400	5.73210900	-0.18909200
O	-4.12813300	4.81074800	1.65969600
C	-2.30545700	2.77650500	2.78880300
H	-3.12670400	2.29650400	3.34264100
O	-2.22322800	4.13657300	2.99241300
H	-3.41003200	3.37367700	1.14708500
H	-3.13860000	4.56648400	2.48094100
H	-1.90068100	2.73926300	0.71111300
C	-3.72399000	1.20863600	-0.50937100
C	-2.95498500	0.48028900	-1.42489200
C	-4.85042600	1.90877500	-0.96603600
C	-3.30717000	0.44672200	-2.77600800
H	-2.08157400	-0.06416300	-1.07644000
C	-5.20047600	1.87851200	-2.31586400
H	-5.44729800	2.48101700	-0.26034400

C	-4.43016000	1.14531200	-3.22333500
H	-2.70577300	-0.12530000	-3.47622000
H	-6.07579200	2.42189900	-2.65899500
H	-4.70548500	1.11870700	-4.27341800
C	-1.00321900	2.05404900	3.06057700
C	-1.00299100	0.79206900	3.66498600
C	0.21570100	2.64249700	2.69611400
C	0.20011600	0.12041900	3.89627200
H	-1.94522300	0.33870700	3.96080200
C	1.41620800	1.97153100	2.92558600
H	0.21718200	3.62883600	2.24298100
C	1.41064500	0.70811600	3.52488000
H	0.19057000	-0.85724900	4.36862700
H	2.35638100	2.43454200	2.64085700
H	2.34667500	0.18796200	3.70559900
C	-4.13461600	7.24795300	1.31458700
C	-4.94928000	7.41320200	2.43878800
C	-3.69410000	8.39227800	0.63196700
C	-5.31673300	8.69038600	2.87477400
H	-5.28944000	6.53165200	2.97172400
C	-4.05959500	9.66767700	1.06184000
H	-3.05756300	8.28006200	-0.24346800
C	-4.87423600	9.82239200	2.18890900
H	-5.94904900	8.79876500	3.75199200
H	-3.70745500	10.54217500	0.52147500
H	-5.15840300	10.81484000	2.52674000

Sol-TS5

E= -1018.471534 (au)

C	-0.93407600	-1.22298800	-0.60578400
H	-1.86315000	-0.66554300	-0.57238800
O	-0.74239500	-0.84074800	1.70273900
H	-0.15367800	-0.07427000	1.66844600
N	-1.03767400	-2.52399300	-0.57918000
H	-0.18362800	-3.06477400	-0.44634800
C	0.37558100	-3.62015400	2.75593400
H	-0.70195000	-3.56137800	3.01324000
H	0.54031200	-4.68326100	2.49178000
O	0.71001900	-2.78798700	1.68766400
H	-0.02121900	-1.75230300	1.73036800
C	-2.26285400	-3.20935100	-0.13362000
H	-3.10148500	-2.54222900	-0.34179100
H	-2.19309100	-3.34531500	0.95015900
C	-2.44052500	-4.54186300	-0.82305000
C	-2.02544200	-5.72286900	-0.19594700
C	-3.00685400	-4.61119500	-2.10330500
C	-2.17233400	-6.95487900	-0.83754800
H	-1.59126800	-5.67600200	0.79935300
C	-3.15435100	-5.84084100	-2.74552900
H	-3.33350200	-3.69834300	-2.59441400
C	-2.73634900	-7.01549900	-2.11339900
H	-1.84959700	-7.86465200	-0.34013700
H	-3.59710800	-5.88366400	-3.73620300
H	-2.85365200	-7.97308600	-2.61200200
C	0.26907000	-0.49584600	-0.99688100

C	0.12351600	0.87178100	-1.29024200
C	1.53454500	-1.09929600	-1.11957300
C	1.22032700	1.62331300	-1.70444100
H	-0.85367900	1.33597500	-1.19553400
C	2.62629500	-0.34220100	-1.53103900
H	1.67505100	-2.14714100	-0.87746100
C	2.47243500	1.01704200	-1.82595600
H	1.09844300	2.67744900	-1.93166600
H	3.60094400	-0.81069400	-1.62218400
H	3.32930100	1.60072200	-2.14812100
C	1.15303600	-3.36085600	4.04732600
C	2.20181800	-2.43777000	4.08878500
C	0.83340300	-4.06412100	5.21901900
C	2.91573800	-2.21649100	5.27104400
H	2.45027100	-1.89560400	3.18210500
C	1.54340200	-3.84927000	6.40018900
H	0.01885400	-4.78598900	5.20319100
C	2.58909400	-2.91965100	6.43148100
H	3.72707800	-1.49335100	5.28426700
H	1.28020700	-4.40180600	7.29824700
H	3.14142300	-2.74842000	7.35102400

