Supplementary Information

Mechanistic insights and computational design of half-sandwich iridium and rhodium complexes for hydrogenation of quinoline

Xiuli Yan,[a,b] and Xinzheng Yang[*,a,b]

[a] Beijing National Laboratory for Molecular Sciences, State Key Laboratory for Structural Chemistry of Unstable and Stable Species, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, People's Republic of China. E-mail: xyang@iccas.ac.cn

[b] University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China.

S1. Evaluation of density functionals

In order to evaluate the density functional dependency of the iridium complex, we also optimized the structures of **1** and **$TS_{4,5}$**, which are rate-determining states in the hydrogenation of quinoline to 1,2,3,4-tetrahydroquinoline catalysed by **2** using other eight widely-used and/or recently developed density functionals, including ωB97X-D,[1] B3LYP,[2, 3] B3PW91,[4-6] HSE06,[7, 8] PBEh1PBE,[9] TPSSh,[10] M06L,[11] and TPSS.[10] As shown in Table S1, The ωB97X-D functional has the lowest relative energy of 18.3 kcal/mol, while the TPSSh functional has the highest relative energy of 28.0 kcal/mol. The difference between them is 9.7 kcal/mol, which indicates that the quinoline hydrogenation reactions catalysed by **1** has a moderate dependence of density functionals. The M06 result of 25.1 kcal/mol is in the middle of them, and close to the results of B3LYP and B3PW91 functionals. More importantly, the free energy barrier obtained by the M06 functional matches well with the experimental reaction conditions of 70−90 °C and 16 hours. Consider the M06 functional is parametrized for the calculations of transition metals and non-covalent interactions with the semiempirical kinetic-energy-density dependence introduced in it, we use the M06 functional in our computational study for this catalytic system.

Table S1. Absolute and relative free energies of rate-limiting states **1** and **TS$_{4,5}$** obtained by using different density functionals.[a]

Density functionals	Absolute free energies (Hartree)		Total barriers (kcal/mol)
	1	**TS$_{4,5}$**	**1 → TS$_{4,5}$**
M06	-1521.5382610	-1463.8539440	25.1
HSE06	-1521.0981690	-1463.4047250	22.9
M06L	-1522.2325340	-1464.8028790	22.4
PBEh1PBE	-1521.1220250	-1463.4348100	23.1
TPSSh	-1522.3672730	-1465.0010880	28.0
TPSS	-1522.4974000	-1465.1722920	27.5
ωB97X-D	-1522.0344370	-1464.5189330	18.3
B3LYP	-1522.3119060	-1464.9129980	26.3
B3PW91	-1521.9625190	-1464.4624910	26.0

[a] Both structures (**1** and **TS$_{4,5}$**) and related small molecules (H_2, H_2O, $Cl^-(H_2O)$, and quinoline) are optimized individually using different density functionals.

S2. Influence of counter ion on the free energy barrier

We have examined the influence of counter ions by calculating the interaction between OTf^- (OTf = trifluoromethanesulfonate) and **1**, and found that the neutral complex **1$_{OTf}$** is 8.5 kcal/mol less stable than separated **1** and OTf^-. Therefore, we believe the addition of dissociative OTf^- anions will not change the reaction mechanism. The OTf^- anion will stay away from **1** in the solvent and not decrease the stability of the catalyst or lead to a higher free energy barrier.

S3. Influence of solvents on the free energy barrier

In order to find out the influence of different solvents, we have also calculated the free energy barriers of the reactions catalysed by **1**, $\mathbf{1}_{\mathbf{Ir\text{-}OCOCH3}}$ and $\mathbf{1}_{\mathbf{Rh\text{-}OCH3}}$ using another experimental solvent of isopropanol. The relative free energies of $\mathbf{1}_{\mathbf{M\text{-}R}}$ and $\mathbf{TS}_{\mathbf{4,5\text{-}M\text{-}R}}$ are listed in Table S2. We can see that the solvent effect has significant influence to free energy barriers. **1**, $\mathbf{1}_{\mathbf{Ir\text{-}OCOCH3}}$ and $\mathbf{1}_{\mathbf{Rh\text{-}OCH3}}$ all have near 8.0 kcal/mol higher free energy barriers in isopropanol. This is not unexpected because the experimental observations indicate that the reactions in isopropanol need about 50 °C higher temperature and 15 bar higher H_2 pressure to reach similar catalytic activities in water.[12] We use water as the solvent in our computational study because it is the optimal solvent in the experimental study.

Table S2. Influence of solvents to the free energy barriers of the reactions catalysed by **1**, $\mathbf{1}_{\mathbf{Ir\text{-}OCOCH3}}$ and $\mathbf{1}_{\mathbf{Rh\text{-}OCH3}}$.

catalyst	solvent	Relative free energies (kcal/mol)	
		$\mathbf{1}_{\mathbf{M\text{-}R}}$	$\mathbf{TS}_{\mathbf{4,5\text{-}M\text{-}R}}$
1	^{i}PrOH	0.0	33.3
$\mathbf{1}_{\mathbf{Ir\text{-}OCOCH3}}$	^{i}PrOH	0.0	32.1
$\mathbf{1}_{\mathbf{Rh\text{-}OCH3}}$	^{i}PrOH	0.0	34.5
1	water	0.0	25.1
$\mathbf{1}_{\mathbf{Ir\text{-}OCOCH3}}$	water	0.0	24.0
$\mathbf{1}_{\mathbf{Rh\text{-}OCH3}}$	water	0.0	26.9

S4. Absolute free energies (Hartree) and Cartesian coordinates (Ångström) of all structures optimized in water

H_2O Gsolv= -76.407718

O	0.000000	0.000000	0.118252
H	0.000000	0.762582	-0.473009
H	0.000000	-0.762582	-0.473009

H_2 Gsolv= -1.168428

H	0.000000	0.000000	0.371430
H	0.000000	0.000000	-0.371430

$Cl^-(H_2O)$ Gsolv= -536.758228

O	-1.997332	-0.108355	0.000039
H	-2.328290	0.797184	0.000028
H	-1.017817	-0.021126	-0.000502
Cl	1.136751	0.005340	0.000009

Q(quinoline) Gsolv= -401.537817

C	-2.406747	0.703449	0.000000
C	-1.224430	1.404133	-0.000002

C	0.014692	0.717842	-0.000001
C	0.027187	-0.707110	0.000001
C	-1.206234	-1.402090	0.000003
C	-2.395159	-0.711050	0.000003
H	1.279122	2.477256	-0.000005
H	-3.355960	1.233906	0.000000
H	-1.218166	2.493291	-0.000003
C	1.259865	1.388368	-0.000003
H	-1.185553	-2.490258	0.000005
H	-3.337481	-1.254116	0.000004
C	2.417935	0.653214	-0.000002
H	3.394349	1.129082	-0.000003
N	1.188718	-1.426900	0.000001
C	2.323526	-0.755577	0.000000
H	3.238846	-1.347929	0.000000

protonated Q Gsolv= -401.977483

C	2.435506	0.694438	-0.000033
C	1.266692	1.415604	0.000149
C	0.020013	0.744902	0.000111
C	0.017387	-0.672814	0.000121
C	1.214371	-1.406673	-0.000028
C	2.406513	-0.719171	-0.000137
H	-1.221748	2.508870	-0.000079
H	3.392496	1.208795	-0.000037
H	1.272081	2.503265	0.000233
C	-1.219032	1.420711	-0.000132
H	1.178033	-2.493802	-0.000115
H	3.342247	-1.271773	-0.000314
C	-2.405799	0.718178	-0.000079
H	-3.366598	1.219895	-0.000213
C	-2.364388	-0.673976	-0.000099
H	-3.253949	-1.294499	0.000129
N	-1.196137	-1.311007	0.000167
H	-1.197170	-2.330901	-0.000013

1,4-dihydro-Q Gsolv= -402.704659

C	-2.465764	-0.708662	0.103612
C	-1.251392	-1.390355	0.041746
C	-0.036154	-0.714917	-0.071136
C	-0.053622	0.690248	-0.099211
C	-1.267818	1.382499	-0.032273
C	-2.467458	0.685956	0.061776
H	-3.400049	-1.259585	0.182900
H	-1.237990	-2.480129	0.073363
H	-1.257305	2.471936	-0.050989
H	-3.404670	1.236334	0.110576
C	2.335327	0.740885	0.154562
H	3.170959	1.397543	0.380335
C	1.268837	-1.465322	-0.193071
H	1.233693	-2.368872	0.431728
H	1.388850	-1.836894	-1.226350
N	1.150545	1.394185	-0.183407
H	1.098832	2.381850	0.034454
C	2.433236	-0.595069	0.183997
H	3.382708	-1.053057	0.447824

3,4-dihydro-Q Gsolv= -402.708552

C	-2.459341	0.710619	0.094145
C	-1.247517	1.391147	-0.027729
C	-0.043786	0.696554	-0.121021
C	-0.063741	-0.709506	-0.101579
C	-1.278097	-1.389364	0.011235
C	-2.473654	-0.683310	0.116407
H	-3.389866	1.268654	0.171647
H	-1.231094	2.480820	-0.044161
H	-1.270569	-2.478120	0.019518
H	-3.414745	-1.220399	0.210973
C	2.234550	-0.883642	0.022183
H	3.142666	-1.488606	-0.043424
N	1.121796	-1.477150	-0.217084
C	2.365887	0.554205	0.407740
H	2.262131	0.614552	1.504371
H	3.370187	0.917738	0.168835
C	1.284294	1.376996	-0.275578
H	1.521515	1.467073	-1.347841
H	1.245631	2.396143	0.124854

protonated 3,4-dihydro-Q Gsolv= -403.147951

C	-2.489005	0.702653	0.089835
C	-1.288277	1.405724	-0.007253
C	-0.074139	0.731025	-0.094948
C	-0.111071	-0.665690	-0.080137
C	-1.294933	-1.388439	0.007295
C	-2.495444	-0.691673	0.094417
H	-3.426724	1.248366	0.159822
H	-1.288172	2.494268	-0.017269
H	-1.267445	-2.476397	0.013234

H	-3.432474	-1.236849	0.167602
C	2.277414	-0.823664	0.039663
H	3.145299	-1.478301	0.007828
C	2.384595	0.611486	0.345145
H	2.366304	0.669089	1.448618
H	3.369100	0.977595	0.042255
C	1.248085	1.419337	-0.269922
H	1.439275	1.549948	-1.345114
H	1.218470	2.421709	0.167481
N	1.122688	-1.370866	-0.153104
H	1.074198	-2.377917	-0.317298

1,2,3,4-tetrahydro-Q Gsolv= -403.902451

C	2.554454	0.684931	0.055649
C	1.348989	1.377998	-0.062557
C	0.124458	0.717554	-0.139769
C	0.103287	-0.693261	-0.086283
C	1.314925	-1.392363	0.052096
C	2.523939	-0.709438	0.117320
H	3.497624	1.223619	0.110306
H	1.349091	2.468455	-0.090076
H	1.291275	-2.480992	0.104957
H	3.449545	-1.272857	0.221584
C	-1.184542	1.451065	-0.227827
H	-1.074747	2.460852	0.187313
H	-1.487576	1.576098	-1.280013
C	-2.266633	0.664498	0.503103
H	-3.235667	1.172015	0.437311
H	-2.006722	0.582519	1.568595
C	-2.387402	-0.719631	-0.104705
H	-2.835742	-0.632408	-1.106982
H	-3.057850	-1.349530	0.489937
N	-1.088851	-1.382348	-0.192903
H	-1.056131	-2.359457	0.065221

1 Gsolv= -1521.538261

Ir	0.548922	0.021168	-0.115270
Cl	0.000236	0.011081	-2.537993
C	1.970727	-1.030928	1.153870
C	2.518481	-0.879522	-0.164297
C	2.706474	0.548000	-0.401622
C	2.246018	1.250186	0.733305
C	1.727503	0.284376	1.685886
C	1.741212	-2.300542	1.893567
H	1.744900	-3.168821	1.229066
H	0.793427	-2.285237	2.443487
H	2.545281	-2.438728	2.628562
C	2.990442	-1.959603	-1.073294
H	4.083592	-2.051791	-1.020248
H	2.727326	-1.747992	-2.115758
H	2.560525	-2.930348	-0.804976
C	3.302506	1.133444	-1.630677
H	2.956557	2.159698	-1.796587
H	3.047244	0.543052	-2.516892
H	4.397289	1.154534	-1.547379
C	2.290237	2.718013	0.960111
H	3.188972	2.972090	1.537972
H	1.426807	3.066644	1.538283
H	2.332593	3.279636	0.020718
C	1.219162	0.598872	3.048870
H	0.574537	-0.201946	3.426771
H	0.642016	1.530567	3.056766
H	2.053551	0.719967	3.753174
N	-1.112246	1.434002	0.002662
C	-0.952879	2.751919	-0.165129
H	0.063386	3.099333	-0.335497
C	-2.019568	3.639372	-0.134460
H	-1.838113	4.700746	-0.270744
C	-3.301328	3.138599	0.066149
H	-4.157573	3.806545	0.099133
C	-3.483566	1.768284	0.207875
H	-4.476963	1.351905	0.342236
C	-2.369487	0.937231	0.160728
C	-2.334977	-0.504750	0.201244
C	-1.113155	-1.155537	0.065898
N	-3.305200	-1.452237	0.213154
C	-4.751664	-1.296101	0.297900
H	-5.193814	-2.292216	0.300788
H	-5.104221	-0.734468	-0.570974
H	-5.008638	-0.770472	1.220261
N	-2.796305	-2.657282	0.087022
N	-1.482298	-2.460949	-0.010689
C	-0.633015	-3.625757	-0.211411
H	-0.400025	-4.094236	0.747894
H	0.281972	-3.289606	-0.703489
H	-1.158042	-4.335253	-0.853039

2 Gsolv= -1061.172902

Ir	0.572608	0.033153	-0.288597	N	-1.491350	-2.488772	-0.229566
C	1.705427	-0.660619	1.350583	C	-0.648403	-3.671314	-0.329772
C	2.348148	-1.151648	0.157256	H	-0.143833	-3.844707	0.624586
C	2.775840	-0.003321	-0.592377	H	0.082552	-3.512531	-1.124189
C	2.437105	1.193539	0.115321	H	-1.281822	-4.525428	-0.571678
C	1.757685	0.796619	1.316073				
C	1.178638	-1.473343	2.475805	3 Gsolv= -1062.330706			
H	0.913332	-2.484752	2.150851	Ir	0.586804	0.029595	-0.315746
H	0.292692	-1.010341	2.923661	C	1.734039	-0.956452	1.198608
H	1.943527	-1.559330	3.259144	C	2.483853	-0.993656	-0.020861
C	2.668713	-2.564239	-0.185146	C	2.794625	0.381533	-0.385523
H	3.728560	-2.763370	0.021578	C	2.234630	1.253823	0.575722
H	2.495552	-2.773106	-1.246770	C	1.505019	0.438857	1.535109
H	2.076039	-3.270186	0.403976	C	1.306776	-2.107334	2.034228
C	3.413821	-0.066532	-1.928262	H	1.295047	-3.042381	1.467547
H	3.286579	0.866376	-2.485519	H	0.313831	-1.946307	2.467997
H	3.008079	-0.893144	-2.521936	H	2.014471	-2.226198	2.865239
H	4.491274	-0.246715	-1.811128	C	2.993439	-2.196206	-0.735472
C	2.769266	2.578582	-0.317794	H	4.077821	-2.290023	-0.591408
H	3.840632	2.773718	-0.180915	H	2.808070	-2.133054	-1.813915
H	2.222527	3.326730	0.264852	H	2.526373	-3.113170	-0.363081
H	2.539964	2.736204	-1.378218	C	3.563559	0.778046	-1.591763
C	1.248289	1.693100	2.382957	H	3.228865	1.742613	-1.987818
H	0.348537	1.283363	2.854201	H	3.482160	0.027540	-2.384082
H	1.015145	2.691420	1.999127	H	4.626974	0.872948	-1.334217
H	2.012373	1.802276	3.164217	C	2.383808	2.732506	0.614248
N	-1.086028	1.436745	-0.265462	H	3.316223	2.997076	1.129985
C	-0.915142	2.762236	-0.333236	H	1.562994	3.213888	1.155978
H	0.105865	3.114552	-0.456756	H	2.434171	3.162155	-0.392714
C	-1.979417	3.651274	-0.252379	C	0.795737	0.932952	2.742256
H	-1.791815	4.718514	-0.310251	H	-0.030957	0.266703	3.012660
C	-3.261315	3.143985	-0.090132	H	0.390049	1.938110	2.584676
H	-4.114662	3.811763	-0.012858	H	1.487080	0.978236	3.594277
C	-3.451541	1.765678	-0.030522	N	-1.077018	1.438801	-0.326096
H	-4.447268	1.351232	0.089259	C	-0.911596	2.761013	-0.451163
C	-2.345016	0.934920	-0.128249	H	0.100980	3.105297	-0.645456
C	-2.317147	-0.514041	-0.117455	C	-1.969616	3.654105	-0.349116
C	-1.108241	-1.185085	-0.251685	H	-1.785461	4.717762	-0.460310
N	-3.296322	-1.447423	-0.021069	C	-3.242574	3.155951	-0.101241
C	-4.735377	-1.276084	0.138949	H	-4.090402	3.828275	-0.005446
H	-5.184150	-2.268038	0.186466	C	-3.428956	1.782321	0.016546
H	-5.131931	-0.725294	-0.717149	H	-4.416783	1.371712	0.199673
H	-4.932741	-0.733723	1.066678	C	-2.327893	0.945235	-0.109445
N	-2.799701	-2.663474	-0.090887	C	-2.302443	-0.500998	-0.078441

C	-1.096530	-1.168824	-0.260459
N	-3.277457	-1.437462	0.022940
C	-4.707867	-1.268850	0.250884
H	-5.153945	-2.261374	0.309672
H	-5.145924	-0.708731	-0.578591
H	-4.859244	-0.735056	1.192050
N	-2.785553	-2.650838	-0.097561
N	-1.479337	-2.471640	-0.272724
C	-0.652010	-3.656304	-0.455196
H	-0.514911	-4.165383	0.502259
H	0.309442	-3.334304	-0.857693
H	-1.144805	-4.325149	-1.163018
H	0.623867	-0.459121	-2.675395
H	0.759689	0.280800	-2.775852

4 Gsolv= -1463.857897

Ir	-0.473822	-0.444530	0.224804
C	-0.974994	-2.116670	1.560885
C	0.344014	-2.320629	1.045249
C	1.197272	-1.264186	1.568367
C	0.397907	-0.380834	2.321846
C	-0.980194	-0.856407	2.266369
C	-2.134197	-3.038575	1.454049
H	-2.013529	-3.761243	0.642415
H	-3.077037	-2.498747	1.315364
H	-2.216350	-3.602409	2.392706
C	0.828924	-3.477872	0.245335
H	1.309370	-4.217738	0.899083
H	1.571104	-3.160397	-0.497035
H	0.009204	-3.975476	-0.282600
C	2.665287	-1.183039	1.356555
H	3.041757	-0.161932	1.482008
H	2.948965	-1.541560	0.360460
H	3.177901	-1.820895	2.089383
C	0.864923	0.805265	3.084392
H	1.144731	0.493790	4.099585
H	0.082318	1.564632	3.184421
H	1.747670	1.268534	2.628581
C	-2.137802	-0.264384	2.991484
H	-3.082623	-0.514372	2.495936
H	-2.059954	0.827459	3.042022
H	-2.185366	-0.644259	4.020480
N	-1.102169	1.654167	0.116831
C	-0.374195	2.664581	0.605348
H	0.620656	2.414536	0.965325
C	-0.850154	3.967819	0.648291
H	-0.219317	4.753676	1.052016
C	-2.128967	4.230632	0.170875
H	-2.533293	5.238468	0.199142
C	-2.888497	3.191213	-0.354607
H	-3.886146	3.371424	-0.742896
C	-2.344766	1.912877	-0.378710
C	-2.925245	0.710697	-0.929343
C	-2.217331	-0.479568	-0.840469
N	-4.032143	0.465758	-1.673182
C	-5.091761	1.379256	-2.081100
H	-5.790638	0.821660	-2.704345
H	-4.654059	2.201582	-2.652301
H	-5.602056	1.761387	-1.194029
N	-4.075921	-0.787923	-2.065750
N	-2.973668	-1.340217	-1.565974
C	-2.702823	-2.737589	-1.876434
H	-3.377451	-3.384213	-1.310501
H	-1.664279	-2.941845	-1.608009
H	-2.848303	-2.895683	-2.946819
H	0.085127	-0.674778	-1.500511
H	0.649236	-0.118451	-1.230155
C	4.405684	2.570608	0.462331
C	5.189377	1.478976	0.172982
C	4.751640	0.510751	-0.763304
C	3.493947	0.678619	-1.411397
C	2.710591	1.816939	-1.099596
C	3.156698	2.738498	-0.180210
H	6.467671	-0.798811	-0.585770
H	4.742585	3.311089	1.183830
H	6.152800	1.335681	0.660262
C	5.503201	-0.647479	-1.068421
H	1.751608	1.942845	-1.601839
H	2.545588	3.608742	0.054089
C	4.996974	-1.560297	-1.958539
H	5.536802	-2.467479	-2.215346
N	3.011709	-0.228632	-2.312388
C	3.741467	-1.300936	-2.551715
H	3.333043	-2.018078	-3.264690

5 Gsolv= -1061.906539

Ir	0.529375	0.009772	-0.316064
C	1.864934	-0.679096	1.357296

C	2.378960	-1.087464	0.059576	H	-0.061176	-3.823433	0.627303
C	2.737618	0.113401	-0.658252	H	0.096622	-3.434244	-1.114338
C	2.373054	1.234830	0.132236	H	-1.224583	-4.494406	-0.548270
C	1.829250	0.739861	1.386783	H	0.162722	-0.111537	-1.901982
C	1.462343	-1.600368	2.457200				
H	1.102562	-2.559321	2.068607	6 Gsolv= -1463.883674			
H	0.666388	-1.169648	3.074639	Ir	-0.978191	0.071362	-0.149520
H	2.316017	-1.813880	3.114591	C	-2.974192	-0.552161	-1.039118
C	2.776269	-2.469647	-0.336436	C	-2.525067	-1.463437	-0.002469
H	3.837926	-2.641269	-0.109508	C	-2.516519	-0.731517	1.241298
H	2.638211	-2.637781	-1.410776	C	-2.863263	0.618689	0.965950
H	2.198522	-3.229881	0.199824	C	-3.162713	0.724496	-0.451904
C	3.412455	0.157887	-1.985271	C	-3.217849	-0.922920	-2.461946
H	3.155187	1.067953	-2.538003	H	-2.520668	-1.697655	-2.799810
H	3.143264	-0.704282	-2.604772	H	-3.110862	-0.061024	-3.129366
H	4.503180	0.144076	-1.853862	H	-4.234213	-1.319767	-2.589867
C	2.649858	2.663758	-0.191565	C	-2.391981	-2.944609	-0.122089
H	3.700436	2.908662	0.016991	H	-3.325930	-3.439343	0.179671
H	2.037288	3.342181	0.412669	H	-1.591521	-3.330747	0.521810
H	2.465367	2.886690	-1.249206	H	-2.175643	-3.250484	-1.151095
C	1.361306	1.604280	2.506285	C	-2.238618	-1.314789	2.584116
H	0.747867	1.042521	3.218756	H	-1.902699	-0.550880	3.294661
H	0.763350	2.448876	2.140138	H	-1.474843	-2.100377	2.534627
H	2.213133	2.026399	3.056509	H	-3.151305	-1.769656	2.993135
N	-1.117234	1.417788	-0.237095	C	-3.050251	1.695676	1.980177
C	-0.958599	2.748442	-0.305575	H	-4.024295	1.592844	2.477867
H	0.056040	3.106615	-0.458657	H	-3.026876	2.692368	1.525393
C	-2.020931	3.633824	-0.203232	H	-2.278854	1.658191	2.759814
H	-1.833367	4.701453	-0.260709	C	-3.607976	1.973189	-1.132076
C	-3.306611	3.128413	-0.033314	H	-3.479732	1.908580	-2.217717
H	-4.159261	3.796686	0.048300	H	-3.043653	2.845984	-0.779510
C	-3.490098	1.754009	0.028132	H	-4.669489	2.172704	-0.931156
H	-4.481684	1.331101	0.157622	N	0.213014	1.875646	-0.236051
C	-2.378875	0.921577	-0.072722	C	-0.037964	2.957575	0.518757
C	-2.344446	-0.516182	-0.035381	H	-0.930476	2.916885	1.137630
C	-1.111471	-1.158514	-0.145948	C	0.785587	4.071669	0.527142
N	-3.305417	-1.472229	0.021526	H	0.527668	4.921204	1.151889
C	-4.751516	-1.326198	0.119364	C	1.931692	4.069736	-0.264881
H	-5.187635	-2.325070	0.123446	H	2.600491	4.925872	-0.276125
H	-5.115906	-0.763884	-0.743876	C	2.214653	2.954557	-1.039765
H	-5.005190	-0.805212	1.045660	H	3.105285	2.923277	-1.659832
N	-2.786046	-2.677130	-0.042302	C	1.338793	1.870245	-1.008723
N	-1.471950	-2.473068	-0.148433	C	1.453729	0.616357	-1.703861
C	-0.605605	-3.631034	-0.300843	C	0.479873	-0.360972	-1.487865

N	2.398403	0.085543	-2.520753	H	1.724127	2.237054	2.169630
C	3.651900	0.663535	-2.984315	H	0.259157	3.186978	2.499857
H	4.150907	-0.078572	-3.608044	C	2.707262	1.684695	-0.551703
H	4.278789	0.905707	-2.121064	H	2.969674	0.957870	-1.328104
H	3.447444	1.564230	-3.568171	H	2.936583	1.254385	0.430603
N	2.111806	-1.155219	-2.841046	H	3.349624	2.566466	-0.683295
N	0.955887	-1.405421	-2.223903	C	0.951235	1.539668	-3.156731
C	0.412215	-2.750837	-2.309664	H	1.645944	2.272181	-3.587030
H	-0.536177	-2.739690	-2.852803	H	0.125655	1.416306	-3.864607
H	0.261632	-3.135268	-1.296149	H	1.487235	0.583618	-3.083548
H	1.131552	-3.377931	-2.838547	C	-2.026428	2.527506	-2.356946
H	0.206449	-0.405697	0.823963	H	-2.950281	2.296254	-1.815687
C	2.859923	-2.971164	0.304704	H	-1.944398	1.842526	-3.206801
C	3.304626	-1.672908	0.363522	H	-2.118274	3.547956	-2.751743
C	2.826765	-0.803579	1.373685	N	-1.534453	-0.847296	-1.155354
C	1.907154	-1.315374	2.324513	C	-1.449828	-1.103974	-2.466605
C	1.473224	-2.650856	2.275031	H	-0.858906	-0.411733	-3.060318
C	1.941664	-3.458494	1.264216	C	-2.085720	-2.191950	-3.051925
H	3.887315	0.957445	0.715305	H	-1.994024	-2.353483	-4.121152
H	3.210615	-3.632382	-0.484002	C	-2.821431	-3.049703	-2.245847
H	4.011609	-1.283314	-0.367641	H	-3.327948	-3.911396	-2.671111
C	3.178127	0.561275	1.441327	C	-2.905932	-2.799468	-0.878453
H	0.764194	-3.012343	3.017253	H	-3.468808	-3.461532	-0.228167
H	1.598819	-4.488206	1.200233	C	-2.253280	-1.690556	-0.360295
C	2.619628	1.384511	2.397659	C	-2.190198	-1.259804	1.020015
H	2.859889	2.440829	2.454337	C	-1.403738	-0.166668	1.362804
C	1.720296	0.841181	3.313083	N	-2.764143	-1.725791	2.157171
H	1.243081	1.425002	4.093370	C	-3.652629	-2.865438	2.354947
N	1.419639	-0.455702	3.273512	H	-3.928507	-2.891148	3.408952
H	0.740189	-0.821019	3.941646	H	-3.127736	-3.784282	2.082491
				H	-4.544775	-2.738107	1.737607
7 Gsolv= -1463.870971				N	-2.396951	-1.012196	3.199392
Ir	-0.406290	0.748640	-0.204428	N	-1.584042	-0.085834	2.708319
C	-0.829262	2.827987	-0.060269	C	-0.986748	0.868144	3.631346
C	0.506635	2.618491	0.439827	H	-1.440140	1.852142	3.485532
C	1.286716	2.091799	-0.646668	H	0.087518	0.915768	3.441018
C	0.472735	2.000982	-1.823395	H	-1.171256	0.522463	4.648841
C	-0.843750	2.441060	-1.464553	H	0.620012	-1.099082	-0.088996
C	-1.971617	3.422419	0.678474	C	3.753686	-0.784376	2.599964
H	-1.876483	3.264521	1.757862	C	2.590262	-1.228091	1.980408
H	-2.925182	2.995798	0.350260	C	2.576521	-1.606003	0.636097
H	-2.009002	4.504952	0.497440	C	3.773516	-1.530858	-0.095190
C	1.053025	3.006647	1.768978	C	4.951705	-1.091998	0.524061
H	1.634883	3.932828	1.672612	C	4.939121	-0.719385	1.860646

H	0.698778	-2.673757	0.617878
H	3.741287	-0.492003	3.647195
H	1.656264	-1.281919	2.542229
C	1.295650	-2.010450	-0.028017
H	5.869632	-1.044996	-0.060422
H	5.858262	-0.376857	2.330710
C	1.490658	-2.563506	-1.392729
H	0.655567	-3.039336	-1.902195
C	2.674835	-2.457044	-2.026387
H	2.831409	-2.830428	-3.034446
N	3.783426	-1.890870	-1.436281
H	4.673549	-1.932183	-1.915997

8 Gsolv= -1465.034755

Ir	-0.707588	-0.669564	0.146656
C	-1.704335	-2.301967	1.074938
C	-0.865989	-2.827562	0.032811
C	0.504582	-2.524300	0.392963
C	0.530597	-1.819533	1.622050
C	-0.845073	-1.627503	2.033094
C	-3.173323	-2.465244	1.222141
H	-3.636111	-2.812196	0.294027
H	-3.655497	-1.529727	1.526214
H	-3.379064	-3.212037	2.000242
C	-1.273234	-3.664904	-1.128601
H	-1.010209	-4.715366	-0.947278
H	-0.763434	-3.349807	-2.046711
H	-2.352453	-3.616072	-1.303415
C	1.691119	-2.861071	-0.430027
H	2.499846	-2.134502	-0.287889
H	1.444651	-2.912408	-1.496075
H	2.075015	-3.846618	-0.131806
C	1.754606	-1.396838	2.354964
H	2.212774	-2.263799	2.848602
H	1.531844	-0.659590	3.132992
H	2.507816	-0.972917	1.677474
C	-1.306694	-0.978538	3.285484
H	-2.308848	-0.553562	3.165181
H	-0.627613	-0.179949	3.601826
H	-1.350783	-1.721760	4.092878
N	-0.461334	1.440677	0.755781
C	0.524027	1.861665	1.556253
H	1.225944	1.104918	1.896479
C	0.652548	3.188316	1.947188
H	1.465954	3.475515	2.606660
C	-0.268041	4.114725	1.474962
H	-0.196351	5.161161	1.757683
C	-1.292749	3.691030	0.634149
H	-2.024716	4.397061	0.255360
C	-1.368772	2.345942	0.296121
C	-2.359378	1.698510	-0.538232
C	-2.287369	0.330672	-0.762892
N	-3.419968	2.172007	-1.240221
C	-3.936730	3.531676	-1.343898
H	-4.807591	3.507567	-1.998863
H	-3.167492	4.180050	-1.770127
H	-4.226004	3.884901	-0.351365
N	-4.018577	1.207453	-1.904032
N	-3.324411	0.113387	-1.612145
C	-3.717556	-1.139473	-2.241686
H	-4.309747	-1.737914	-1.545084
H	-2.812008	-1.677050	-2.530478
H	-4.311750	-0.909044	-3.126611
H	0.235995	-0.501313	-2.230159
H	0.534468	0.125579	-1.929087
C	5.119447	-1.561025	-1.205864
C	5.073001	-0.629370	-0.168630
C	4.255225	0.495903	-0.251398
C	3.455652	0.675330	-1.395027
C	3.500988	-0.261175	-2.431539
C	4.335827	-1.371637	-2.343573
H	5.769316	-2.429752	-1.126667
H	5.689717	-0.767645	0.719494
H	2.874955	-0.103752	-3.308513
H	4.368393	-2.091934	-3.158104
C	2.750615	2.778641	-0.748308
H	2.068152	3.626519	-0.866680
N	2.573354	1.776537	-1.530779
C	3.847458	2.886509	0.261974
H	4.724921	3.304997	-0.259611
H	3.576208	3.607915	1.039853
C	4.179371	1.520264	0.843428
H	3.399369	1.224649	1.565310
H	5.120257	1.549669	1.404471

9 Gsolv= -1465.048829

Ir	-0.548821	-0.700398	0.137125
C	-1.183805	-2.830005	0.493122

C	-0.137721	-2.746817	-0.510326	H	-2.832815	-1.937424	-2.837474
C	1.049047	-2.250834	0.139268	H	-1.299556	-1.169970	-3.356035
C	0.734952	-1.957232	1.496642	H	-2.839936	-0.719310	-4.143404
C	-0.656624	-2.320333	1.710120	H	0.342057	0.346818	-0.727827
C	-2.552617	-3.372325	0.261692	C	5.897059	0.410200	0.042430
H	-2.904905	-3.148558	-0.752123	C	4.837712	0.979036	0.748850
H	-3.277958	-2.954363	0.968120	C	3.685347	1.402178	0.091741
H	-2.564305	-4.464538	0.379160	C	3.636085	1.234741	-1.295073
C	-0.173571	-3.361759	-1.868203	C	4.679600	0.669693	-2.019959
H	0.237042	-4.380519	-1.829208	C	5.819822	0.253857	-1.341146
H	0.425122	-2.794270	-2.589998	H	6.787439	0.086722	0.576035
H	-1.194887	-3.437130	-2.255344	H	4.897772	1.094822	1.830055
C	2.385793	-2.116391	-0.505552	H	4.589343	0.556543	-3.098843
H	2.998621	-1.349972	-0.015293	H	6.644864	-0.190083	-1.891496
H	2.297521	-1.857995	-1.567134	C	1.481672	2.277045	-1.437735
H	2.929019	-3.069389	-0.442548	H	0.622834	2.506178	-2.066234
C	1.699552	-1.539243	2.553143	C	1.611098	2.806676	-0.069354
H	2.180335	-2.418585	3.003856	H	2.055867	3.809267	-0.205597
H	1.207281	-0.995343	3.367541	H	0.617013	2.975760	0.357444
H	2.496931	-0.901577	2.151354	C	2.486407	1.935562	0.821900
C	-1.366431	-2.205514	3.013862	H	1.891923	1.078727	1.177225
H	-2.453960	-2.218039	2.884926	H	2.796593	2.496524	1.709749
H	-1.098301	-1.280474	3.539780	N	2.454827	1.620658	-1.984671
H	-1.097283	-3.040605	3.674758	H	2.370723	1.332310	-2.960587
N	-1.138077	1.052947	1.264922				
C	-0.615584	1.373742	2.459308	10 Gsolv= -1465.071792			
H	0.108555	0.677566	2.874899	Ir	0.405637	0.646197	0.224625
C	-0.962215	2.530370	3.140825	C	0.946864	2.661103	0.506517
H	-0.510366	2.736645	4.106143	C	-0.248602	2.646931	-0.299631
C	-1.882291	3.402666	2.565819	C	-1.298414	2.073385	0.505366
H	-2.170083	4.319425	3.072833	C	-0.786391	1.723145	1.787438
C	-2.433985	3.085913	1.332299	C	0.615116	2.063551	1.793213
H	-3.155916	3.746087	0.861560	C	2.261902	3.254432	0.152016
C	-2.049389	1.903172	0.705440	H	2.388273	3.336839	-0.932305
C	-2.492518	1.388411	-0.562598	H	3.089858	2.658318	0.550916
C	-1.959982	0.183120	-1.021031	H	2.339920	4.263137	0.578376
N	-3.346082	1.850796	-1.511015	C	-0.446591	3.257806	-1.642581
C	-4.149164	3.066057	-1.521024	H	-0.992300	4.205789	-1.545763
H	-4.721697	3.080975	-2.448350	H	-1.034391	2.605429	-2.299191
H	-3.489742	3.936349	-1.476202	H	0.506637	3.469551	-2.135344
H	-4.827323	3.060394	-0.664303	C	-2.696917	1.890532	0.048988
N	-3.396644	1.041815	-2.544127	H	-3.204514	1.074555	0.575526
N	-2.560181	0.049580	-2.236925	H	-2.752607	1.709478	-1.029912
C	-2.370835	-1.017463	-3.205016	H	-3.253151	2.816908	0.250730