Sol-TS6

E= -1288.581714 (au)

N	-1.78899400	3.22927200	-3.27105700
H	-1.97403600	4.09587500	-2.52803100
C	-2.08879500	3.78493400	-4.63653200
H	-1.43901700	4.65599300	-4.74278000

H	-1.76997300	3.04749700	-5.37710200
C	-2.61406800	2.00994200	-2.92697100
H	-3.61763100	2.37911200	-2.71505400
H	-2.20961800	1.61437000	-1.99596600
C	-2.68733000	0.92833000	-3.98727900
C	-1.61746000	0.05214600	-4.22644700
C	-3.86917900	0.75676000	-4.72310500
C	-1.71796400	-0.95007600	-5.19226200
H	-0.70536400	0.14331800	-3.64715100
C	-3.97427600	-0.24961500	-5.68535700
H	-4.71354600	1.41361200	-4.53793200
C	-2.89577800	-1.10205200	-5.92774900
H	-0.87849200	-1.61760300	-5.36291200
H	-4.89874200	-0.36718600	-6.24292400
H	-2.97462900	-1.88467600	-6.67653400
C	-3.53057300	4.17560500	-4.89095300
C	-4.38077200	4.69925600	-3.90682800
C	-4.01577600	4.05561900	-6.20167400
C	-5.68346400	5.08855400	-4.22836700
H	-4.03817800	4.79794900	-2.88284400
C	-5.31202000	4.45702800	-6.52593000
H	-3.37080600	3.64304500	-6.97281500
C	-6.15313700	4.97353800	-5.53765000
H	-6.32947800	5.48492900	-3.45055100
H	-5.66700900	4.35650600	-7.54735300
H	-7.16563000	5.27864100	-5.78435000
C	1.64376400	0.58328800	-0.98424800

C	1.12414100	1.27453500	-2.08155400
C	0.18937700	2.30236300	-1.90431600
C	-0.20897000	2.64002900	-0.60063300
C	0.30576300	1.94490700	0.49361300
C	1.23253300	0.91508900	0.30663600
H	2.36779600	-0.21058800	-1.14122200
H	1.45305100	1.01750200	-3.08481900
H	-0.91672500	3.44770000	-0.44492500
H	-0.01494100	2.21145200	1.49637900
H	1.63177700	0.37867200	1.16220300
C	-0.25645900	3.08206800	-3.13482700
H	0.09406100	2.56506400	-4.03173700
O	0.27109400	4.38533600	-3.14191400
O	-1.68951100	5.19955000	-1.68208500
H	-0.30230700	4.88744000	-2.47035700
C	-1.29242600	7.59850000	-1.35968800
C	-0.25807500	7.31813900	-0.46158200
C	0.47520100	8.35187700	0.13127300
C	0.18051200	9.68315000	-0.16414500
C	-0.85490200	9.97484000	-1.05933700
C	-1.58159200	8.94155800	-1.64942600
H	-0.02746500	6.28323600	-0.23241700
H	1.27713800	8.11369100	0.82495000
H	0.74874400	10.48650400	0.29575600
H	-1.09283000	11.00805400	-1.29733100
H	-2.38401800	9.17669200	-2.34585100
C	-2.11021600	6.49214400	-2.01867000

H	-3.16766000	6.65734900	-1.73734700
H	-2.07917100	6.66895900	-3.11077500

Sol-TS7

E= -1288.577602 (au)

N	-1.86895400	2.50314200	-2.65052100
H	1.13207500	4.49806900	-2.90154400
C	-1.88004100	2.43479100	-4.14514700
H	-0.85561800	2.22861400	-4.45651700
H	-2.49654900	1.57162000	-4.40641400
C	-3.17691300	2.36240400	-1.98044100
H	-3.00096100	1.88202100	-1.01499300
H	-3.75195800	1.65372800	-2.58009800
C	-3.98222600	3.63922300	-1.80330200
C	-5.37739400	3.52174300	-1.72906500
C	-3.39558700	4.90362700	-1.66536600
C	-6.17503900	4.64517400	-1.51221000
H	-5.83964000	2.54473900	-1.84398500
C	-4.19914500	6.02845300	-1.45595100
H	-2.31722000	5.02230300	-1.73596600
C	-5.58686800	5.90517600	-1.37565200
H	-7.25432100	4.53685200	-1.45878700
H	-3.73378900	7.00490000	-1.35671400
H	-6.20587600	6.78247700	-1.21329200
C	-2.39461100	3.67682400	-4.83996500
C	-1.53011300	4.75373000	-5.08194300
C	-3.71996400	3.75011400	-5.28656200
C	-1.99102600	5.89264600	-5.74291900

H	-0.49566400	4.68814300	-4.75881900
C	-4.18111900	4.88968400	-5.94853100
H	-4.39050500	2.91199700	-5.11833900
C	-3.31837800	5.96444700	-6.17436200
H	-1.31272500	6.72033900	-5.92775500
H	-5.21050600	4.93536900	-6.29130200
H	-3.67551300	6.84997300	-6.69173300
C	1.27262300	1.78962400	0.98892500
C	0.86665700	1.99266500	-0.32644200
C	-0.41029900	2.51906300	-0.61230600
C	-1.24844900	2.89144100	0.45753500
C	-0.82850300	2.69863700	1.77075800
C	0.42245900	2.13693400	2.04104300
H	2.25286600	1.37054500	1.19165200
H	1.53359400	1.74173500	-1.14539500
H	-2.20152200	3.37234000	0.27764500
H	-1.47856400	2.99634900	2.58712700
H	0.73948800	1.98773700	3.06851800
C	-0.71686600	2.62677100	-2.03835200
H	0.14290000	2.59081200	-2.69451400
O	0.05173200	5.06067800	-2.10193600
H	0.33832900	4.89016800	-1.19479400
C	6.10597000	5.67036000	-2.28772200
C	5.14526400	5.28086300	-3.22624800
C	3.78148200	5.48426700	-2.98499200
C	3.39529500	6.08731800	-1.77720600
C	4.35000700	6.47540800	-0.83747100

C	5.71034600	6.26850700	-1.09035700
H	7.16009600	5.50418100	-2.49172200
H	5.45844100	4.81305100	-4.15660900
H	2.33751400	6.24363000	-1.58150300
H	4.03545600	6.94300100	0.09148900
H	6.45390600	6.57203900	-0.35910000
C	2.73089100	5.06014800	-3.99851300
H	3.23750100	4.68524500	-4.89719800
H	2.15677600	5.94841300	-4.30841600
O	1.85866100	4.04805700	-3.51773800

2-H₂O-S-TS1

E= -554.8457711 (au)

C	-2.30908100	-1.17637500	-0.45402200
H	-1.25542500	-1.48022500	-0.49390500
O	-2.46340700	0.18780400	-0.29353100
N	-2.85196600	-1.56545400	-1.83224200
H	-2.80367600	-2.57797800	-1.97114900
H	-3.83396900	-1.28412200	-1.89014300
H	-2.25322900	-1.04506600	-2.61478200
O	-1.36997000	-0.26519100	-3.52991400
H	-1.71878500	0.66524100	-0.86079800
C	-3.03566600	-1.96984000	0.61309700
C	-2.57401900	-3.24340900	0.96619000
C	-4.18176500	-1.45828900	1.23343600
C	-3.25051200	-3.99937900	1.92516100
H	-1.68060400	-3.64105500	0.49132700

C	-4.85682800	-2.21338800	2.19376200
H	-4.53653800	-0.46750200	0.97013300
C	-4.39384000	-3.48518900	2.54105000
H	-2.88120100	-4.98426600	2.19494400
H	-5.74263900	-1.80767200	2.67351800
H	-4.91822400	-4.07032300	3.29069700
H	-0.61784900	-0.85647900	-3.67937300
O	-0.69778800	1.23801900	-1.74523800
H	-0.99291800	0.48450800	-2.70851500
H	0.12520400	0.86446200	-1.39851300

2-H₂O-S-TS2

E= -554.8295968 (au)