C	-1.575841	1.159296	2.916513	C	-1.191472	-2.431526	-0.931565
H	-2.173919	1.947739	3.391542	H	-1.554217	-3.403448	-1.295476
H	-0.928529	0.731791	3.689122	H	-0.134045	-2.558661	-0.665111
H	-2.270298	0.380627	2.577806	C	-2.000601	-1.983219	0.276210
C	1.555495	1.914027	2.931498	H	-1.498788	-1.105273	0.727330
H	2.577712	1.734855	2.581249	H	-2.022726	-2.756495	1.056425
H	1.266404	1.090716	3.592955	N	-2.728816	-1.307106	-2.433749
H	1.563715	2.837097	3.526254	H	-2.902628	-0.696681	-3.224747
N	1.278118	-1.111193	1.215890				
C	0.807913	-1.610757	2.364362	$TS_{4,5}$ Gsolv= -1463.853944			
H	-0.041280	-1.096100	2.807000	Ir	-0.487704	-0.371239	0.305484
C	1.364286	-2.729174	2.971182	C	-1.110603	-1.830506	1.797872
H	0.947354	-3.094886	3.903926	C	0.142146	-2.250960	1.218944
C	2.447629	-3.349693	2.362473	C	1.148964	-1.288006	1.625647
H	2.908684	-4.224926	2.811271	C	0.521425	-0.254169	2.350874
C	2.941907	-2.842484	1.164487	C	-0.898908	-0.563543	2.433669
H	3.783259	-3.315698	0.668493	C	-2.395116	-2.580389	1.793925
C	2.333538	-1.723992	0.611104	H	-2.412420	-3.355960	1.022877
C	2.656905	-1.069546	-0.639799	H	-3.253660	-1.916463	1.642826
C	1.903902	0.016605	-1.064278	H	-2.527691	-3.074264	2.765456
N	3.567000	-1.339951	-1.610021	C	0.441643	-3.553424	0.559902
C	4.600767	-2.366669	-1.660511	H	0.914434	-4.242694	1.272820
H	5.144912	-2.244083	-2.596893	H	1.133582	-3.422672	-0.281182
H	4.132357	-3.353263	-1.628265	H	-0.465699	-4.035396	0.181790
H	5.277899	-2.237177	-0.813375	C	2.606096	-1.435413	1.378858
N	3.440540	-0.511029	-2.623005	H	3.136043	-0.478183	1.440455
N	2.435083	0.287672	-2.285185	H	2.812939	-1.895328	0.405796
C	2.009391	1.301077	-3.240492	H	3.031071	-2.099435	2.144291
H	2.350763	2.287069	-2.915162	C	1.201672	0.906366	2.987527
H	0.919478	1.278865	-3.306907	H	1.622191	0.605929	3.956419
H	2.445644	1.062221	-4.210898	H	0.508613	1.732647	3.176836
H	-0.943604	-0.425860	-1.683919	H	2.030071	1.281785	2.373315
C	-5.687874	-1.041966	0.546692	C	-1.927307	0.233226	3.157154
C	-4.407860	-1.497868	0.857581	H	-2.918468	0.100555	2.707649
C	-3.399794	-1.577624	-0.103461	H	-1.691222	1.303366	3.143245
C	-3.692286	-1.201037	-1.429793	H	-1.990559	-0.079335	4.207873
C	-4.981315	-0.745003	-1.745112	N	-1.146502	1.707572	0.058610
C	-5.965972	-0.660900	-0.767049	C	-0.497530	2.757090	0.577796
H	-6.454833	-0.984384	1.315595	H	0.460140	2.550589	1.049433
H	-4.168943	-1.792774	1.880639	C	-1.005864	4.047731	0.525162
H	-5.197791	-0.451400	-2.772413	H	-0.438330	4.864160	0.960113
H	-6.956424	-0.297749	-1.034503	C	-2.236683	4.259463	-0.084610
C	-1.331846	-1.406642	-2.041032	H	-2.663754	5.256810	-0.139075
H	-0.738417	-1.680781	-2.920638	C	-2.921651	3.179502	-0.628561

H	-3.885287	3.318448	-1.108333
C	-2.352162	1.914212	-0.544142
C	-2.873945	0.672089	-1.065644
C	-2.150719	-0.496681	-0.865109
N	-3.932932	0.361335	-1.854729
C	-4.990013	1.223819	-2.369046
H	-5.651425	0.610773	-2.981217
H	-4.542875	2.013550	-2.977717
H	-5.544565	1.656453	-1.533263
N	-3.931541	-0.912947	-2.177354
N	-2.848865	-1.411937	-1.584309
C	-2.531603	-2.817578	-1.796587
H	-3.120340	-3.445545	-1.122942
H	-1.464714	-2.949718	-1.605234
H	-2.757730	-3.075204	-2.832557
H	0.117580	-0.227294	-1.334675
H	1.001267	-0.087161	-1.203900
C	5.480188	2.131031	0.034500
C	5.810195	0.966820	-0.617504
C	4.800860	0.173926	-1.216288
C	3.448062	0.603471	-1.131956
C	3.131388	1.813259	-0.475046
C	4.132593	2.557270	0.102889
H	6.098712	-1.385058	-1.967650
H	6.256322	2.735453	0.497203
H	6.844311	0.633416	-0.683823
C	5.068539	-1.042469	-1.886370
H	2.090486	2.130529	-0.439094
H	3.889809	3.485219	0.615680
C	4.033202	-1.778232	-2.412163
H	4.204657	-2.719511	-2.925197
N	2.444303	-0.151743	-1.659166
C	2.720739	-1.295176	-2.253985
H	1.864823	-1.867424	-2.618101

$TS_{6,7}$ Gsolv= -1463.863439

Ir	-0.423051	0.745712	-0.046322
C	-0.749753	2.853964	0.567722
C	0.601968	2.441284	0.876377
C	1.260762	2.156536	-0.371867
C	0.330451	2.336859	-1.437079
C	-0.920345	2.767901	-0.851334
C	-1.760899	3.324411	1.553676
H	-1.622626	2.842260	2.527860
H	-2.781645	3.116687	1.215782
H	-1.673768	4.408540	1.707416
C	1.284575	2.537710	2.197792
H	1.845366	3.480022	2.265480
H	1.999692	1.719155	2.344786
H	0.569633	2.519433	3.026386
C	2.682397	1.749075	-0.514394
H	2.850337	1.199200	-1.447421
H	3.008040	1.121590	0.324796
H	3.328105	2.637898	-0.527169
C	0.634805	2.197117	-2.889617
H	1.245748	3.039088	-3.241260
H	-0.278931	2.187302	-3.494138
H	1.193658	1.275594	-3.101132
C	-2.153760	3.097158	-1.614609
H	-3.043784	3.055363	-0.978227
H	-2.302922	2.408321	-2.454679
H	-2.085860	4.110966	-2.031509
N	-1.642982	-0.595024	-1.218280
C	-1.661199	-0.570036	-2.559353
H	-1.089498	0.221831	-3.036929
C	-2.363723	-1.499865	-3.311711
H	-2.353306	-1.428177	-4.394712
C	-3.060813	-2.508422	-2.654396
H	-3.615265	-3.255461	-3.215364
C	-3.039271	-2.555697	-1.265838
H	-3.568697	-3.337648	-0.730418
C	-2.325509	-1.584419	-0.571247
C	-2.153725	-1.454094	0.853407
C	-1.328091	-0.443551	1.343658
N	-2.611970	-2.165219	1.914353
C	-3.473346	-3.340172	1.937357
H	-3.659335	-3.597290	2.980159
H	-2.968319	-4.167055	1.431802
H	-4.416683	-3.108181	1.437557
N	-2.137589	-1.693373	3.044873
N	-1.370248	-0.665450	2.687521
C	-0.666297	0.063226	3.731141
H	-1.107798	1.055792	3.854963
H	0.385786	0.153085	3.449990
H	-0.754483	-0.498147	4.661937
H	0.628056	-0.589716	-0.134262
C	3.970154	-1.275184	2.194205
C	2.746481	-1.578294	1.634323

C	2.608714	-1.701951	0.238979
C	3.742682	-1.501616	-0.574794
C	4.988315	-1.194114	-0.005345
C	5.093398	-1.083147	1.366367
H	0.557590	-2.412711	0.241797
H	4.070892	-1.180914	3.272254
H	1.862582	-1.718719	2.256505
C	1.330817	-1.957786	-0.379370
H	5.849771	-1.048744	-0.653962
H	6.055808	-0.844157	1.811793
C	1.308335	-2.190715	-1.778055
H	0.397195	-2.508820	-2.276759
C	2.442146	-1.981096	-2.520932
H	2.470432	-2.117800	-3.597076
N	3.609715	-1.635030	-1.939905
H	4.435081	-1.510222	-2.519795

$TS_{8,5}$ Gsolv= -1465.027023

Ir	-0.667407	-0.657799	0.032777
C	-1.752053	-2.138997	1.197833
C	-1.214549	-2.780054	0.017360
C	0.219029	-2.728344	0.113958
C	0.584137	-2.038645	1.307616
C	-0.643405	-1.671451	1.980437
C	-3.189345	-2.044583	1.573088
H	-3.837480	-2.074388	0.690263
H	-3.402509	-1.118923	2.118888
H	-3.467314	-2.886253	2.220822
C	-1.959840	-3.589483	-0.985604
H	-1.856716	-4.657147	-0.747533
H	-1.569384	-3.440885	-1.998749
H	-3.028165	-3.355327	-0.988051
C	1.131473	-3.369811	-0.866863
H	2.178062	-3.108988	-0.687637
H	0.870425	-3.104011	-1.897801
H	1.034580	-4.460588	-0.779513
C	1.968731	-1.843604	1.824216
H	2.307799	-2.739217	2.361574
H	2.024938	-1.005318	2.527288
H	2.682176	-1.654605	1.011259
C	-0.741086	-0.982350	3.293556
H	-1.668022	-0.404849	3.377572
H	0.103364	-0.306239	3.465680
H	-0.736735	-1.726352	4.101048
N	-0.342131	1.368470	0.776733
C	0.721202	1.704673	1.519167
H	1.434616	0.911200	1.732086
C	0.916921	2.994096	1.994396
H	1.790063	3.214117	2.601301
C	-0.007368	3.978384	1.663113
H	0.122488	4.999353	2.010893
C	-1.104026	3.646296	0.876382
H	-1.835340	4.398398	0.597686
C	-1.250485	2.330005	0.452377
C	-2.299618	1.770349	-0.365075
C	-2.244300	0.425169	-0.711346
N	-3.399361	2.301169	-0.956040
C	-3.908354	3.666764	-0.913749
H	-4.828540	3.697812	-1.497028
H	-3.167018	4.341636	-1.348776
H	-4.112082	3.943386	0.123264
N	-4.045902	1.396683	-1.655776
N	-3.337847	0.280091	-1.504808
C	-3.794399	-0.919755	-2.189487
H	-4.376009	-1.541945	-1.503598
H	-2.918203	-1.465130	-2.544933
H	-4.416210	-0.621488	-3.034497
H	0.004561	-0.138202	-1.548899
H	0.811976	0.198540	-1.331888
C	5.668139	-1.109311	-0.612007
C	5.513928	0.186415	-0.116340
C	4.358394	0.918249	-0.377688
C	3.344256	0.314832	-1.138505
C	3.498707	-0.972466	-1.649219
C	4.663987	-1.687121	-1.387493
H	6.579255	-1.663880	-0.399261
H	6.306113	0.643154	0.475893
H	2.698166	-1.399753	-2.251088
H	4.784770	-2.692916	-1.783735
C	2.057723	2.258839	-1.217548
H	1.088390	2.731985	-1.405978
N	2.125159	0.988237	-1.383454
C	3.227589	3.090151	-0.816498
H	3.770651	3.353652	-1.739546
H	2.884294	4.031411	-0.375460
C	4.131944	2.311659	0.132932
H	3.661828	2.261281	1.127810
H	5.088121	2.829001	0.266203

$TS_{9,10}$ Gsolv= -1465.045746

Ir	0.476553	0.669751	0.189830
C	1.057897	2.776440	0.614220
C	-0.002892	2.729891	-0.371558
C	-1.162580	2.167054	0.265246
C	-0.827852	1.819235	1.608684
C	0.554530	2.200218	1.818933
C	2.412459	3.356163	0.397466
H	2.754563	3.196938	-0.631959
H	3.153739	2.912786	1.070874
H	2.403564	4.439659	0.578179
C	-0.005547	3.409456	-1.697728
H	-0.475200	4.398636	-1.605555
H	-0.573073	2.845593	-2.446932
H	1.008472	3.563743	-2.079394
C	-2.497667	2.031678	-0.379645
H	-3.118086	1.276741	0.117231
H	-2.407529	1.762830	-1.439104
H	-3.030979	2.991136	-0.330368
C	-1.772527	1.320456	2.648374
H	-2.289566	2.159481	3.133890
H	-1.255997	0.764196	3.438814
H	-2.541300	0.665214	2.219913
C	1.294148	2.052039	3.101185
H	2.375895	1.989827	2.941122
H	0.977640	1.157219	3.649401
H	1.100328	2.915202	3.752018
N	1.240981	-1.064148	1.230796
C	0.769543	-1.468355	2.420425
H	0.009500	-0.841305	2.878990
C	1.210757	-2.625212	3.044664
H	0.795903	-2.902357	4.008681
C	2.176203	-3.404815	2.414613
H	2.539013	-4.318127	2.877532
C	2.673035	-3.002263	1.182105
H	3.425259	-3.590992	0.665960
C	2.188338	-1.828530	0.612761
C	2.543495	-1.246054	-0.654494
C	1.904542	-0.075011	-1.058286
N	3.394198	-1.616428	-1.644365
C	4.265859	-2.780587	-1.731309
H	4.810299	-2.718866	-2.673630
H	3.658789	-3.689049	-1.709489
H	4.968133	-2.773471	-0.894521
N	3.345638	-0.776442	-2.653022
N	2.447869	0.138257	-2.288671
C	2.161995	1.224891	-3.211366
H	2.622023	2.148310	-2.849463
H	1.078797	1.346475	-3.282525
H	2.572719	0.965769	-4.187843
H	-0.407886	-0.453563	-0.665708
C	-5.905471	-0.831222	0.035146
C	-4.807042	-1.407505	0.671440
C	-3.595954	-1.578455	0.003773
C	-3.522175	-1.147541	-1.325395
C	-4.610024	-0.576651	-1.980250
C	-5.807953	-0.417524	-1.293397
H	-6.840209	-0.707818	0.576560
H	-4.882621	-1.731913	1.708559
H	-4.504158	-0.253319	-3.014621
H	-6.662653	0.029529	-1.794362
C	-1.219379	-1.811314	-1.502993
H	-0.347041	-1.881602	-2.149433
C	-1.374888	-2.691891	-0.319578
H	-1.734184	-3.650249	-0.733303
H	-0.400810	-2.893944	0.135877
C	-2.376043	-2.137627	0.683269
H	-1.897043	-1.336918	1.268853
H	-2.664153	-2.918086	1.395963
N	-2.292794	-1.255015	-2.018636
H	-2.216855	-0.763890	-2.907673

$1_{Ir\text{-}OCOCH3}$ Gsolv= -1749.276665

Ir	-1.132604	-0.259875	-0.133680
Cl	-0.707142	-0.030009	-2.571790
C	-2.839364	-0.194322	1.200150
C	-3.255510	-0.673141	-0.090197
C	-2.597820	-1.954853	-0.314682
C	-1.761834	-2.227645	0.787870
C	-1.853839	-1.109407	1.714719
C	-3.354388	1.001563	1.919105
H	-3.862200	1.695392	1.243423
H	-2.553488	1.541104	2.436724
H	-4.081179	0.681964	2.677360
C	-4.310745	-0.098932	-0.969942
H	-5.239582	-0.677920	-0.878768
H	-4.009409	-0.122932	-2.023491
H	-4.537485	0.938993	-0.705270

C	-2.798970	-2.807457	-1.514749
H	-1.950594	-3.480166	-1.679823
H	-2.932063	-2.199640	-2.415916
H	-3.700630	-3.422213	-1.392073
C	-0.945088	-3.451142	1.001590
H	-1.543397	-4.205265	1.530045
H	-0.061399	-3.250242	1.616889
H	-0.616001	-3.896549	0.056082
C	-1.179820	-1.025891	3.038879
H	-1.115161	0.010713	3.386884
H	-0.162545	-1.432379	2.995215
H	-1.734660	-1.600577	3.792820
N	1.047006	-0.382555	0.050945
C	1.727233	-1.532380	-0.023533
H	1.146401	-2.428621	-0.227061
C	3.101266	-1.603638	0.142118
H	3.618741	-2.555952	0.090560
C	3.782054	-0.417587	0.382057
C	3.108785	0.792330	0.436430
H	3.656015	1.713290	0.613664
C	1.731230	0.775773	0.256672
C	0.834440	1.905918	0.208147
C	-0.519041	1.680745	-0.018895
N	1.031563	3.248695	0.205647
C	2.264871	4.005306	0.383435
H	2.014857	5.065362	0.344952
H	2.960307	3.756084	-0.421920
H	2.701598	3.758426	1.353760
N	-0.089801	3.893947	-0.019708
N	-1.008095	2.939495	-0.161919
C	-2.367831	3.342672	-0.489395
H	-2.902719	3.643475	0.414973
H	-2.863099	2.491678	-0.961122
H	-2.326402	4.178174	-1.190387
O	5.136565	-0.403771	0.644571
C	6.008858	-0.878805	-0.300901
O	5.638249	-1.239871	-1.394658
C	7.399024	-0.849754	0.213234
H	7.465306	-1.442527	1.131213
H	8.083427	-1.242743	-0.539144
H	7.672979	0.179514	0.467450

$1_{Rh\text{-}OCH3}$ Gsolv= -1642.161858

Rh	-0.943048	-0.272222	-0.198452
Cl	-0.817610	-0.080187	-2.653734
C	-2.248074	-0.167883	1.512696
C	-3.030866	-0.361846	0.321841
C	-2.679824	-1.656849	-0.223682
C	-1.662658	-2.228491	0.574140
C	-1.361136	-1.288301	1.639133
C	-2.349038	0.956612	2.480087
H	-2.846046	1.828683	2.044287
H	-1.363378	1.266338	2.845005
H	-2.936440	0.637976	3.351506
C	-4.144516	0.489781	-0.176256
H	-5.110576	0.027613	0.068480
H	-4.105390	0.605741	-1.265914
H	-4.127352	1.486582	0.274937
C	-3.308884	-2.268813	-1.419510
H	-2.664914	-3.028637	-1.873863
H	-3.546152	-1.516172	-2.178404
H	-4.249679	-2.754488	-1.125832
C	-1.059252	-3.574385	0.378179
H	-1.753959	-4.352520	0.720880
H	-0.130024	-3.693475	0.943911
H	-0.846055	-3.771233	-0.679846
C	-0.367788	-1.479340	2.728032
H	0.071067	-0.522164	3.033673
H	0.446450	-2.145628	2.423940
H	-0.850548	-1.921015	3.610198
N	1.233208	-0.550625	-0.199666
C	1.845103	-1.726665	-0.347107
H	1.205612	-2.584252	-0.546844
C	3.220242	-1.890973	-0.266938
H	3.646147	-2.880033	-0.395727
C	4.003181	-0.761033	-0.019821
C	3.379592	0.486836	0.107124
H	3.987866	1.369779	0.279212
C	2.003037	0.554012	0.007868
C	1.176447	1.742279	0.057228
C	-0.200960	1.632377	-0.087446
N	1.474383	3.065768	0.119319
C	2.766912	3.723323	0.265052
H	2.590764	4.798419	0.300711
H	3.398130	3.478231	-0.592784
H	3.239884	3.390929	1.192032
N	0.392264	3.804715	0.013125
N	-0.600538	2.927383	-0.120419

C	-1.950748	3.441616	-0.300203
H	-2.440873	3.562013	0.669409
H	-2.502497	2.731776	-0.919569
H	-1.891037	4.406321	-0.806120
O	5.338336	-0.770628	0.103009
C	6.018255	-2.021873	-0.015939
H	7.075004	-1.802853	0.140131
H	5.670945	-2.725931	0.748392
H	5.873527	-2.446770	-1.015428