C	-1.07703700	-1.18614700	-0.47745100
H	-0.08983300	-1.62370700	-0.54012900
O	-0.01972100	0.14057000	0.97621700
H	-0.82347300	0.46453700	1.40751000
N	-1.96290600	-1.86943300	0.19974300
H	-2.92789500	-1.56284300	0.25088700
H	-1.62202400	-2.59803100	0.86617700
O	-0.74335200	-3.54882000	1.99801100
H	-0.07416700	-2.78976800	2.20456600
C	-1.41736400	-0.14938100	-1.45598200
C	-0.43832700	0.21279000	-2.39563300
C	-2.67930100	0.46731900	-1.50177400
C	-0.71958700	1.16272200	-3.37461100
H	0.53932500	-0.25812900	-2.35493400
C	-2.95471200	1.42039700	-2.47854800

H	-3.44528700	0.21646000	-0.77438500
C	-1.97835300	1.76700300	-3.41785900
H	0.04046100	1.43206000	-4.10097800
H	-3.93082100	1.89396900	-2.50744400
H	-2.19883800	2.50918600	-4.17892000
H	-0.24419000	-4.15339700	1.43051300
O	0.85731000	-1.59141100	2.44806600
H	0.57847200	-1.31978600	3.33418700
H	0.39134700	-0.67833500	1.69998500

H-bond-S-TS1

E= -631.2903035 (au)

C	-1.55889800	-1.69736500	-0.22623600
H	-0.97060800	-2.54615300	-0.60718700
O	-0.79348700	-0.72905500	0.38567500
N	-2.15224000	-1.07512100	-1.50660200
H	-2.64982500	-1.76296900	-2.07472600
H	-2.77732800	-0.27031900	-1.25581100
H	-1.33697600	-0.66759900	-2.01347400
O	0.10325000	0.36633200	-1.58425400
H	-0.24690800	-0.21468800	-0.44139400
C	-2.68487400	-2.21522800	0.64677900
C	-3.16804100	-3.51595400	0.46360500
C	-3.26512500	-1.39794200	1.62447400
C	-4.22376500	-3.99391000	1.24228500
H	-2.71264200	-4.15597600	-0.28805700
C	-4.31913000	-1.87585600	2.40436300
H	-2.87851200	-0.39552700	1.77701200

C	-4.80161600	-3.17360600	2.21402200
H	-4.58927700	-5.00585400	1.09474600
H	-4.76207800	-1.23706800	3.16278900
H	-5.62022500	-3.54533400	2.82318000
H	1.06057200	0.32984400	-1.71029200
O	-1.11216800	2.59714600	-1.09624300
H	-0.55571600	1.77147100	-1.30523600
H	-1.25141800	3.00881500	-1.96094300
O	-3.49429500	1.29780200	-0.81847400
H	-3.62044800	1.16464200	0.13233000
H	-2.64421400	1.81263400	-0.87827300

H-bond-S-TS2

E= -631.2583648 (au)

C	-0.88518700	-2.60226600	-0.12938200
H	0.14773700	-2.75099200	0.15824200
O	-0.71491400	-0.91428100	1.14207700
H	-1.60705000	-0.54437000	1.05702800
N	-1.76640500	-3.36051500	0.51295000
H	-2.74981900	-3.26694600	0.27863100
H	-1.53904500	-3.45047100	1.52841600
O	-0.88322600	-2.57384900	2.93727700
H	-0.77527200	-1.60469600	2.02852600
C	-1.12009500	-2.01003800	-1.44622200
C	-0.00337800	-1.55314500	-2.16696100
C	-2.40385000	-1.88168100	-2.00457500
C	-0.16438200	-0.98585300	-3.42809400
H	0.98652200	-1.64791000	-1.73061900

C	-2.56018600	-1.31351100	-3.26549100
H	-3.28138500	-2.21821400	-1.46185200
C	-1.44311800	-0.86517500	-3.97791700
H	0.70294200	-0.63864300	-3.98024600
H	-3.55299900	-1.21656300	-3.69287100
H	-1.57125800	-0.42171800	-4.96062300
H	0.02677200	-2.88491800	3.05125500
O	-1.36813800	-1.60209300	5.38851500
H	-1.19756200	-1.95985600	4.47151400
H	-1.77554800	-2.35188800	5.84216300
O	-0.40136200	-5.95244900	-0.64762300
H	-0.98748200	-5.27164600	-0.28047400
H	0.01593800	-6.32543700	0.14134400

3-H₂O-S-TS1

E= -631.2707977 (au)

C	-1.29893100	-1.03503200	-0.45196200
H	-0.31349300	-1.48034100	-0.45032000
O	-0.27196700	0.40908000	0.91652500
H	-0.52027300	-0.05453700	1.72984600
N	-2.20339600	-1.66826000	0.24965200
H	-3.16497200	-1.35110100	0.28161600
H	-1.87989800	-2.38923500	0.92352300
O	-0.99738100	-3.49981000	1.96061300
H	-0.12506300	-3.04090500	2.10621800
C	-1.59799000	-0.08041000	-1.52324300
C	-0.51541500	0.42621100	-2.26294600
C	-2.90568200	0.30592300	-1.85960300

C	-0.73624600	1.30243200	-3.32142900
H	0.49360500	0.13638200	-1.98559200
C	-3.12171300	1.18326300	-2.92018600
H	-3.76000400	-0.07930400	-1.31136700
C	-2.04026200	1.68183600	-3.65202700
H	0.10494900	1.68926700	-3.88780000
H	-4.13477800	1.47489000	-3.17831900
H	-2.21423500	2.36312200	-4.47932200
H	-0.78210700	-4.22175200	1.35280300
O	1.36659600	-2.26118700	2.41028100
H	1.11891600	-1.62789300	3.09904100
H	1.58374500	-1.67229200	1.60957600
O	1.80622300	-0.70332400	0.36491300
H	2.54369200	-0.13833100	0.63566300
H	0.79115800	-0.08244000	0.65956100

4-H₂O-S-TS1

E= -707.7082936 (au)

C	-1.30404600	-1.32366900	-0.52279500
H	-0.37895400	-1.86935000	-0.65480100
O	-0.26494900	-0.22664500	0.93248700
H	-0.29250400	-0.86803500	1.67238000
N	-2.27226200	-1.99087900	0.06860600
H	-3.18237700	-1.56686900	0.19833400
H	-2.04443600	-2.83163300	0.62368200
O	-1.44330900	-4.20865600	1.64083500
H	-0.82587000	-3.61753200	2.13911900
C	-1.56581100	-0.21034300	-1.45506000

C	-0.46968900	0.42516900	-2.06235100
C	-2.86721900	0.20182000	-1.78133600
C	-0.67301700	1.46148200	-2.96960400
H	0.53569700	0.11595900	-1.79173400
C	-3.06561800	1.24020900	-2.69039400
H	-3.73287400	-0.28988500	-1.34841200
C	-1.97131600	1.87230500	-3.28506400
H	0.17984600	1.94926100	-3.43135300
H	-4.07582800	1.55012000	-2.93865300
H	-2.12957200	2.67897400	-3.99444100
H	-0.86839800	-4.66245100	1.00767400
O	2.65146300	-2.15633900	2.00899300
H	3.02717700	-1.56002500	2.67239100
H	2.44167700	-1.53369900	1.20792600
O	2.00121600	-0.62962300	0.06192000
H	2.48737400	0.19347200	0.21438800
H	0.76768900	-0.36178300	0.54741100
O	0.12125700	-2.33224500	2.81577200
H	1.09365800	-2.32730500	2.57085600
H	0.09104800	-2.23102500	3.77739600

Waters-1

C	-0.72467900	-0.80865700	-0.54159800
H	0.23652500	-1.24977500	-0.81984200
O	-0.26349693	0.28416464	1.19133361
H	-1.08653693	0.74790364	1.41479861
N	-1.59442269	-1.79733190	-0.35460106
H	-2.51274069	-1.42217090	-0.12318906

H	-1.34453374	-2.54394619	0.53000354
O	-1.09753045	-3.14618402	1.76947882
H	-0.63459694	-2.20942227	2.29417196
C	-1.17335000	0.13480800	-1.64441300
C	-0.30435600	0.43612700	-2.69898300
C	-2.44523200	0.72695400	-1.61569300
C	-0.69503500	1.31905900	-3.71117000
H	0.66857900	-0.04629800	-2.72235700
C	-2.83696400	1.60696900	-2.62309700
H	-3.12240200	0.48518400	-0.80157700
C	-1.96579900	1.89746600	-3.67749700
H	-0.01222700	1.54680400	-4.52546500
H	-3.82632800	2.05208700	-2.58439600
H	-2.26973000	2.58416800	-4.46220000
H	-0.68153351	-3.97480699	1.49272874
O	-0.01856262	-1.25901397	2.89051562
H	0.19015165	-1.23107442	3.83583897
H	-0.37335183	-0.12489558	2.27124177
O	2.32157600	0.38425700	-5.19031400
H	1.89681900	-0.11022900	-5.90494800
H	3.03239100	0.89697100	-5.60073900
O	2.92276200	-1.18496100	-2.96332200
H	2.81659200	-0.67197800	-3.79353000
H	3.54079800	-0.66558500	-2.43150300
O	-2.74241900	4.19757500	-6.40670300
H	-2.86716000	5.15700500	-6.39573000
H	-3.64600700	3.86757200	-6.50763200