$2_{Ir\text{-}OCOCH3}$ Gsolv= -1288.910696

Ir	-1.214516	-0.296486	-0.369983
C	-2.724433	-0.194267	1.135192
C	-3.305559	-0.760244	-0.041105
C	-2.656215	-2.043316	-0.287067
C	-1.653572	-2.241668	0.680608
C	-1.622773	-1.056267	1.529849
C	-3.172267	1.014124	1.872875
H	-3.787097	1.669014	1.249176
H	-2.327569	1.590541	2.265178
H	-3.781750	0.698276	2.729747
C	-4.470771	-0.251349	-0.812705
H	-5.374458	-0.817426	-0.549332
H	-4.312997	-0.367666	-1.890822
H	-4.665238	0.805778	-0.607281
C	-2.997916	-2.933638	-1.423628
H	-2.245242	-3.712812	-1.574336
H	-3.099619	-2.362841	-2.354087
H	-3.963784	-3.422412	-1.238579
C	-0.776367	-3.429897	0.842268
H	-1.248185	-4.141443	1.532512
H	0.196356	-3.162658	1.269008
H	-0.608030	-3.949222	-0.106902
C	-0.737880	-0.850209	2.705117
H	-0.589293	0.217225	2.902866
H	0.244483	-1.310006	2.548336
H	-1.182572	-1.302865	3.601483
N	0.996735	-0.348827	-0.430872
C	1.707781	-1.478988	-0.521497
H	1.165900	-2.370417	-0.826393
C	3.063371	-1.540422	-0.237755
H	3.601630	-2.480061	-0.304911
C	3.688321	-0.367705	0.162616
C	2.982860	0.825696	0.238849
H	3.487370	1.734942	0.551040
C	1.631722	0.800928	-0.070836
C	0.708995	1.916868	-0.068030
C	-0.641935	1.684227	-0.291394
N	0.882796	3.259561	0.015034
C	2.104523	4.028900	0.220581
H	1.845976	5.085849	0.162072
H	2.822173	3.775137	-0.563322
H	2.518133	3.797598	1.204909
N	-0.254069	3.897247	-0.155112
N	-1.156747	2.938962	-0.341741
C	-2.532482	3.338154	-0.605512
H	-2.982447	3.751069	0.300403
H	-3.077770	2.450985	-0.931404
H	-2.537164	4.089435	-1.397978
O	4.998453	-0.351325	0.583512
C	5.987726	-0.812393	-0.249714
O	5.768809	-1.112123	-1.400667
C	7.284053	-0.866194	0.465868
H	7.226446	-1.632194	1.247364
H	8.086716	-1.109393	-0.230637
H	7.483613	0.089951	0.959151

$2_{Rh\text{-}OCH3}$ Gsolv= -1181.791450

Rh	-0.968708	-0.283424	-0.333824
C	-2.396052	-0.266072	1.234134
C	-3.104341	-0.314892	-0.004787
C	-2.733376	-1.546408	-0.661098
C	-1.816855	-2.266983	0.155468
C	-1.571623	-1.463650	1.319109
C	-2.497618	0.759468	2.300971
H	-2.988093	1.670266	1.946237
H	-1.511613	1.023750	2.699021
H	-3.090169	0.356481	3.133333
C	-4.130966	0.631450	-0.513583
H	-5.128569	0.183209	-0.414065
H	-3.977690	0.854977	-1.575425
H	-4.129352	1.572864	0.042992
C	-3.207555	-1.941828	-2.004922
H	-2.618027	-2.761209	-2.424822
H	-3.182279	-1.090775	-2.695930
H	-4.254805	-2.268346	-1.940014
C	-1.255382	-3.610650	-0.146143
H	-2.031401	-4.376760	-0.022308

H	-0.430748	-3.865997	0.526214
H	-0.893880	-3.676812	-1.178954
C	-0.676343	-1.784896	2.454549
H	-0.185334	-0.882080	2.834697
H	0.093129	-2.511211	2.176568
H	-1.267356	-2.210606	3.276959
N	1.184553	-0.557274	-0.320328
C	1.791587	-1.746528	-0.371685
H	1.147858	-2.613364	-0.499759
C	3.164236	-1.911988	-0.274475
H	3.584228	-2.910339	-0.326908
C	3.951686	-0.771611	-0.105576
C	3.331537	0.486980	-0.057298
H	3.946167	1.372723	0.070036
C	1.959577	0.555931	-0.166529
C	1.139616	1.753706	-0.142845
C	-0.241039	1.664190	-0.255742
N	1.457441	3.070883	-0.051727
C	2.758710	3.714153	0.086705
H	2.593194	4.790748	0.125196
H	3.381149	3.464249	-0.775835
H	3.233662	3.376140	1.010683
N	0.379818	3.823470	-0.108647
N	-0.624895	2.966049	-0.233269
C	-1.974686	3.502377	-0.342287
H	-2.499094	3.382156	0.608939
H	-2.498800	2.965258	-1.134689
H	-1.904874	4.561388	-0.592811
O	5.282113	-0.776391	0.020771
C	5.962231	-2.034414	-0.003408
H	7.018480	-1.803848	0.137203
H	5.613106	-2.677246	0.812061
H	5.817591	-2.532347	-0.968246

$3_{Ir\text{-}OCOCH3}$ Gsolv= -1290.070880

Ir	-1.209704	-0.295024	-0.346132
C	-2.697685	-0.175211	1.185435
C	-3.304053	-0.719178	0.009703
C	-2.678268	-2.008975	-0.257787
C	-1.668527	-2.234709	0.697996
C	-1.608835	-1.059592	1.560550
C	-3.108978	1.038156	1.936324
H	-3.711877	1.714854	1.324294
H	-2.246081	1.588941	2.325678
H	-3.718935	0.731082	2.796006
C	-4.458586	-0.171474	-0.753469
H	-5.359902	-0.768312	-0.560946
H	-4.268335	-0.200461	-1.833025
H	-4.674671	0.864274	-0.473775
C	-3.043856	-2.890202	-1.395191
H	-2.231200	-3.574390	-1.658380
H	-3.308068	-2.305482	-2.283056
H	-3.921963	-3.494679	-1.130981
C	-0.814142	-3.442785	0.831950
H	-1.307492	-4.168614	1.491549
H	0.158207	-3.207541	1.277853
H	-0.644977	-3.933562	-0.132491
C	-0.709036	-0.882350	2.729672
H	-0.539994	0.180037	2.937902
H	0.263547	-1.357063	2.557515
H	-1.151963	-1.337727	3.625401
N	1.000896	-0.360735	-0.391760
C	1.705365	-1.494863	-0.484001
H	1.157674	-2.383199	-0.788103
C	3.061921	-1.564046	-0.206029
H	3.594032	-2.506786	-0.276384
C	3.696286	-0.393907	0.187355
C	2.996855	0.802345	0.270123
H	3.507848	1.709520	0.578059
C	1.643571	0.785321	-0.031729
C	0.728220	1.906765	-0.031124
C	-0.621079	1.679049	-0.266797
N	0.907026	3.249929	0.039577
C	2.130264	4.014967	0.251797
H	1.875646	5.073021	0.195737
H	2.850475	3.760886	-0.529696
H	2.539305	3.779229	1.236955
N	-0.224438	3.891203	-0.151979
N	-1.129415	2.934463	-0.339469
C	-2.498523	3.328986	-0.640746
H	-2.993512	3.693997	0.262501
H	-3.016493	2.449991	-1.029631
H	-2.481218	4.115108	-1.398213
H	-1.426135	0.150706	-2.843583
H	-1.027528	-0.491962	-2.876412
O	5.012799	-0.377733	0.589492
C	5.991300	-0.831476	-0.260017
O	5.749520	-1.176709	-1.393505

C	7.314237	-0.790631	0.406937
H	8.078124	-1.199432	-0.254966
H	7.558096	0.246358	0.661676
H	7.278879	-1.357571	1.342489

$3_{Rh\text{-}OCH3}$ Gsolv= -1182.950876

Rh	-0.973606	-0.293185	-0.371821
C	-2.722163	-0.083658	0.888924
C	-3.083797	-0.776753	-0.295579
C	-2.344905	-2.036506	-0.337126
C	-1.508584	-2.093530	0.794268
C	-1.663379	-0.841796	1.522076
C	-3.336680	1.147466	1.444143
H	-3.916695	1.692707	0.694453
H	-2.590705	1.822037	1.877241
H	-4.022571	0.858911	2.251911
C	-4.085840	-0.351461	-1.303682
H	-5.037899	-0.869916	-1.126241
H	-3.761545	-0.603623	-2.318989
H	-4.273868	0.725741	-1.256766
C	-2.465656	-3.054858	-1.410477
H	-1.551868	-3.650838	-1.505292
H	-2.678728	-2.591067	-2.379133
H	-3.293742	-3.740391	-1.185614
C	-0.623849	-3.208775	1.210558
H	-1.135742	-3.797983	1.983252
H	0.312556	-2.847675	1.650180
H	-0.388226	-3.882603	0.381173
C	-0.978436	-0.483783	2.787291
H	-0.938910	0.601897	2.923650
H	0.044068	-0.875758	2.814313
H	-1.522425	-0.912118	3.640522
N	1.179383	-0.540144	-0.363180
C	1.798165	-1.713572	-0.519067
H	1.165564	-2.566503	-0.757020
C	3.169509	-1.875886	-0.400128
H	3.602495	-2.860038	-0.541208
C	3.939574	-0.751491	-0.094118
C	3.308132	0.493591	0.044898
H	3.909125	1.371147	0.263124
C	1.938900	0.563242	-0.103326
C	1.109319	1.752236	-0.066934
C	-0.261214	1.650062	-0.271047
N	1.409030	3.072711	0.022794
C	2.698743	3.726338	0.211430
H	2.523105	4.801278	0.251215
H	3.351742	3.486643	-0.631472
H	3.145829	3.386019	1.148089
N	0.334086	3.816253	-0.124126
N	-0.655316	2.946897	-0.304190
C	-1.990749	3.476520	-0.548866
H	-2.419012	3.859113	0.380344
H	-2.602019	2.664060	-0.945060
H	-1.922546	4.279580	-1.285287
H	-0.984262	0.153628	-2.756570
H	-0.779590	-0.571520	-2.824822
O	5.266423	-0.760230	0.074260
C	5.958139	-2.005610	-0.051717
H	7.007745	-1.783345	0.142390
H	5.590553	-2.727360	0.685901
H	5.846806	-2.407564	-1.064643

$4_{Ir\text{-}OCOCH3}$ Gsolv= -1691.600596

Ir	0.433165	-0.970196	0.205523
C	1.016557	-2.598488	1.581044
C	2.199848	-2.001462	1.040174
C	2.261050	-0.629672	1.518236
C	1.103020	-0.365319	2.279896
C	0.276415	-1.569067	2.265533
C	0.613755	-4.025093	1.495753
H	1.132273	-4.551846	0.690262
H	-0.466467	-4.140317	1.356957
H	0.876979	-4.517632	2.441054
C	3.280315	-2.671197	0.266795
H	4.118830	-2.924165	0.929074
H	3.668311	-2.013722	-0.520083
H	2.931134	-3.596518	-0.201737
C	3.391428	0.297043	1.254204
H	3.112573	1.341229	1.430995
H	3.756838	0.201454	0.224767
H	4.229935	0.054403	1.920890
C	0.796427	0.883786	3.023532
H	1.222757	0.817576	4.033167
H	-0.281336	1.040729	3.137805
H	1.228739	1.767754	2.539598
C	-1.009669	-1.756823	2.991329
H	-1.639634	-2.500608	2.490255
H	-1.574331	-0.819778	3.052857

H	-0.826227	-2.105712	4.015920	O	-4.385642	4.029152	-0.771789
N	-1.356854	0.260976	0.097343	C	-6.579379	3.908803	0.232628
C	-1.423394	1.498567	0.601754	H	-6.690966	3.913848	1.321841
H	-0.489480	1.931946	0.949402	H	-6.744864	4.909517	-0.167326
C	-2.608292	2.209803	0.691796	H	-7.324939	3.215088	-0.169593
H	-2.619373	3.206702	1.119715				
C	-3.765166	1.592049	0.234340	$4_{Rh\text{-}OCH3}$ Gsolv= -1584.481103			
C	-3.723438	0.314797	-0.306660	Rh	-0.279659	-0.937574	0.237184
H	-4.635175	-0.154550	-0.662302	C	-0.450447	-2.662388	1.570976
C	-2.494879	-0.326855	-0.367904	C	0.862172	-2.614645	1.012149
C	-2.198579	-1.625986	-0.926793	C	1.513439	-1.404951	1.495876
C	-0.893441	-2.096408	-0.869650	C	0.586806	-0.687281	2.278786
N	-2.918721	-2.524400	-1.644118	C	-0.669357	-1.423034	2.270931
C	-4.332270	-2.503973	-2.000896	C	-1.414870	-3.787582	1.506025
H	-4.538822	-3.394480	-2.594059	H	-1.177372	-4.487689	0.701095
H	-4.540075	-1.606340	-2.588502	H	-2.446934	-3.440924	1.388328
H	-4.934700	-2.512336	-1.089807	H	-1.363077	-4.339139	2.454427
N	-2.165850	-3.520059	-2.053427	C	1.528670	-3.655864	0.188664
N	-0.949953	-3.243309	-1.589553	H	2.182837	-4.271896	0.820194
C	0.136729	-4.156191	-1.917947	H	2.153658	-3.202124	-0.589545
H	0.011490	-5.094182	-1.371767	H	0.804174	-4.318853	-0.293800
H	1.072788	-3.671615	-1.634531	C	2.922338	-1.032158	1.217595
H	0.126837	-4.346987	-2.992853	H	3.080320	0.049295	1.295766
H	1.050784	-0.701840	-1.483202	H	3.234656	-1.361890	0.220265
H	1.016576	0.081006	-1.166132	H	3.583870	-1.520778	1.945942
C	2.395557	4.365935	0.668380	C	0.840789	0.572763	3.019584
C	3.675754	3.994622	0.332374	H	1.187326	0.328373	4.032710
C	3.900658	3.043594	-0.692944	H	-0.065019	1.179008	3.124220
C	2.789466	2.476075	-1.380803	H	1.619511	1.180353	2.543995
C	1.481507	2.882007	-1.017862	C	-1.907198	-1.038764	2.996173
C	1.291454	3.804521	-0.014814	H	-2.797664	-1.443347	2.502860
H	6.061047	3.018956	-0.538557	H	-2.011757	0.049833	3.057391
H	2.225759	5.093354	1.458625	H	-1.883024	-1.430566	4.021890
H	4.536216	4.416737	0.849642	N	-1.252896	1.017988	0.090368
C	5.195572	2.602784	-1.052120	C	-0.723792	2.162839	0.525885
H	0.635183	2.448034	-1.550123	H	0.292953	2.110841	0.909617
H	0.281793	4.109261	0.256661	C	-1.395763	3.375285	0.499968
C	5.332608	1.654880	-2.034047	H	-0.896340	4.266194	0.865377
H	6.307537	1.283453	-2.337010	C	-2.699517	3.393768	-0.001225
N	2.941835	1.546477	-2.370850	C	-3.269298	2.200116	-0.465672
C	4.168429	1.160746	-2.663483	H	-4.279020	2.213482	-0.864494
H	4.267802	0.413900	-3.452013	C	-2.521735	1.041414	-0.411219
O	-5.004143	2.175163	0.367032	C	-2.900379	-0.268486	-0.900852
C	-5.220450	3.439929	-0.125657	C	-2.008376	-1.327049	-0.806975

N	-3.981373	-0.715448	-1.590001
C	-5.196926	-0.007002	-1.973696
H	-5.840216	-0.712642	-2.499413
H	-4.937179	0.823707	-2.634408
H	-5.700028	0.361735	-1.077067
N	-3.832781	-1.970930	-1.950138
N	-2.638186	-2.318818	-1.481114
C	-2.152828	-3.660633	-1.777426
H	-2.690571	-4.396521	-1.175174
H	-1.085832	-3.686085	-1.548930
H	-2.309404	-3.863566	-2.838585
H	0.384748	-0.972211	-1.505256
H	0.756836	-0.317239	-1.200640
C	3.813200	3.120815	0.511145
C	4.869887	2.262033	0.323431
C	4.781459	1.213309	-0.624345
C	3.587159	1.050667	-1.384753
C	2.514920	1.951495	-1.171545
C	2.629410	2.963989	-0.246537
H	6.754171	0.393838	-0.267886
H	3.883312	3.926312	1.238316
H	5.788549	2.369192	0.898462
C	5.832040	0.290915	-0.838068
H	1.605219	1.826775	-1.758872
H	1.803749	3.657629	-0.097454
C	5.663757	-0.715845	-1.754087
H	6.442304	-1.448860	-1.945716
N	3.438924	0.051337	-2.305342
C	4.442998	-0.789210	-2.461416
H	4.302619	-1.584218	-3.194529
O	-3.469329	4.484712	-0.081946
C	-2.932035	5.728608	0.374101
H	-3.720607	6.466044	0.222117
H	-2.678869	5.672492	1.438475
H	-2.049025	6.006251	-0.211983

$5_{Ir\text{-}OCOCH3}$ Gsolv= -1289.645959

Ir	-1.138660	-0.222942	-0.287955
C	-2.746234	-0.467563	1.301187
C	-3.307491	-0.398541	-0.035628
C	-2.858370	-1.562854	-0.755435
C	-1.966269	-2.290537	0.079315
C	-1.904559	-1.607642	1.359936
C	-3.035058	0.494461	2.402100
H	-3.176964	1.511713	2.019224
H	-2.224388	0.522715	3.138259
H	-3.955903	0.212713	2.930864
C	-4.406690	0.507460	-0.477554
H	-5.380135	0.016612	-0.337385
H	-4.319851	0.767287	-1.538735
H	-4.424646	1.437463	0.100087
C	-3.297617	-1.953989	-2.123747
H	-2.534454	-2.547032	-2.638990
H	-3.522682	-1.077259	-2.740388
H	-4.211000	-2.561903	-2.065976
C	-1.349895	-3.610615	-0.239650
H	-2.082776	-4.420002	-0.116301
H	-0.508970	-3.836974	0.425495
H	-0.986153	-3.652313	-1.273193
C	-1.099178	-2.071207	2.523863
H	-0.946410	-1.269848	3.254417
H	-0.111740	-2.433557	2.210536
H	-1.599422	-2.902934	3.038075
N	1.012871	-0.368069	-0.057685
C	1.675006	-1.534998	-0.012428
H	1.080991	-2.434778	-0.146586
C	3.042208	-1.618029	0.186799
H	3.539981	-2.581524	0.230032
C	3.747409	-0.429838	0.332669
C	3.099979	0.790780	0.280035
H	3.660748	1.713011	0.399107
C	1.721766	0.789005	0.088517
C	0.842487	1.923586	0.015198
C	-0.523046	1.700099	-0.165470
N	1.044084	3.265571	0.041884
C	2.285430	4.011947	0.199724
H	2.043155	5.074168	0.168869
H	2.965449	3.760658	-0.617922
H	2.737719	3.759857	1.161858
N	-0.082907	3.919945	-0.112206
N	-1.011230	2.970880	-0.239899
C	-2.389563	3.379388	-0.456194
H	-2.976698	3.209306	0.450045
H	-2.799483	2.796807	-1.284434
H	-2.398958	4.440580	-0.707643
H	-0.791390	-0.006818	-1.857899
O	5.102357	-0.431035	0.610783
C	5.969477	-0.914354	-0.331537

O	5.594430	-1.284222	-1.421873
C	7.362316	-0.887643	0.176610
H	7.430728	-1.476561	1.096880
H	8.042577	-1.286400	-0.576514
H	7.640848	0.141801	0.424972

$5_{Rh\text{-}OCH3}$ Gsolv= -1182.520326

Rh	-0.954580	-0.228822	-0.386804
C	-2.371654	-0.352331	1.342901
C	-3.065242	-0.270274	0.069595
C	-2.759236	-1.465950	-0.675219
C	-1.824219	-2.222858	0.074491
C	-1.591775	-1.531528	1.333663
C	-2.480444	0.638139	2.451092
H	-2.686460	1.645459	2.072510
H	-1.561483	0.685680	3.045666
H	-3.302173	0.371641	3.129602
C	-4.133092	0.705485	-0.290258
H	-5.121593	0.286244	-0.055077
H	-4.123825	0.940840	-1.360731
H	-4.034239	1.643559	0.265194
C	-3.362842	-1.853457	-1.980473
H	-2.690129	-2.491969	-2.563166
H	-3.609752	-0.976397	-2.588181
H	-4.293538	-2.414030	-1.815778
C	-1.299930	-3.569607	-0.289028
H	-2.052191	-4.342857	-0.079956
H	-0.405525	-3.829319	0.287980
H	-1.051856	-3.636504	-1.355093
C	-0.694924	-2.024904	2.414576
H	-0.447553	-1.231771	3.127982
H	0.245267	-2.420555	2.009875
H	-1.172622	-2.840964	2.973727
N	1.197688	-0.543202	-0.339911
C	1.799645	-1.734545	-0.413710
H	1.153738	-2.591601	-0.590078
C	3.168633	-1.914940	-0.289833
H	3.580274	-2.915882	-0.360845
C	3.965185	-0.786698	-0.079654
C	3.357400	0.471861	-0.016083
H	3.974012	1.351542	0.142100
C	1.983045	0.556509	-0.146117
C	1.172241	1.751917	-0.109033
C	-0.211672	1.651277	-0.239208
N	1.482250	3.070646	-0.015175
C	2.780908	3.714153	0.135789
H	2.615531	4.790799	0.177063
H	3.411315	3.467674	-0.722077
H	3.250572	3.373479	1.061633
N	0.405607	3.821164	-0.080980
N	-0.597724	2.954850	-0.221803
C	-1.945595	3.483590	-0.358062
H	-2.497299	3.350278	0.576037
H	-2.446959	2.952943	-1.170398
H	-1.877827	4.546096	-0.595104
O	5.298892	-0.811078	0.070484
C	5.959393	-2.076488	0.022924
H	7.016849	-1.867489	0.188433
H	5.587701	-2.738934	0.812757
H	5.826110	-2.546515	-0.957841
H	-0.811054	0.083875	-1.958958

$6_{Ir\text{-}OCOCH3}$ Gsolv= -1691.621354

Ir	1.345904	-0.527254	-0.077350
C	3.185328	-1.451531	-1.003039
C	3.518801	-0.450136	-0.002818
C	3.058225	-0.944797	1.274116
C	2.380764	-2.174927	1.057956
C	2.466925	-2.491539	-0.359050
C	3.557905	-1.376815	-2.443722
H	3.520920	-0.346302	-2.815114
H	2.890138	-1.981871	-3.066260
H	4.581855	-1.743442	-2.598308
C	4.437867	0.708470	-0.195026
H	5.471206	0.420964	0.044388
H	4.171541	1.549564	0.456498
H	4.428098	1.066208	-1.229845
C	3.273273	-0.276471	2.588989
H	2.462749	-0.502279	3.291989
H	3.333600	0.812428	2.478987
H	4.213985	-0.617531	3.042225
C	1.812868	-3.056265	2.117707
H	2.607176	-3.644037	2.597988
H	1.088649	-3.770147	1.709253
H	1.313822	-2.476551	2.904476
C	1.908820	-3.724285	-0.982301
H	1.839602	-3.629636	-2.071104
H	0.905246	-3.948670	-0.598939

H	2.541401	-4.594657	-0.760911	O	-5.467737	-0.056046	0.358722
N	-0.756293	-1.089852	-0.164438	C	-7.095756	-1.658654	-0.424717
C	-1.303821	-2.038843	0.609313	H	-7.213948	-2.669219	-0.023208
H	-0.638349	-2.540927	1.306634	H	-7.854840	-0.992602	-0.013148
C	-2.647067	-2.373879	0.553062	H	-7.213044	-1.721489	-1.512476
H	-3.056606	-3.150289	1.191342				
C	-3.450676	-1.681806	-0.341599	$6_{Rh\text{-}OCH3}$ Gsolv= -1584.497098			
C	-2.922693	-0.689484	-1.148771	Rh	1.131789	-0.643663	-0.131627
H	-3.555265	-0.151614	-1.848953	C	2.980913	-1.534290	-1.055502
C	-1.564506	-0.412001	-1.031825	C	3.283979	-0.599599	0.014684
C	-0.809159	0.583473	-1.743031	C	2.777734	-1.157482	1.242653
C	0.554240	0.709281	-1.471890	C	2.084850	-2.353831	0.926201
N	-1.148871	1.560754	-2.621750	C	2.225822	-2.593230	-0.502748
C	-2.457085	1.908269	-3.160371	C	3.409054	-1.376808	-2.474023
H	-2.333874	2.789174	-3.790667	H	3.374104	-0.328307	-2.792121
H	-3.138520	2.132370	-2.334277	H	2.774235	-1.954440	-3.154398
H	-2.843942	1.075261	-3.752469	H	4.442751	-1.723568	-2.609230
N	-0.114224	2.306755	-2.929467	C	4.210752	0.565169	-0.070874
N	0.899202	1.782731	-2.238381	H	5.216911	0.272090	0.260921
C	2.184965	2.459272	-2.286952	H	3.883572	1.393323	0.569781
H	2.902895	1.869709	-2.863647	H	4.300211	0.941559	-1.095158
H	2.546688	2.592958	-1.263536	C	2.975006	-0.583330	2.603419
H	2.044184	3.432287	-2.760126	H	2.155531	-0.854163	3.279578
H	0.802955	0.654100	0.882642	H	3.045253	0.510213	2.573994
C	0.166344	4.123393	0.302720	H	3.907572	-0.960668	3.045662
C	-1.016140	3.424434	0.281202	C	1.457686	-3.282152	1.909313
C	-1.309238	2.491762	1.305480	H	2.226377	-3.875443	2.423558
C	-0.363221	2.313756	2.346082	H	0.777694	-3.990929	1.423903
C	0.829788	3.054981	2.382488	H	0.894727	-2.741227	2.680896
C	1.086868	3.940506	1.361069	C	1.667855	-3.774336	-1.218349
H	-3.213861	1.841849	0.521307	H	1.656767	-3.619718	-2.302303
H	0.401017	4.823708	-0.495310	H	0.640435	-3.991432	-0.899235
H	-1.740021	3.561111	-0.521357	H	2.264493	-4.673890	-1.014302
C	-2.477833	1.700524	1.312715	N	-0.968532	-1.158880	-0.307281
H	1.533466	2.900842	3.197733	C	-1.573816	-2.138788	0.371959
H	2.014379	4.507425	1.365891	H	-0.940536	-2.746203	1.014779
C	-2.683247	0.756982	2.298623	C	-2.933002	-2.401339	0.298863
H	-3.569974	0.131264	2.315039	H	-3.346973	-3.217251	0.881186
C	-1.720634	0.602278	3.293580	C	-3.719138	-1.588586	-0.522359
H	-1.808367	-0.120562	4.098115	C	-3.108246	-0.552010	-1.234746
N	-0.631855	1.370002	3.302927	H	-3.715588	0.088374	-1.867743
H	0.057216	1.231970	4.043061	C	-1.742821	-0.363489	-1.101615
O	-4.780092	-2.047402	-0.456279	C	-0.939350	0.669997	-1.711842
C	-5.743024	-1.134102	-0.119342	C	0.424853	0.741848	-1.430757

N	-1.254615	1.732666	-2.496157
C	-2.551639	2.155015	-3.004508
H	-2.404239	3.074736	-3.571410
H	-3.227475	2.340407	-2.164484
H	-2.960258	1.378545	-3.655867
N	-0.202423	2.481222	-2.735128
N	0.795409	1.868742	-2.095810
C	2.096367	2.517531	-2.077117
H	2.831369	1.898948	-2.598223
H	2.400287	2.666226	-1.036385
H	2.006810	3.482742	-2.577806
H	0.600661	0.471740	0.863947
C	0.063953	4.128091	0.441937
C	-1.124353	3.439121	0.429191
C	-1.372728	2.434192	1.395736
C	-0.374985	2.171131	2.368131
C	0.827983	2.896706	2.393252
C	1.038980	3.856431	1.430322
H	-3.319003	1.855187	0.665330
H	0.264505	4.885683	-0.311817
H	-1.884640	3.636667	-0.325772
C	-2.545346	1.649188	1.403715
H	1.573546	2.674126	3.153626
H	1.972523	4.413508	1.426392
C	-2.704573	0.629971	2.320309
H	-3.591556	0.005191	2.333504
C	-1.692638	0.394859	3.248783
H	-1.741897	-0.391616	3.995029
N	-0.603016	1.160949	3.265599
H	0.129710	0.954020	3.945989
O	-5.046158	-1.719211	-0.681181
C	-5.715270	-2.744060	0.055379
H	-5.600007	-2.582440	1.133377
H	-6.768780	-2.668185	-0.215651
H	-5.335375	-3.733683	-0.221895

$7_{Ir\text{-}OCOCH3}$ Gsolv= -1691.608158

Ir	-0.805309	-0.764240	-0.495712
C	-2.047731	-2.295674	-1.295839
C	-2.905695	-1.222661	-0.854127
C	-2.567426	-0.063704	-1.633634
C	-1.534968	-0.394280	-2.567653
C	-1.194250	-1.772545	-2.352491
C	-2.074023	-3.706152	-0.832673
H	-2.496552	-3.792192	0.173608
H	-1.068818	-4.140867	-0.823019
H	-2.692583	-4.308801	-1.510983
C	-4.044342	-1.304012	0.100706
H	-4.989295	-1.361019	-0.455632
H	-4.095588	-0.418037	0.745155
H	-3.979936	-2.191045	0.737392
C	-3.166677	1.279727	-1.445115
H	-2.523885	2.069785	-1.847878
H	-3.355861	1.485165	-0.383139
H	-4.132163	1.330203	-1.966987
C	-0.958696	0.531906	-3.581675
H	-1.683601	0.719499	-4.384076
H	-0.058509	0.115186	-4.044771
H	-0.699592	1.502513	-3.140029
C	-0.178160	-2.556836	-3.097400
H	0.283050	-3.318762	-2.459881
H	0.612969	-1.915976	-3.500108
H	-0.655933	-3.073077	-3.940540
N	1.363101	-0.622016	-0.529584
C	2.015667	-0.012237	-1.528077
H	1.419734	0.303341	-2.380706
C	3.381280	0.217904	-1.494872
H	3.882384	0.707621	-2.323483
C	4.074042	-0.189368	-0.364614
C	3.423593	-0.823067	0.685153
H	3.980751	-1.128049	1.565460
C	2.055312	-1.021612	0.572143
C	1.155457	-1.578437	1.557474
C	-0.216400	-1.525588	1.336885
N	1.356362	-2.132799	2.778672
C	2.604630	-2.410806	3.479527
H	2.360339	-2.956989	4.390522
H	3.099223	-1.468923	3.729626
H	3.245192	-3.020880	2.838535
N	0.214268	-2.422354	3.359509
N	-0.716397	-2.047809	2.489123
C	-2.112339	-2.222663	2.864141
H	-2.529538	-3.090004	2.346404
H	-2.663402	-1.319504	2.594947
H	-2.159383	-2.380211	3.942168
H	-0.215130	1.054804	0.397027
C	-3.441880	2.778177	2.326553
C	-2.206500	2.168657	2.135597

C	-1.259977	2.700446	1.257607
C	-1.574973	3.874783	0.555680
C	-2.815798	4.497128	0.746271
C	-3.741214	3.949880	1.624277
H	0.446680	1.556092	1.926135
H	-4.166863	2.347097	3.012924
H	-1.958305	1.247321	2.666362
C	0.029594	1.983735	1.002537
H	-3.039859	5.409912	0.195892
H	-4.702540	4.439408	1.763366
C	1.015147	2.796588	0.244346
H	2.047358	2.459627	0.169174
C	0.639383	3.925146	-0.388098
H	1.330985	4.522182	-0.975453
N	-0.646943	4.417344	-0.324706
H	-0.843533	5.326467	-0.723938
O	5.438843	-0.023402	-0.269203
C	5.944050	1.254431	-0.291398
O	5.223835	2.226223	-0.296072
C	7.425591	1.230451	-0.290574
H	7.813657	2.249147	-0.272803
H	7.786010	0.673411	0.580136
H	7.781007	0.707006	-1.184411

$7_{Rh\text{-}OCH3}$ Gsolv= -1584.492672

Rh	-0.209901	-0.930969	-0.599014
C	-0.824242	-2.718234	-1.582729
C	-1.995971	-2.062051	-1.078555
C	-2.078917	-0.784725	-1.728145
C	-0.981247	-0.638535	-2.638357
C	-0.201979	-1.833017	-2.554651
C	-0.351323	-4.081698	-1.241013
H	-0.738989	-4.409423	-0.271189
H	0.742366	-4.129790	-1.212013
H	-0.694909	-4.795952	-2.001545
C	-3.034716	-2.614563	-0.169607
H	-3.914724	-2.910277	-0.756386
H	-3.366228	-1.867382	0.561732
H	-2.681270	-3.497925	0.369585
C	-3.121677	0.229511	-1.465525
H	-2.814653	1.225642	-1.799771
H	-3.378125	0.272375	-0.399384
H	-4.037447	-0.044512	-2.008491
C	-0.740855	0.552655	-3.497486
H	-1.541775	0.654237	-4.240726
H	0.206551	0.476481	-4.039790
H	-0.726889	1.477923	-2.904035
C	1.033302	-2.145503	-3.311278
H	1.743390	-2.712370	-2.699216
H	1.530044	-1.240038	-3.672865
H	0.782908	-2.765682	-4.182577
N	1.755272	-0.007219	-0.507184
C	2.253087	0.769954	-1.473334
H	1.684416	0.819947	-2.399409
C	3.431342	1.490255	-1.344616
H	3.778478	2.094331	-2.175599
C	4.119969	1.411224	-0.132677
C	3.602637	0.610753	0.897591
H	4.131967	0.561356	1.844149
C	2.430196	-0.081096	0.676708
C	1.725764	-0.936688	1.613340
C	0.495344	-1.486969	1.274643
N	2.022198	-1.340950	2.875799
C	3.182660	-1.040096	3.705852
H	3.085454	-1.609223	4.630187
H	3.203237	0.029734	3.927409
H	4.091542	-1.338795	3.178291
N	1.071279	-2.107468	3.363724
N	0.168691	-2.183806	2.394150
C	-1.028932	-2.977120	2.630015
H	-1.028591	-3.839694	1.958738
H	-1.908457	-2.356070	2.446841
H	-1.019677	-3.314192	3.666845
H	-0.483211	0.876884	0.333981
C	-4.045548	1.384956	2.349000
C	-2.681000	1.261098	2.111884
C	-2.024109	2.078622	1.189505
C	-2.769718	3.044505	0.492904
C	-4.144718	3.176414	0.728496
C	-4.775705	2.350327	1.648079
H	0.004122	1.667701	1.802393
H	-4.539164	0.737125	3.069322
H	-2.095786	0.505217	2.639036
C	-0.573702	1.866864	0.887200
H	-4.704568	3.932795	0.179933
H	-5.843812	2.460151	1.822045
C	0.015970	2.949262	0.058774
H	1.094604	2.998418	-0.072151

C	-0.764687	3.851967	-0.566169
H	-0.357768	4.633765	-1.201140
N	-2.135551	3.867519	-0.427618
H	-2.665757	4.623158	-0.842610
O	5.260457	2.054856	0.139661
C	5.809472	2.912926	-0.863702
H	6.714158	3.338536	-0.429003
H	6.066988	2.342206	-1.762619
H	5.106075	3.715593	-1.110619

$8_{Ir\text{-}OCOCH3}$ Gsolv= -1692.774715

Ir	1.338211	-0.424781	0.218821
C	2.928112	-1.124520	1.441890
C	3.462582	-0.117031	0.565361
C	2.795333	1.127388	0.888610
C	1.860862	0.910504	1.932162
C	1.897725	-0.501608	2.255921
C	3.372862	-2.535868	1.565607
H	3.912550	-2.869740	0.674407
H	2.526863	-3.210724	1.734443
H	4.049981	-2.629831	2.424801
C	4.587528	-0.266438	-0.397355
H	5.511187	0.140435	0.034811
H	4.393480	0.274199	-1.330853
H	4.768025	-1.317418	-0.643884
C	3.021799	2.420177	0.196269
H	2.117729	3.041370	0.197891
H	3.349788	2.276845	-0.838488
H	3.809961	2.979945	0.718368
C	1.033306	1.964300	2.581726
H	1.661160	2.582574	3.236440
H	0.237862	1.536928	3.200575
H	0.577181	2.635682	1.841408
C	1.126257	-1.180820	3.327045
H	0.934743	-2.229207	3.074150
H	0.164939	-0.689259	3.509357
H	1.698570	-1.160401	4.263975
N	-0.843723	-0.734056	0.432719
C	-1.623933	0.075314	1.157887
H	-1.138817	0.931992	1.617102
C	-2.978941	-0.149050	1.337979
H	-3.577651	0.524931	1.943159
C	-3.531019	-1.260187	0.717996
C	-2.746934	-2.118747	-0.039878
H	-3.194309	-2.988164	-0.510668
C	-1.394926	-1.826579	-0.161284
C	-0.395213	-2.570717	-0.899623
C	0.918715	-2.123902	-0.926073
N	-0.463290	-3.678270	-1.682555
C	-1.598545	-4.547596	-1.968762
H	-1.251836	-5.340010	-2.631731
H	-2.384866	-3.968793	-2.459000
H	-1.965866	-4.976053	-1.033247
N	0.704636	-3.952356	-2.219012
N	1.519276	-3.008185	-1.760962
C	2.902546	-3.000740	-2.217442
H	3.550571	-3.450189	-1.461108
H	3.195122	-1.964653	-2.400723
H	2.962674	-3.575415	-3.142411
H	1.618466	0.522777	-2.113373
H	0.972322	0.893939	-1.977906
C	1.044917	5.477171	-0.986940
C	-0.026306	5.161797	-0.151101
C	-0.863133	4.083351	-0.433133
C	-0.598933	3.293598	-1.566770
C	0.473149	3.613793	-2.404596
C	1.288700	4.705735	-2.122578
H	1.683763	6.326625	-0.755493
H	-0.229193	5.769519	0.730798
H	0.656148	2.994100	-3.281090
H	2.117199	4.948386	-2.784381
C	-2.517165	2.029354	-1.312900
H	-3.106910	1.140873	-1.564308
N	-1.372022	2.147409	-1.881373
C	-3.112655	3.039002	-0.384880
H	-3.638897	3.779611	-1.010707
H	-3.874480	2.570499	0.247383
C	-2.028763	3.718696	0.439414
H	-1.687266	3.040623	1.239280
H	-2.420100	4.610064	0.942708
O	-4.857800	-1.589420	0.892324
C	-5.820857	-0.708354	0.462936
O	-5.540978	0.295780	-0.150300
C	-7.170958	-1.184570	0.844783
H	-7.243346	-1.233754	1.936507
H	-7.928925	-0.506846	0.450991
H	-7.330625	-2.196718	0.460087