O	-5.89284300	2.15393000	-1.09631300
H	-5.89431300	3.08014400	-1.37595300
H	-6.50150100	1.74598200	-1.72810100
O	-5.13959900	-0.11244900	0.47658700
H	-5.24429300	0.69461700	-0.05876000
H	-5.88281700	-0.04013100	1.09293800

Waters-2

C	-1.04631500	-2.61872500	-0.43168600
H	-0.04245400	-2.59388100	-0.03747100
O	-0.85516176	-1.04737316	0.87093207
H	-1.74965976	-0.85047316	0.56609507
N	-1.93832700	-3.23301900	0.28745300
H	-2.92365000	-3.27190000	0.01645100
H	-1.60845571	-3.31645643	1.44862617
O	-0.94703500	-2.75720100	2.69127300
H	-1.01853540	-1.73616003	1.87301456
C	-1.20623000	-2.00974300	-1.73308000
C	-0.03321500	-1.51552100	-2.33347600
C	-2.44920200	-1.83242700	-2.37050000
C	-0.08796000	-0.89869400	-3.57717100
H	0.91012400	-1.61598800	-1.80641000
C	-2.49506000	-1.20579100	-3.60941200
H	-3.36501400	-2.17227300	-1.89920800
C	-1.31876600	-0.75670200	-4.22285700
H	0.81612400	-0.52327000	-4.04299900
H	-3.45383500	-1.06960000	-4.09613000

H	-1.35592400	-0.29988000	-5.20704000
H	-0.01669200	-2.97747700	2.52836100
O	-0.87649322	-1.48802093	5.31646487
H	-0.87014522	-1.92839793	4.41036387
H	-1.33594522	-2.14169793	5.86319887
O	0.05590900	-5.58563500	-0.49604400
H	-0.79688500	-5.15847400	-0.32715000
H	0.29509800	-5.94382700	0.37253900
O	-0.71529100	0.57639100	-7.53294800
H	0.13445100	0.72066100	-7.06809800
H	-1.18676800	1.41387700	-7.38681900
O	1.69042600	0.84761700	-6.10454100
H	2.41689100	0.34378900	-6.49214200
H	2.05690100	1.73479500	-5.98190600
O	1.69617526	-3.22895588	0.14541746
H	2.44110865	-3.11753752	-0.45281315
H	1.34531776	-4.07897724	-0.10642191
O	-5.99601400	-1.86359800	-2.91526900
H	-5.93418400	-0.93573200	-3.15507500
H	-5.97737400	-2.29646800	-3.78549100
O	-4.85651300	-3.32781300	-0.27951000
H	-5.23524900	-2.50099500	-0.56973200
H	-4.93388700	-3.86648400	-1.07413300

Waters-3

C	-1.34673100	-1.17370600	-0.51799900
H	-0.47532200	-1.81020600	-0.58498000

O	0.01752931	-0.19786254	0.58953130
H	-0.51199769	0.51825546	0.97378730
N	-2.28606500	-1.55410900	0.30321800
H	-3.17308600	-1.04776300	0.43660000
H	-2.05491132	-2.38140477	1.02193191
O	-1.47578457	-3.29962882	1.84112469
H	-0.35999588	-2.82009990	2.24363489
C	-1.51382800	-0.16032200	-1.55884600
C	-0.44441100	0.03626000	-2.45263900
C	-2.69355000	0.58932300	-1.71651700
C	-0.54950000	0.96921800	-3.48106400
H	0.46648800	-0.54125300	-2.32271500
C	-2.79251100	1.51985400	-2.74807900
H	-3.53498300	0.45223400	-1.04505300
C	-1.72437200	1.71352400	-3.62971100
H	0.27984300	1.12347700	-4.16551500
H	-3.70961700	2.09022000	-2.85674800
H	-1.80737500	2.43800100	-4.43579200
H	-1.26190057	-3.83392282	1.05947869
O	0.61308100	-1.75721500	2.49745700
H	0.32558100	-1.38772300	3.34400500
H	0.46284200	-0.98007000	1.76439900
O	2.00381000	2.03181900	-6.02366800
H	1.48514100	1.98072600	-6.84508900
H	1.98518400	2.97905600	-5.81890700
O	2.48308400	-1.82940400	-1.40961700
H	2.75747300	-1.68596100	-2.32493200