$8_{Rh\text{-}OCH3}$ Gsolv= -1585.652773

Rh	-1.216922	-0.630012	0.204743
C	-2.747793	-1.506723	1.407855
C	-2.350966	-2.460364	0.423168
C	-0.957166	-2.777436	0.664811
C	-0.487574	-2.027410	1.769219
C	-1.577939	-1.190646	2.208820
C	-4.103008	-0.953145	1.651544
H	-4.794624	-1.193656	0.839783
H	-4.077679	0.134290	1.783341
H	-4.505623	-1.385242	2.577403
C	-3.199082	-3.125221	-0.600616
H	-3.382129	-4.169332	-0.314083
H	-2.705067	-3.138020	-1.579340
H	-4.168769	-2.631148	-0.711267
C	-0.147999	-3.718364	-0.141466
H	0.917827	-3.464664	-0.107972
H	-0.475709	-3.747428	-1.186052
H	-0.261050	-4.732439	0.267658
C	0.871830	-2.132170	2.365621
H	0.991292	-3.112806	2.844211
H	1.043575	-1.368981	3.131011
H	1.659980	-2.048786	1.603679
C	-1.562473	-0.237768	3.343202
H	-2.228428	0.611301	3.154115
H	-0.556277	0.143804	3.542215
H	-1.918057	-0.743519	4.251424
N	0.017437	1.144772	0.492606
C	1.157981	1.158829	1.185784
H	1.464812	0.215495	1.630348
C	1.944118	2.288058	1.351974
H	2.858147	2.217910	1.932631
C	1.529762	3.470772	0.736999
C	0.326540	3.479699	0.015427
H	-0.004124	4.403066	-0.450296
C	-0.401775	2.311930	-0.077734
C	-1.671215	2.121780	-0.752654
C	-2.282050	0.876110	-0.753277
N	-2.456909	2.960927	-1.476227
C	-2.278896	4.375090	-1.784256
H	-3.136481	4.695755	-2.375589
H	-1.358435	4.508329	-2.357655
H	-2.234535	4.944372	-0.852990
N	-3.513015	2.334303	-1.947127
N	-3.388324	1.087009	-1.509510
C	-4.400453	0.113982	-1.896955
H	-5.082973	-0.063707	-1.062533
H	-3.894756	-0.812018	-2.179562
H	-4.951558	0.512053	-2.749583
H	-0.733471	-1.115547	-2.219510
H	-0.000750	-1.088152	-2.034806
C	3.344384	-3.853091	-1.243651
C	3.863522	-2.982392	-0.285760
C	3.737131	-1.601354	-0.427136
C	3.055981	-1.089143	-1.546387
C	2.530986	-1.965043	-2.501391
C	2.680624	-3.341428	-2.357951
H	3.459827	-4.927736	-1.120086
H	4.390466	-3.375560	0.583847
H	2.015146	-1.549506	-3.365806
H	2.274033	-4.013256	-3.110812
C	3.632059	1.098435	-1.082454
H	3.508190	2.170770	-1.265828
N	2.881506	0.302832	-1.754063
C	4.691814	0.665443	-0.120071
H	5.618536	0.526933	-0.702180
H	4.896976	1.465258	0.600049
C	4.302296	-0.633405	0.571402
H	3.550697	-0.428725	1.351972
H	5.162584	-1.076644	1.085499
O	2.203243	4.625169	0.776043
C	3.451654	4.655994	1.473047
H	3.829250	5.672700	1.361398
H	3.306749	4.430788	2.535185
H	4.159368	3.948233	1.025931

$9_{Ir\text{-}OCOCH3}$ Gsolv= -1692.787344

Ir	-0.558610	-1.004898	-0.366717
C	-1.350342	-2.650095	-1.721683
C	-2.376811	-2.132554	-0.835712
C	-2.606103	-0.756264	-1.191051
C	-1.690708	-0.398180	-2.222865
C	-0.918702	-1.581849	-2.551503
C	-0.871023	-4.060912	-1.748690
H	-0.873387	-4.502878	-0.745505
H	0.148026	-4.134900	-2.143553
H	-1.519482	-4.682515	-2.381482
C	-3.266891	-2.945008	0.041628

H	-4.178522	-3.223385	-0.505680	H	-4.742803	5.097715	-0.881080
H	-3.576670	-2.391346	0.935432	H	-2.321745	4.681390	-1.235812
H	-2.784646	-3.873257	0.363940	H	-4.655464	2.579725	2.612580
C	-3.670542	0.111259	-0.612539	H	-5.922402	4.052615	1.042882
H	-3.423869	1.175759	-0.707196	C	-0.819434	1.790913	2.387818
H	-3.841657	-0.109979	0.447412	H	-0.396669	1.082440	3.098315
H	-4.618690	-0.060191	-1.140804	C	0.028886	2.628737	1.522533
C	-1.657621	0.894237	-2.965469	H	0.284170	3.501221	2.150891
H	-2.367166	0.874295	-3.804326	H	0.975858	2.115814	1.325432
H	-0.667841	1.096268	-3.391366	C	-0.673745	3.062304	0.242756
H	-1.931840	1.742239	-2.325366	H	-0.636168	2.234695	-0.483905
C	0.126559	-1.634859	-3.610197	H	-0.143305	3.905591	-0.211550
H	0.784184	-2.501616	-3.487302	N	-2.102863	1.961831	2.418233
H	0.750461	-0.731956	-3.606773	H	-2.657507	1.418457	3.081527
H	-0.335615	-1.702405	-4.604402	O	4.926001	2.084223	-0.020529
N	1.377432	-0.024117	-0.391617	C	5.918208	1.963510	-0.956076
C	1.705530	0.919287	-1.289173	O	5.836978	1.186557	-1.881363
H	0.981789	1.112604	-2.076444	C	7.038618	2.886684	-0.655842
C	2.889630	1.633058	-1.233185	H	7.856953	2.721725	-1.357241
H	3.117881	2.392376	-1.974564	H	6.684575	3.920277	-0.733913
C	3.765325	1.350534	-0.191782	H	7.383742	2.736424	0.371751
C	3.464253	0.379633	0.745659				
H	4.155017	0.169671	1.556076	$9_{Rh\text{-}OCH3}$ Gsolv= -1585.664034			
C	2.255272	-0.298747	0.616567	Rh	-0.173483	-1.053527	0.377251
C	1.726549	-1.331098	1.463945	C	-0.223505	-2.893655	1.645177
C	0.462433	-1.849446	1.176287	C	0.899542	-2.897216	0.727379
N	2.193843	-1.962248	2.571478	C	1.777821	-1.817137	1.102491
C	3.453461	-1.780029	3.282165	C	1.168977	-1.103146	2.164362
H	3.472465	-2.485543	4.112782	C	-0.074409	-1.777621	2.502628
H	3.511966	-0.756563	3.660398	C	-1.328261	-3.892942	1.670661
H	4.285115	-1.980348	2.602441	H	-1.500385	-4.328245	0.680064
N	1.330536	-2.844405	3.015696	H	-2.269633	-3.445853	2.008696
N	0.299815	-2.765688	2.173735	H	-1.089976	-4.719824	2.353364
C	-0.844516	-3.631154	2.406795	C	1.261081	-3.987147	-0.222346
H	-0.921712	-4.362619	1.598308	H	1.980787	-4.670800	0.249898
H	-1.749567	-3.020938	2.451238	H	1.732420	-3.595520	-1.131114
H	-0.698580	-4.147109	3.356527	H	0.390244	-4.580902	-0.516981
H	-0.856243	0.089333	0.783750	C	3.118132	-1.555576	0.506621
C	-4.198031	4.458565	-0.190600	H	3.429276	-0.512425	0.640401
C	-2.837317	4.228668	-0.390133	H	3.137714	-1.786574	-0.564812
C	-2.115002	3.412720	0.476794	H	3.872354	-2.191954	0.990566
C	-2.805961	2.838438	1.547385	C	1.771770	0.026228	2.926533
C	-4.162086	3.054977	1.766788	H	2.438428	-0.358945	3.710725
C	-4.862035	3.873380	0.887087	H	1.011808	0.634708	3.429871

H	2.371210	0.685186	2.285659
C	-0.987876	-1.358439	3.600181
H	-1.974622	-1.823633	3.504886
H	-1.126487	-0.269884	3.618029
H	-0.574466	-1.644643	4.576986
N	-1.368776	0.753157	0.588215
C	-1.110511	1.747784	1.443746
H	-0.257208	1.610968	2.104083
C	-1.859086	2.912339	1.522499
H	-1.586605	3.669450	2.249803
C	-2.939817	3.060855	0.649388
C	-3.227510	2.033322	-0.255395
H	-4.069727	2.141520	-0.932358
C	-2.430859	0.902300	-0.257269
C	-2.561769	-0.258828	-1.106120
C	-1.652072	-1.307919	-0.987185
N	-3.420831	-0.569976	-2.111096
C	-4.543904	0.191159	-2.642959
H	-5.001093	-0.400711	-3.435900
H	-4.181543	1.138866	-3.048745
H	-5.270650	0.371207	-1.847503
N	-3.130503	-1.734066	-2.645144
N	-2.066245	-2.159282	-1.963944
C	-1.463237	-3.423635	-2.356487
H	-1.634816	-4.175741	-1.582581
H	-0.391619	-3.269865	-2.503858
H	-1.923279	-3.748049	-3.290558
H	0.468794	-0.358471	-0.926254
C	5.607669	2.053837	0.067629
C	4.293258	2.440421	0.328116
C	3.256803	2.065153	-0.522145
C	3.585856	1.292925	-1.639675
C	4.888480	0.895610	-1.918963
C	5.906757	1.280467	-1.053404
H	6.402279	2.356916	0.744926
H	4.060129	3.037573	1.208477
H	5.092071	0.290319	-2.800391
H	6.930855	0.978633	-1.255559
C	1.319927	1.298974	-2.425439
H	0.606887	0.900617	-3.144594
C	0.970126	2.388282	-1.496974
H	1.142509	3.312914	-2.077230
H	-0.103615	2.360521	-1.282762
C	1.815667	2.368379	-0.231501
H	1.430902	1.580689	0.436563
H	1.719370	3.317891	0.305790
N	2.538519	0.866095	-2.501136
H	2.771469	0.161270	-3.202479
O	-3.746816	4.132038	0.607382
C	-3.519289	5.184722	1.545562
H	-2.526316	5.625569	1.403038
H	-4.284478	5.934840	1.343594
H	-3.625449	4.816330	2.571990

$10_{Ir\text{-}OCOCH3}$ Gsolv= -1692.813373

Ir	-0.602814	-0.867257	-0.448472
C	-1.303696	-2.551901	-1.504587
C	-2.442619	-1.933805	-0.872965
C	-2.597032	-0.624547	-1.458150
C	-1.570752	-0.404000	-2.419042
C	-0.744896	-1.587192	-2.440344
C	-0.822667	-3.945788	-1.327788
H	-1.170088	-4.376939	-0.383674
H	0.271495	-3.996641	-1.350094
H	-1.203653	-4.571714	-2.145495
C	-3.418626	-2.562163	0.058732
H	-4.343367	-2.806875	-0.480560
H	-3.685177	-1.885438	0.879390
H	-3.029880	-3.488585	0.491131
C	-3.647760	0.343591	-1.063024
H	-3.357176	1.379647	-1.270471
H	-3.899108	0.250967	-0.000147
H	-4.562813	0.130127	-1.632867
C	-1.410795	0.810461	-3.263872
H	-2.076563	0.758808	-4.135202
H	-0.387867	0.910791	-3.641485
H	-1.663959	1.724088	-2.712331
C	0.418908	-1.834017	-3.327074
H	1.161928	-2.474775	-2.839787
H	0.907255	-0.901246	-3.627343
H	0.082259	-2.346228	-4.238361
N	1.466894	-0.009157	-0.523210
C	1.836651	0.957581	-1.369887
H	1.068265	1.348099	-2.032827
C	3.130228	1.454170	-1.419548
H	3.400779	2.233201	-2.124725
C	4.059408	0.910075	-0.544586
C	3.701681	-0.090211	0.348146

H	4.440657	-0.498627	1.030242
C	2.384616	-0.526048	0.335255
C	1.777704	-1.510965	1.204816
C	0.421580	-1.790001	1.094311
N	2.263579	-2.241621	2.240543
C	3.619702	-2.320540	2.771577
H	3.616614	-3.051459	3.580089
H	3.917678	-1.341402	3.154020
H	4.297910	-2.644312	1.978843
N	1.313861	-2.950962	2.806563
N	0.217265	-2.665225	2.114106
C	-1.033317	-3.291469	2.517737
H	-1.264237	-4.123037	1.847248
H	-1.824528	-2.539865	2.480777
H	-0.920044	-3.661884	3.537110
H	-1.503068	0.239627	1.715994
C	-3.908087	4.446684	-0.233796
C	-2.600501	3.966742	-0.286268
C	-2.099581	3.082977	0.670259
C	-2.940501	2.679137	1.726755
C	-4.256194	3.162720	1.782459
C	-4.736697	4.032651	0.810510
H	-4.274315	5.132941	-0.993788
H	-1.940549	4.275687	-1.098333
H	-4.898049	2.842213	2.603276
H	-5.762090	4.391849	0.872735
C	-1.280045	1.048016	2.448906
H	-0.946874	0.561728	3.372638
C	-0.209006	1.950860	1.868175
H	0.006301	2.758521	2.581976
H	0.722818	1.390021	1.719800
C	-0.706150	2.522712	0.549616
H	-0.720379	1.707933	-0.201092
H	-0.020355	3.285819	0.156359
N	-2.470780	1.832712	2.733047
H	-3.209995	1.317503	3.198672
O	5.383769	1.288991	-0.576349
C	5.709325	2.599773	-0.328093
O	4.880141	3.412938	0.009657
C	7.162808	2.819443	-0.514967
H	7.417242	3.851282	-0.271363
H	7.726677	2.130449	0.121951
H	7.433770	2.601191	-1.553323

$10_{Rh\text{-}OCH3}$ Gsolv= -1585.692672

Rh	0.031591	-0.904278	0.559023
C	0.105760	-2.637768	1.750377
C	1.332572	-2.578018	1.007480
C	2.006419	-1.375312	1.401380
C	1.235635	-0.694925	2.399286
C	0.057122	-1.469444	2.619998
C	-0.904196	-3.722949	1.723475
H	-0.852285	-4.297942	0.793332
H	-1.919353	-3.325713	1.831228
H	-0.726260	-4.411250	2.560838
C	1.908457	-3.612222	0.108523
H	2.730288	-4.125408	0.625426
H	2.323961	-3.170808	-0.804874
H	1.169606	-4.366498	-0.174419
C	3.308725	-0.926977	0.861216
H	3.449571	0.154716	0.961214
H	3.432954	-1.213873	-0.188952
H	4.109276	-1.424361	1.427967
C	1.640767	0.556305	3.092821
H	2.431607	0.340882	3.823138
H	0.805658	1.009681	3.635965
H	2.041044	1.297408	2.389595
C	-1.033898	-1.177828	3.578142
H	-2.005536	-1.501228	3.190152
H	-1.089340	-0.113289	3.825503
H	-0.850979	-1.731128	4.509420
N	-1.569319	0.587320	0.617827
C	-1.570194	1.635982	1.445035
H	-0.768036	1.678247	2.179017
C	-2.523635	2.640983	1.404901
H	-2.461141	3.462564	2.109913
C	-3.532731	2.549716	0.443427
C	-3.544109	1.455885	-0.435289
H	-4.324042	1.392291	-1.187968
C	-2.551147	0.504478	-0.324344
C	-2.348617	-0.656911	-1.171316
C	-1.230077	-1.464578	-1.006407
N	-3.055033	-1.146184	-2.223459
C	-4.303592	-0.676172	-2.811685
H	-4.579138	-1.372450	-3.603391
H	-4.155938	0.322626	-3.229455
H	-5.078726	-0.657687	-2.042280
N	-2.464392	-2.199810	-2.742519

N	-1.374813	-2.372842	-2.004977
C	-0.484781	-3.472741	-2.344827
H	-0.591979	-4.272947	-1.607935
H	0.541265	-3.098899	-2.355150
H	-0.757352	-3.842298	-3.333924
H	1.175372	-0.212481	-1.666009
C	5.009927	2.798064	0.145169
C	3.619521	2.857346	0.221371
C	2.800542	2.220355	-0.712099
C	3.403353	1.511947	-1.770976
C	4.802732	1.454806	-1.851926
C	5.597448	2.085012	-0.901342
H	5.624840	3.299073	0.889182
H	3.142627	3.406004	1.035202
H	5.258709	0.900531	-2.672291
H	6.680884	2.020826	-0.981254
C	1.238731	0.605842	-2.417417
H	0.720304	0.256501	-3.317507
C	0.591444	1.853257	-1.846995
H	0.665459	2.665440	-2.583691
H	-0.477108	1.681062	-1.663327
C	1.301807	2.234668	-0.557495
H	1.021196	1.498924	0.220473
H	0.966229	3.212487	-0.185046
N	2.625058	0.895513	-2.754025
H	3.106035	0.134857	-3.222142
O	-4.513262	3.444221	0.282894
C	-4.527522	4.591470	1.136740
H	-5.390100	5.182307	0.827791
H	-4.642300	4.292024	2.184116
H	-3.612067	5.178909	1.007664

$TS_{4,5\text{-Ir-}OCOCH_3}$ Gsolv= -1691.594112

Ir	0.500508	-0.952069	0.291612
C	1.206892	-2.504318	1.640776
C	2.340452	-1.839039	1.056878
C	2.344795	-0.467420	1.543424
C	1.199448	-0.276443	2.344321
C	0.450697	-1.525778	2.374945
C	0.880841	-3.952330	1.558714
H	1.379452	-4.437680	0.715080
H	-0.197892	-4.123625	1.474239
H	1.221674	-4.448421	2.476983
C	3.446086	-2.456627	0.273209
H	4.313399	-2.643934	0.920663
H	3.776743	-1.794957	-0.536728
H	3.146613	-3.412424	-0.168792
C	3.427284	0.518702	1.293830
H	3.081628	1.551334	1.418348
H	3.853651	0.406111	0.290672
H	4.242447	0.351274	2.011070
C	0.852123	0.959000	3.095006
H	1.393666	0.967343	4.050284
H	-0.216386	1.014139	3.326449
H	1.140373	1.866193	2.549948
C	-0.795577	-1.783374	3.147025
H	-1.394184	-2.570522	2.673928
H	-1.416712	-0.883169	3.216261
H	-0.561539	-2.106626	4.170039
N	-1.385835	0.188342	0.172279
C	-1.595886	1.356495	0.793219
H	-0.733886	1.823761	1.261894
C	-2.840001	1.962239	0.866117
H	-2.965955	2.900687	1.395856
C	-3.907428	1.316152	0.257428
C	-3.722540	0.111266	-0.401892
H	-4.565344	-0.388807	-0.868475
C	-2.444141	-0.428938	-0.424649
C	-2.031643	-1.665907	-1.042722
C	-0.721169	-2.096929	-0.880228
N	-2.646152	-2.537036	-1.881756
C	-4.013027	-2.531081	-2.390366
H	-4.113626	-3.368093	-3.081069
H	-4.196816	-1.589645	-2.913773
H	-4.711304	-2.646923	-1.558321
N	-1.823702	-3.484428	-2.269469
N	-0.671155	-3.203983	-1.665313
C	0.469370	-4.068605	-1.934051
H	0.385386	-4.990191	-1.352607
H	1.373163	-3.523901	-1.655051
H	0.489937	-4.301744	-3.000081
H	0.811913	-0.426502	-1.389077
H	1.366889	0.268655	-1.368494
C	2.570467	4.912019	0.268533
C	3.700923	4.465624	-0.374313
C	3.673878	3.255265	-1.109609
C	2.462360	2.514100	-1.171913
C	1.303236	3.009411	-0.535828