H	2.51499900	-0.91993200	-1.02331000
O	-1.89092000	4.00985300	-6.48004000
H	-2.25776300	4.70515200	-5.91772500
H	-2.67824500	3.55502800	-6.80632100
O	-6.11965700	2.49758400	-2.00173000
H	-5.96622300	3.41788700	-2.26219300
H	-6.21956700	2.04778300	-2.85284600
O	-4.80631700	-0.33023400	0.94709400
H	-4.53901400	0.04670000	1.79847500
H	-5.31007100	-1.12146700	1.19265200
O	2.47107711	0.58471772	-0.34758810
H	3.12106211	0.48874972	0.36588290
H	1.68524786	0.40320042	0.05181627
O	2.81531307	-3.67814607	3.17812577
H	3.24391407	-3.32058007	3.97319477
H	2.17355707	-2.97031807	2.91422477
O	0.82436668	-5.11257644	4.09010496
H	1.62211668	-4.61538144	3.82648696
H	0.14362168	-4.74155744	3.49829696
O	-4.59751138	-3.39198554	-0.76357858
H	-5.28468551	-2.73769718	-0.52984147
H	-3.83358204	-3.06820518	-0.24459550

OH-S

C	-1.75531600	-1.76888700	-0.49857500
H	-0.86798600	-2.44775900	-0.39917700
O	-1.47179800	-0.46566900	-0.36222000

N	-2.28444400	-2.07533300	-1.89499000
H	-2.73241600	-2.99357900	-1.91565400
H	-3.02366300	-1.38544000	-2.05308800
H	-0.89118800	-0.85859700	-3.04348200
O	-0.42259000	-0.02200800	-2.87367800
H	-2.50646100	0.42823600	-1.33845300
C	-2.77663700	-2.27752600	0.55577600
C	-2.98620300	-3.64186300	0.79678100
C	-3.51151000	-1.35268200	1.30462400
C	-3.91984000	-4.07553500	1.74070800
H	-2.40157900	-4.37570200	0.24129700
C	-4.45117500	-1.77714400	2.24497400
H	-3.29881000	-0.30373700	1.12111300
C	-4.66215900	-3.14116700	2.46767400
H	-4.06524300	-5.14047000	1.91478600
H	-5.01808400	-1.04314300	2.81521000
H	-5.38929700	-3.47304400	3.20593100
H	-0.56795600	-0.01028100	-1.89336400
O	-3.12304800	0.96214600	-1.92086400
H	-2.53804600	1.04318400	-2.69034000

H₃O⁺-S

C	-2.24213000	-1.33038600	-0.33319800
H	-1.18390500	-1.61945600	-0.33623300
O	-2.45156900	0.02372000	-0.27972300
N	-2.74918300	-1.81451100	-1.74358600

H	-2.66489800	-2.83055600	-1.83641100
H	-3.74177800	-1.57193300	-1.81691600
H	-2.21934800	-1.32904700	-2.51953400
O	-1.41178300	-0.33662100	-3.57087400
H	-1.72128700	0.52362600	-0.69740000
C	-3.02270400	-2.08121100	0.71559100
C	-2.67923100	-3.40778200	1.01006900
C	-4.10997400	-1.47874500	1.36101300
C	-3.42790800	-4.13349500	1.93585800
H	-1.81568100	-3.87258900	0.53507000
C	-4.85257200	-2.20812100	2.29043200
H	-4.35574600	-0.44378200	1.15038200
C	-4.51720100	-3.53357000	2.57402900
H	-3.15580100	-5.15850600	2.16660500
H	-5.69069500	-1.73809400	2.79703400
H	-5.09749100	-4.09646700	3.29854600
H	-0.97620300	-0.51287900	-4.41706000
O	-0.63274300	1.63253300	-1.77303100
H	-1.01472800	0.46538800	-3.18501500
H	0.28254700	1.81202200	-1.50251400
H	-1.05476700	2.50251700	-1.85325400