C	1.361960	4.181400	0.180004
H	5.740060	3.285065	-1.751234
H	2.597134	5.836124	0.840498
H	4.632190	5.027332	-0.326865
C	4.804681	2.728566	-1.775402
H	0.378001	2.444975	-0.628098
H	0.470454	4.553966	0.680655
C	4.712779	1.523118	-2.429181
H	5.563675	1.087603	-2.943892
N	2.404593	1.313591	-1.816172
C	3.485264	0.833317	-2.400723
H	3.387980	-0.147406	-2.868092
O	-5.197898	1.788417	0.354884
C	-5.490749	3.060087	-0.069619
O	-4.670385	3.759992	-0.617479
C	-6.904489	3.392534	0.226705
H	-7.060792	3.378420	1.310709
H	-7.146508	4.377952	-0.172219
H	-7.563938	2.635279	-0.208862

$TS_{4,5\text{-}Rh\text{-}OCH3}$ Gsolv= -1584.474690

Rh	-0.114140	-0.793127	0.367901
C	-0.316138	-2.224905	1.990922
C	1.001721	-2.313303	1.420895
C	1.686640	-1.066683	1.704442
C	0.780503	-0.194406	2.340570
C	-0.485658	-0.895941	2.490020
C	-1.329536	-3.308615	2.085779
H	-1.098204	-4.145996	1.421341
H	-2.338222	-2.947716	1.856212
H	-1.347668	-3.694611	3.113680
C	1.652698	-3.519851	0.842371
H	2.279529	-4.012117	1.598505
H	2.303317	-3.254781	-0.000051
H	0.917815	-4.250352	0.489431
C	3.125857	-0.807448	1.450144
H	3.351833	0.264315	1.410105
H	3.472890	-1.282169	0.525409
H	3.714504	-1.239945	2.271296
C	1.096154	1.163457	2.858764
H	1.660482	1.076943	3.797059
H	0.191909	1.741190	3.074427
H	1.718097	1.735564	2.158458
C	-1.715856	-0.368733	3.137741
H	-2.615543	-0.810541	2.692865
H	-1.789209	0.720329	3.044155
H	-1.720651	-0.610853	4.209070
N	-1.384109	0.967446	-0.020153
C	-1.149123	2.201777	0.433318
H	-0.170800	2.383054	0.875196
C	-2.073449	3.233671	0.370338
H	-1.805181	4.209037	0.761147
C	-3.321197	2.967846	-0.198303
C	-3.584562	1.681970	-0.688132
H	-4.553455	1.471273	-1.131000
C	-2.602174	0.716914	-0.582511
C	-2.678031	-0.656520	-1.036998
C	-1.635121	-1.530652	-0.765505
N	-3.565028	-1.320638	-1.821900
C	-4.814965	-0.854989	-2.409620
H	-5.210759	-1.659507	-3.029277
H	-4.615006	0.026696	-3.023638
H	-5.523870	-0.611445	-1.615161
N	-3.157319	-2.544606	-2.075475
N	-1.993155	-2.650667	-1.439099
C	-1.246831	-3.895392	-1.558804
H	-1.513877	-4.576234	-0.746699
H	-0.182271	-3.653528	-1.516154
H	-1.486109	-4.353607	-2.519457
H	0.475015	-0.725788	-1.275994
H	1.292008	-0.315324	-1.299521
C	4.443693	3.398172	-0.045520
C	5.236815	2.405920	-0.571532
C	4.649051	1.262422	-1.164983
C	3.231737	1.163294	-1.205699
C	2.433555	2.206346	-0.689410
C	3.033747	3.299480	-0.110953
H	6.489164	0.254128	-1.690523
H	4.898020	4.270297	0.417867
H	6.322381	2.477977	-0.537816
C	5.402272	0.193904	-1.703934
H	1.351154	2.116084	-0.757276
H	2.420044	4.098003	0.300782
C	4.760389	-0.906699	-2.221134
H	5.310702	-1.746426	-2.633808
N	2.628432	0.052463	-1.714882
C	3.354625	-0.944528	-2.181778
H	2.804697	-1.819306	-2.532296

O	-4.311048	3.861855	-0.320016
C	-4.089829	5.187195	0.167369
H	-5.012915	5.734147	-0.026431
H	-3.888454	5.174721	1.244213
H	-3.260367	5.662127	-0.368108

$TS_{6,7\text{-}Ir\text{-}OCOCH3}$ Gsolv= -1691.602187

Ir	-0.743322	-0.808689	-0.446753
C	-2.051139	-2.386371	-1.305259
C	-2.849297	-1.272225	-0.837174
C	-2.492417	-0.123836	-1.625478
C	-1.456160	-0.492860	-2.536359
C	-1.183376	-1.899843	-2.335602
C	-2.156804	-3.790993	-0.824715
H	-2.453952	-3.830495	0.229310
H	-1.206716	-4.325541	-0.929387
H	-2.913997	-4.338757	-1.402094
C	-4.004477	-1.335721	0.102165
H	-4.942501	-1.432160	-0.461563
H	-4.080030	-0.426936	0.711627
H	-3.935576	-2.194634	0.777055
C	-3.110144	1.222014	-1.504358
H	-2.450504	2.003807	-1.897125
H	-3.351037	1.461074	-0.460932
H	-4.048737	1.256942	-2.074240
C	-0.853170	0.401338	-3.566248
H	-1.563686	0.591057	-4.381657
H	0.042037	-0.043583	-4.014489
H	-0.573502	1.375003	-3.141350
C	-0.188302	-2.697933	-3.100782
H	0.141077	-3.578217	-2.538820
H	0.697333	-2.102776	-3.352479
H	-0.625439	-3.046730	-4.045908
N	1.397984	-0.637304	-0.481075
C	2.065200	-0.152758	-1.540616
H	1.479793	0.052568	-2.432739
C	3.428255	0.087000	-1.522817
H	3.938163	0.470548	-2.401160
C	4.113492	-0.169728	-0.343320
C	3.455419	-0.658445	0.771876
H	4.001508	-0.846025	1.690974
C	2.087825	-0.887684	0.669904
C	1.192931	-1.356312	1.695517
C	-0.172239	-1.413080	1.419113
N	1.373807	-1.751526	2.981449
C	2.606087	-1.871331	3.751478
H	2.351538	-2.297816	4.721599
H	3.051456	-0.882140	3.882914
H	3.296603	-2.532578	3.222762
N	0.229608	-2.051023	3.550586
N	-0.685503	-1.843260	2.605913
C	-2.082036	-2.083981	2.933444
H	-2.442624	-2.956913	2.382764
H	-2.668182	-1.201582	2.665888
H	-2.157035	-2.268615	4.005635
H	-0.553273	0.726690	0.264553
C	-3.505140	2.800715	2.288390
C	-2.269863	2.205729	2.136002
C	-1.362141	2.677493	1.169490
C	-1.743514	3.761726	0.353769
C	-3.000153	4.367869	0.508051
C	-3.867144	3.886812	1.468219
H	0.315710	1.431042	1.757841
H	-4.202166	2.431931	3.036325
H	-1.975512	1.355786	2.751523
C	-0.086939	2.039766	0.946488
H	-3.268304	5.206799	-0.130953
H	-4.841649	4.352688	1.590907
C	0.817526	2.664737	0.049861
H	1.837196	2.305242	-0.058908
C	0.391745	3.717735	-0.718614
H	1.031897	4.211092	-1.442774
N	-0.848281	4.231870	-0.582768
H	-1.118189	5.031642	-1.148992
O	5.482592	0.007033	-0.270289
C	5.971734	1.284842	-0.345226
O	5.240368	2.248712	-0.391281
C	7.454097	1.280409	-0.348082
H	7.812227	0.750949	-1.237472
H	7.829948	2.303819	-0.346485
H	7.825783	0.738114	0.526982

$TS_{6,7\text{-}Rh\text{-}OCH3}$ Gsolv= -1584.481549

Rh	-0.184243	-0.881998	-0.539305
C	-0.798886	-2.774803	-1.537093
C	-1.946973	-2.049924	-1.041016
C	-2.020604	-0.803929	-1.752089
C	-0.898140	-0.715693	-2.624040

C	-0.149346	-1.947711	-2.498200
C	-0.403303	-4.150394	-1.128140
H	-0.639070	-4.337710	-0.074183
H	0.669202	-4.321692	-1.269080
H	-0.940664	-4.901568	-1.723146
C	-3.025338	-2.578910	-0.160073
H	-3.865531	-2.931794	-0.774599
H	-3.417257	-1.805125	0.511618
H	-2.686630	-3.423887	0.446997
C	-3.105270	0.200421	-1.607741
H	-2.809735	1.172915	-2.016154
H	-3.394416	0.336470	-0.557644
H	-4.001233	-0.134198	-2.148962
C	-0.622377	0.408524	-3.563523
H	-1.339749	0.406121	-4.395013
H	0.379303	0.335417	-4.000506
H	-0.706867	1.383108	-3.062282
C	1.082644	-2.280113	-3.261863
H	1.677167	-3.048254	-2.756303
H	1.717620	-1.398412	-3.408624
H	0.822928	-2.660092	-4.259172
N	1.772983	0.032200	-0.463605
C	2.305651	0.754465	-1.454627
H	1.736562	0.803372	-2.380452
C	3.515508	1.424474	-1.353695
H	3.886855	1.981541	-2.206917
C	4.207953	1.353309	-0.142709
C	3.656508	0.619875	0.914476
H	4.191322	0.569539	1.858005
C	2.448842	-0.025396	0.721739
C	1.714425	-0.818050	1.682731
C	0.473331	-1.348069	1.336263
N	1.966072	-1.164710	2.972349
C	3.110911	-0.849242	3.817349
H	2.957918	-1.336729	4.780224
H	3.173872	0.233311	3.953694
H	4.022948	-1.227494	3.349663
N	0.983207	-1.877368	3.474826
N	0.099096	-1.974457	2.484104
C	-1.141697	-2.690211	2.736141
H	-1.155929	-3.618699	2.159534
H	-1.981451	-2.054067	2.445347
H	-1.200017	-2.916664	3.801424
H	-0.601026	0.521270	0.234814
C	-4.121116	1.374820	2.256471
C	-2.752895	1.292784	2.112133
C	-2.085723	2.087976	1.159284
C	-2.846715	2.958319	0.350392
C	-4.240303	3.043376	0.499542
C	-4.863888	2.256284	1.445356
H	-0.065174	1.536512	1.730238
H	-4.631413	0.759437	2.992692
H	-2.162162	0.609274	2.721456
C	-0.668412	1.992410	0.944896
H	-4.804242	3.725479	-0.133435
H	-5.942685	2.316038	1.564496
C	-0.063405	2.891292	0.041250
H	1.015715	2.925893	-0.076583
C	-0.852691	3.715036	-0.725808
H	-0.444417	4.407395	-1.454829
N	-2.190799	3.737026	-0.576550
H	-2.740242	4.378411	-1.143491
O	5.386842	1.945495	0.098532
C	6.010084	2.663971	-0.967479
H	6.955566	3.031184	-0.567248
H	6.202849	2.000412	-1.817762
H	5.389716	3.511073	-1.280772

$TS_{8,5\text{-}Ir\text{-}OCOCH3}$ Gsolv= -1692.766717

Ir	1.393682	-0.268250	0.124693
C	2.737044	-1.113973	1.621825
C	3.472111	-0.202999	0.768975
C	2.937954	1.119702	0.991040
C	1.849238	1.033931	1.899065
C	1.720991	-0.360295	2.291243
C	3.008903	-2.564426	1.812746
H	3.566333	-2.984236	0.969233
H	2.081597	-3.136341	1.930656
H	3.610750	-2.714017	2.718486
C	4.721555	-0.491593	0.012354
H	5.595891	-0.192631	0.606630
H	4.757335	0.066401	-0.930064
H	4.824057	-1.556812	-0.215762
C	3.486790	2.355127	0.375937
H	2.809216	3.205907	0.495256
H	3.699664	2.217457	-0.690373
H	4.435958	2.608265	0.867715
C	1.057816	2.180282	2.429336

H	1.625280	2.716647	3.201065
H	0.121662	1.846648	2.888764
H	0.810698	2.901689	1.638855
C	0.742483	-0.901971	3.270261
H	0.496982	-1.947475	3.053987
H	-0.188869	-0.325481	3.278821
H	1.165727	-0.859084	4.282503
N	-0.799282	-0.568205	0.214302
C	-1.635713	0.275094	0.832467
H	-1.194715	1.171594	1.264121
C	-3.000369	0.048776	0.919153
H	-3.648728	0.761740	1.418825
C	-3.502085	-1.099765	0.321571
C	-2.660880	-1.985624	-0.334428
H	-3.067836	-2.875668	-0.803672
C	-1.305222	-1.686460	-0.372778
C	-0.259160	-2.436366	-1.026327
C	1.046876	-1.962767	-0.985759
N	-0.260515	-3.565939	-1.779448
C	-1.362667	-4.461966	-2.108405
H	-0.963293	-5.264442	-2.728349
H	-2.128437	-3.911057	-2.659448
H	-1.777408	-4.874307	-1.185499
N	0.943086	-3.841840	-2.224327
N	1.714132	-2.867145	-1.747768
C	3.129826	-2.880409	-2.087273
H	3.703821	-3.334106	-1.274953
H	3.453581	-1.850870	-2.251020
H	3.259010	-3.462593	-3.000470
H	1.311997	0.432591	-1.496477
H	0.622265	1.013215	-1.413770
C	-0.314160	5.873563	-0.318019
C	-1.554918	5.243818	-0.425803
C	-1.658092	3.949275	-0.929024
C	-0.481569	3.290099	-1.318171
C	0.759585	3.917807	-1.224874
C	0.844915	5.213462	-0.723924
H	-0.255010	6.885935	0.075000
H	-2.461184	5.765513	-0.120035
H	1.648265	3.379992	-1.551685
H	1.812608	5.704417	-0.649109
C	-1.632303	1.440823	-2.159243
H	-1.605638	0.400403	-2.499140
N	-0.518508	1.957628	-1.788351
C	-2.919033	2.191803	-2.172167
H	-2.990798	2.691386	-3.152625
H	-3.758174	1.490267	-2.118961
C	-2.961602	3.213006	-1.040311
H	-3.162205	2.695085	-0.089048
H	-3.786636	3.918124	-1.188278
O	-4.853555	-1.361579	0.273983
C	-5.575114	-1.431431	1.439759
O	-5.047582	-1.378251	2.526903
C	-7.018859	-1.589868	1.145279
H	-7.577929	-1.713411	2.073101
H	-7.375991	-0.704508	0.608184
H	-7.172718	-2.453806	0.491223

$TS_{8,5\text{-}Rh\text{-}OCH3}$ Gsolv= -1585.647201

Rh	-1.194152	-0.634444	0.085420
C	-2.821739	-1.194424	1.410377
C	-2.697470	-2.165955	0.352761
C	-1.415608	-2.808345	0.500458
C	-0.722556	-2.210545	1.584345
C	-1.599190	-1.206871	2.153659
C	-4.016634	-0.361128	1.708744
H	-4.639810	-0.218787	0.819641
H	-3.733712	0.626204	2.089894
H	-4.632496	-0.849473	2.475400
C	-3.759672	-2.623437	-0.582050
H	-4.190544	-3.566811	-0.219182
H	-3.358836	-2.812277	-1.584560
H	-4.573880	-1.898077	-0.665602
C	-0.949752	-3.946093	-0.331728
H	0.117424	-4.144544	-0.193537
H	-1.146207	-3.779050	-1.396973
H	-1.501555	-4.849896	-0.038370
C	0.614251	-2.622843	2.098512
H	0.534846	-3.570431	2.647506
H	1.031129	-1.882455	2.789287
H	1.335027	-2.775482	1.283213
C	-1.307525	-0.367639	3.343129
H	-1.823428	0.597287	3.289684
H	-0.234904	-0.182260	3.463848
H	-1.656752	-0.880859	4.249187
N	0.164108	1.014212	0.576446
C	1.296395	0.871825	1.268909
H	1.547385	-0.138102	1.589268

C	2.145799	1.924901	1.570339
H	3.048727	1.732713	2.139757
C	1.807152	3.197758	1.105503
C	0.617759	3.366734	0.384828
H	0.351639	4.355771	0.024755
C	-0.174066	2.260748	0.141270
C	-1.408396	2.213221	-0.614171
C	-2.059066	1.000663	-0.806702
N	-2.109686	3.162577	-1.286017
C	-1.851465	4.591536	-1.414735
H	-2.652206	5.021976	-2.016003
H	-0.889572	4.742439	-1.911022
H	-1.844025	5.047407	-0.422060
N	-3.151576	2.643608	-1.895690
N	-3.102106	1.346662	-1.602070
C	-4.131024	0.476969	-2.153215
H	-4.924468	0.323218	-1.416616
H	-3.667007	-0.475828	-2.415030
H	-4.542376	0.948903	-3.046288
H	-0.546093	-0.872287	-1.520633
H	0.348732	-0.681930	-1.470074
C	4.250030	-3.627987	-0.536192
C	4.712028	-2.317378	-0.407340
C	3.927403	-1.239281	-0.810018
C	2.654100	-1.504626	-1.337114
C	2.191528	-2.811655	-1.482288
C	2.991911	-3.877406	-1.082495
H	4.879530	-4.455971	-0.218358
H	5.701200	-2.124583	0.006632
H	1.205851	-2.978775	-1.913733
H	2.632284	-4.897932	-1.193916
C	2.248859	0.738031	-1.859834
H	1.528708	1.516765	-2.128498
N	1.788924	-0.449614	-1.708584
C	3.691852	1.077903	-1.714368
H	4.153446	0.938222	-2.706027
H	3.798451	2.140777	-1.470491
C	4.367711	0.189760	-0.674305
H	4.113567	0.549554	0.335263
H	5.457261	0.261341	-0.761479
O	2.550974	4.296104	1.292457
C	3.821529	4.144426	1.929778
H	4.459601	3.463038	1.353798
H	4.266716	5.139449	1.947997
H	3.702897	3.776627	2.954836

$TS_{9,10\text{-}Ir\text{-}OCOCH3}$ Gsolv= -1692.786863

Ir	0.570640	-0.941910	0.410043
C	1.320396	-2.536425	1.782625
C	2.392838	-2.028616	0.951858
C	2.590307	-0.644059	1.293223
C	1.629041	-0.274660	2.279290
C	0.841946	-1.452853	2.579626
C	0.848713	-3.948528	1.814312
H	0.889116	-4.405654	0.818946
H	-0.181593	-4.022168	2.177857
H	1.481479	-4.552514	2.478883
C	3.323424	-2.839224	0.117033
H	4.232185	-3.069602	0.690373
H	3.633662	-2.303878	-0.787837
H	2.875786	-3.791958	-0.182639
C	3.663769	0.218602	0.730329
H	3.439900	1.284846	0.852630
H	3.824743	0.017193	-0.335917
H	4.611912	0.012190	1.245842
C	1.543040	1.039849	2.976442
H	2.237690	1.073068	3.826726
H	0.539324	1.222619	3.376647
H	1.799292	1.872717	2.309629
C	-0.258210	-1.507649	3.580083
H	-0.940420	-2.341376	3.383207
H	-0.844956	-0.580982	3.584923
H	0.150582	-1.637776	4.591063
N	-1.400874	-0.014320	0.374943
C	-1.766080	0.970125	1.210367
H	-1.055323	1.234990	1.988942
C	-2.974002	1.638972	1.105632
H	-3.221599	2.439178	1.795078
C	-3.838792	1.256034	0.086634
C	-3.493626	0.242410	-0.791069
H	-4.171417	-0.041091	-1.590509
C	-2.260163	-0.375657	-0.620356
C	-1.684296	-1.421316	-1.422901
C	-0.401329	-1.873059	-1.119461
N	-2.116895	-2.100436	-2.515548
C	-3.375690	-1.985318	-3.240950
H	-3.358764	-2.711902	-4.053238
H	-3.468287	-0.974307	-3.645252

H	-4.205388	-2.201680	-2.563923
N	-1.210403	-2.950895	-2.935866
N	-0.189477	-2.803755	-2.092108
C	0.997698	-3.616280	-2.303488
H	1.084010	-4.356516	-1.503967
H	1.875280	-2.965734	-2.311998
H	0.901219	-4.122268	-3.264720
H	0.854481	0.172384	-0.789546
C	4.036742	4.685044	-0.080875
C	2.676805	4.416883	0.066424
C	2.062158	3.395669	-0.655160
C	2.858433	2.647069	-1.528827
C	4.216077	2.906551	-1.697212
C	4.806779	3.931136	-0.966550
H	4.495309	5.486035	0.493736
H	2.073816	5.006223	0.756051
H	4.797810	2.296151	-2.386176
H	5.866697	4.139129	-1.087872
C	0.997332	1.268671	-2.177730
H	0.658917	0.452398	-2.812485
C	0.055976	2.300336	-1.674825
H	-0.078084	2.995006	-2.522254
H	-0.924387	1.857741	-1.475764
C	0.613436	3.039823	-0.467185
H	0.519279	2.402723	0.426738
H	0.023509	3.942055	-0.272061
N	2.278746	1.563571	-2.231836
H	2.914452	0.917460	-2.696532
O	-5.028030	1.915462	-0.147193
C	-5.955594	2.016333	0.857871
O	-5.801421	1.484353	1.933563
H	-0.603217	-1.660771	4.595725
N	-1.412697	0.700180	0.606005
C	-1.218842	1.716333	1.452615
H	-0.379614	1.624073	2.138539
C	-2.013692	2.851431	1.489577
H	-1.789314	3.631066	2.209164
C	-3.077880	2.940068	0.588250
C	-3.298860	1.886680	-0.306742
H	-4.123742	1.949870	-1.009685
C	-2.454927	0.792004	-0.272015
C	-2.495931	-0.372569	-1.126746
C	-1.525429	-1.362470	-0.992133
N	-3.307520	-0.728668	-2.156395
C	-7.122489	2.813096	0.409806
H	-7.610123	2.303956	-0.428321
H	-7.828853	2.930864	1.232150
H	-6.790448	3.792148	0.050398

$TS_{9,10\text{-}Rh\text{-}OCH3}$ Gsolv= -1585.662885

Rh	-0.109760	-1.023177	0.431160
C	-0.089825	-2.855165	1.686402
C	1.055005	-2.810410	0.802702
C	1.862569	-1.681176	1.186161
C	1.195346	-0.988563	2.230059
C	-0.016285	-1.724563	2.543837
C	-1.141600	-3.909034	1.695280
H	-1.266734	-4.360198	0.704660
H	-2.112179	-3.508836	2.008113
H	-0.875269	-4.715730	2.391571
C	1.494650	-3.876280	-0.140068
H	2.256766	-4.505850	0.340523
H	1.944624	-3.456428	-1.047352
H	0.668244	-4.529775	-0.436217
C	3.193077	-1.353278	0.606645
H	3.479521	-0.313086	0.801879
H	3.218180	-1.524422	-0.476653
H	3.960136	-2.001756	1.052879
C	1.720038	0.190835	2.974424
H	2.468090	-0.125082	3.714175
H	0.926884	0.710203	3.523723
H	2.206051	0.914324	2.307047
C	-0.982155	-1.352523	3.611810
H	-1.954817	-1.832711	3.462041
H	-1.140694	-0.267808	3.653352
C	-4.470695	-0.042036	-2.705288
H	-4.873838	-0.660425	-3.507237
H	-4.166356	0.929880	-3.101387
H	-5.220347	0.084446	-1.920710
N	-2.926513	-1.865481	-2.692984
N	-1.855724	-2.227462	-1.987680
C	-1.167784	-3.453593	-2.361865
H	-1.331651	-4.218893	-1.598987
H	-0.100485	-3.240767	-2.458580
H	-1.566073	-3.795539	-3.317779
H	0.547740	-0.225165	-0.836156
C	5.438229	2.525438	-0.128406
C	4.099453	2.854691	0.077174

C	3.086703	2.235163	-0.651817
C	3.461124	1.269952	-1.591814
C	4.792803	0.932510	-1.817334
C	5.785917	1.565105	-1.078557
H	6.212276	3.021097	0.452370
H	3.826175	3.604275	0.818659
H	5.036442	0.172031	-2.557456
H	6.828867	1.308117	-1.244214
C	1.175818	0.870250	-2.223028
H	0.500387	0.306975	-2.863377
C	0.771322	2.155303	-1.606131
H	0.900679	2.902412	-2.408804
H	-0.295645	2.140306	-1.364478
C	1.631190	2.514135	-0.402961
H	1.305672	1.923125	0.467688
H	1.485697	3.567162	-0.137944
N	2.451487	0.580378	-2.308242
H	2.738000	-0.239418	-2.841502
O	-3.928096	3.974052	0.509008
C	-3.768160	5.053683	1.431140
H	-2.795005	5.539055	1.297426
H	-4.565302	5.761031	1.200422
H	-3.876458	4.699602	2.462320

1_{OTf} Gsolv= -2482.943793

Ir	-1.075628	-0.222470	0.328264
Cl	-1.824642	-0.170962	2.696126
C	0.848725	-1.299005	0.774011
C	1.064446	0.095200	0.424638
C	0.613407	0.270987	-0.933347
C	0.029652	-0.970014	-1.367581
C	0.236045	-1.954843	-0.315872
C	1.236448	-1.911901	2.069784
H	0.594930	-2.762194	2.325363
H	1.188032	-1.185104	2.886966
H	2.271168	-2.276731	2.009925
C	1.810021	1.072624	1.266358
H	2.867970	0.784832	1.344950
H	1.409177	1.112989	2.286286
H	1.767374	2.082950	0.845953
C	0.759194	1.484353	-1.782683
H	1.038768	2.363066	-1.193899
H	-0.162563	1.711183	-2.330347
H	1.549645	1.315700	-2.526221
C	-0.537083	-1.243591	-2.715312
H	-0.952485	-0.333562	-3.161998
H	-1.332692	-1.996074	-2.670291
H	0.241623	-1.624846	-3.389739
C	-0.103436	-3.400516	-0.394683
H	-0.426834	-3.795854	0.575534
H	0.780316	-3.974399	-0.703881
H	-0.891713	-3.595592	-1.129706
O	5.598157	0.743947	1.310694
O	7.082631	0.936606	-0.673171
O	6.772075	-1.264896	0.439009
S	6.224107	0.073878	0.157613
C	4.791421	-0.285340	-0.956256
F	3.916082	-1.085638	-0.350583
F	4.169285	0.841572	-1.298391
F	5.209934	-0.888114	-2.068595
N	-3.080632	-0.975407	-0.097391
C	-3.393270	-2.275372	-0.052882
H	-2.601333	-2.953511	0.255647
C	-4.658408	-2.746773	-0.376348
H	-4.861153	-3.812103	-0.331798
C	-5.638541	-1.833347	-0.748178
C	-5.334401	-0.477382	-0.768612
H	-6.088065	0.255840	-1.037816
C	-4.046452	-0.075562	-0.431624
C	-3.529193	1.269016	-0.331593
C	-2.209216	1.452084	0.064558
N	-4.095894	2.496733	-0.441394
C	-5.452469	2.861907	-0.830059
H	-5.516525	3.949930	-0.833571
H	-6.161601	2.448022	-0.109096
H	-5.656130	2.471829	-1.829999
N	-3.242506	3.446094	-0.127306
N	-2.118721	2.801627	0.182256
C	-0.970110	3.586094	0.612043
H	-0.376331	3.891017	-0.253727
H	-0.371368	2.966599	1.283066
H	-1.329846	4.469169	1.142318
H	-6.637161	-2.169954	-1.012211

$1_{isopropanol}$ Gsolv= -1521.549961

Ir	0.553611	0.017058	-0.130161
Cl	0.016491	-0.006144	-2.554561
C	1.859540	-0.912550	1.326831

C	2.465026	-0.994096	0.021477	H	-0.282940	-4.005728	0.761344
C	2.758074	0.365089	-0.405206	H	0.221938	-3.326437	-0.821945
C	2.301528	1.262313	0.585242	H	-1.206952	-4.394232	-0.717713
C	1.693123	0.479231	1.649550				
C	1.512727	-2.045228	2.228354	$TS_{4,5\text{-isopropanol}}$ Gsolv= -1463.861076			
H	1.505025	-3.001368	1.697380	Ir	-0.500268	-0.375536	0.311463
H	0.534898	-1.907129	2.704151	C	-1.173964	-1.832955	1.786210
H	2.260791	-2.116939	3.029351	C	0.074213	-2.277578	1.213980
C	2.930169	-2.220426	-0.685544	C	1.098588	-1.337597	1.628908
H	4.021427	-2.317371	-0.600998	C	0.487532	-0.294339	2.358024
H	2.686367	-2.190020	-1.754157	C	-0.939332	-0.576451	2.432875
H	2.484657	-3.127470	-0.264003	C	-2.473909	-2.555860	1.763464
C	3.441138	0.726620	-1.673650	H	-2.496028	-3.334033	0.995090
H	3.149998	1.723235	-2.022929	H	-3.318565	-1.877676	1.597159
H	3.220842	0.009559	-2.471017	H	-2.631974	-3.045674	2.733656
H	4.529133	0.728591	-1.519155	C	0.346682	-3.587979	0.558560
C	2.470309	2.740369	0.583200	H	0.771453	-4.296348	1.283461
H	3.458718	3.000717	0.986178	H	1.068873	-3.485361	-0.260761
H	1.725279	3.240210	1.211798	H	-0.565102	-4.038119	0.152430
H	2.410675	3.159966	-0.427921	C	2.554510	-1.517366	1.394546
C	1.132240	1.022923	2.916529	H	3.109537	-0.576217	1.479804
H	0.416217	0.325681	3.365501	H	2.763478	-1.965510	0.416306
H	0.615612	1.976042	2.752720	H	2.952593	-2.205963	2.153275
H	1.932063	1.201822	3.648426	C	1.188333	0.835924	3.025944
N	-1.108970	1.435223	-0.029401	H	1.580601	0.505709	3.997542
C	-0.947634	2.754677	-0.179126	H	0.515709	1.677950	3.220221
H	0.069115	3.101840	-0.346022	H	2.040715	1.199621	2.438508
C	-2.012395	3.644418	-0.136593	C	-1.954057	0.238172	3.155630
H	-1.828096	4.707388	-0.259398	H	-2.949697	0.120285	2.711597
C	-3.295141	3.144670	0.058142	H	-1.702743	1.305035	3.139887
H	-4.149927	3.814694	0.098157	H	-2.018102	-0.070892	4.207764
C	-3.479161	1.773489	0.188292	N	-1.137803	1.712471	0.083229
H	-4.473261	1.358083	0.323534	C	-0.486317	2.749313	0.624577
C	-2.366245	0.940628	0.132972	H	0.457348	2.527747	1.117682
C	-2.333704	-0.502282	0.179427	C	-0.976872	4.046965	0.575392
C	-1.111368	-1.153382	0.053830	H	-0.409108	4.851651	1.032347
N	-3.302389	-1.451734	0.195288	C	-2.191166	4.280652	-0.058571
C	-4.749134	-1.303975	0.278226	H	-2.605900	5.283795	-0.109288
H	-5.185596	-2.303372	0.275301	C	-2.874679	3.215288	-0.632058
H	-5.103989	-0.740734	-0.589337	H	-3.824976	3.373172	-1.132346
H	-5.010437	-0.784760	1.203689	C	-2.323392	1.941450	-0.549441
N	-2.790669	-2.656141	0.083175	C	-2.849887	0.711608	-1.097578
N	-1.477640	-2.459792	-0.009405	C	-2.148110	-0.470869	-0.896452
C	-0.627806	-3.624852	-0.203712	N	-3.904492	0.423118	-1.901085

C	-4.947426	1.298877	-2.420973
H	-5.596739	0.697972	-3.058784
H	-4.486265	2.099110	-3.005991
H	-5.521232	1.715100	-1.588951
N	-3.919475	-0.848040	-2.230872
N	-2.854711	-1.369820	-1.627543
C	-2.565785	-2.779348	-1.851835
H	-3.188158	-3.401095	-1.202411
H	-1.507632	-2.942401	-1.636719
H	-2.772589	-3.016298	-2.897366
H	0.137384	-0.214139	-1.314454
H	1.014503	-0.071353	-1.153648
C	5.575114	2.070813	0.064069
C	5.877354	0.931539	-0.642807
C	4.844943	0.164040	-1.235555
C	3.496753	0.591738	-1.084873
C	3.208560	1.776439	-0.371162
C	4.232513	2.497686	0.195713
H	6.109359	-1.364537	-2.101422
H	6.369892	2.655587	0.521063
H	6.908259	0.600373	-0.758087
C	5.084217	-1.022048	-1.968273
H	2.170319	2.095518	-0.289954
H	4.012563	3.408313	0.749067
C	4.028920	-1.727750	-2.495484
H	4.180307	-2.641749	-3.062184
N	2.472573	-0.142812	-1.600960
C	2.724233	-1.249942	-2.269527
H	1.854468	-1.800244	-2.636346

$1_{\text{Ir-OCOCH3-isopropanol}}$ Gsolv= -1749.288586

Ir	-1.132377	-0.263064	-0.138007
Cl	-0.706408	-0.053064	-2.572832
C	-2.841118	-0.188242	1.194667
C	-3.253075	-0.690751	-0.088145
C	-2.583469	-1.969961	-0.293178
C	-1.745993	-2.217932	0.815148
C	-1.847176	-1.085624	1.723984
C	-3.369505	1.012455	1.896932
H	-3.918048	1.673374	1.219767
H	-2.572914	1.590211	2.379446
H	-4.065935	0.692670	2.683893
C	-4.315122	-0.140555	-0.975264
H	-5.238608	-0.727374	-0.874343
H	-4.016237	-0.175288	-2.029382
H	-4.554700	0.898479	-0.726170
C	-2.777971	-2.843546	-1.479539
H	-1.921493	-3.507542	-1.639389
H	-2.920842	-2.252164	-2.390346
H	-3.671306	-3.468738	-1.345207
C	-0.921106	-3.431622	1.053002
H	-1.513991	-4.177657	1.599835
H	-0.037377	-3.213462	1.662845
H	-0.591109	-3.898135	0.117839
C	-1.169203	-0.970283	3.044165
H	-1.119542	0.072864	3.375919
H	-0.144786	-1.359889	3.004386
H	-1.710731	-1.540991	3.811471
N	1.044455	-0.379571	0.044492
C	1.728674	-1.526524	-0.036391
H	1.149790	-2.423657	-0.242969
C	3.103132	-1.595458	0.127858
H	3.620580	-2.547655	0.069889
C	3.783008	-0.409619	0.374155
C	3.103986	0.797753	0.432078
H	3.650288	1.719140	0.611556
C	1.726482	0.779532	0.252060
C	0.827860	1.909384	0.199810
C	-0.524934	1.679993	-0.030717
N	1.020079	3.252682	0.196716
C	2.245849	4.019543	0.376070
H	1.985692	5.077485	0.329736
H	2.946424	3.771783	-0.426020
H	2.681465	3.784046	1.350413
N	-0.103293	3.893362	-0.027367
N	-1.018096	2.937095	-0.171907
C	-2.376808	3.342510	-0.499295
H	-2.905005	3.658048	0.404703
H	-2.879696	2.488092	-0.957330
H	-2.334003	4.168765	-1.212061
O	5.131470	-0.389245	0.636896
C	6.011047	-0.877697	-0.295392
O	5.649850	-1.259080	-1.382211
C	7.397681	-0.832888	0.230507
H	7.462734	-1.418650	1.153780
H	8.091420	-1.227029	-0.513340
H	7.663911	0.200121	0.479680

$TS_{4,5\text{-Ir-OCOCH3-isopropanol}}$ Gsolv= -1691.601573

Ir	0.477849	-0.986377	0.282455
C	1.114757	-2.585268	1.615082
C	2.276165	-1.994128	1.002833
C	2.378154	-0.626963	1.485309
C	1.265475	-0.358283	2.311845
C	0.444719	-1.561726	2.367878
C	0.687402	-4.007403	1.535337
H	1.152031	-4.529187	0.693826
H	-0.400617	-4.103695	1.446971
H	0.989727	-4.526593	2.454802
C	3.331295	-2.688077	0.213669
H	4.187213	-2.935179	0.857117
H	3.706642	-2.054346	-0.598852
H	2.967082	-3.622296	-0.225294
C	3.516359	0.283971	1.203292
H	3.252634	1.337726	1.350026
H	3.901466	0.151596	0.185702
H	4.340993	0.050123	1.891329
C	1.015515	0.896526	3.070017
H	1.584660	0.877554	4.009368
H	-0.039842	1.015838	3.336283
H	1.336241	1.786620	2.514928
C	-0.792329	-1.738990	3.175755
H	-1.454746	-2.490246	2.729742
H	-1.354488	-0.802317	3.263233
H	-0.544331	-2.072602	4.192572
N	-1.386839	0.187603	0.224399
C	-1.555145	1.356290	0.857380
H	-0.675954	1.788009	1.329571
C	-2.777047	2.004628	0.934043
H	-2.871004	2.945780	1.466913
C	-3.867463	1.402339	0.320058
C	-3.724523	0.194438	-0.345344
H	-4.584520	-0.270349	-0.817574
C	-2.464905	-0.388656	-0.377064
C	-2.089484	-1.624872	-1.023970
C	-0.780656	-2.075282	-0.904131
N	-2.734809	-2.473518	-1.863859
C	-4.112287	-2.447311	-2.341263
H	-4.241740	-3.286273	-3.025691
H	-4.291981	-1.505026	-2.866108
H	-4.792953	-2.548823	-1.492148
N	-1.933316	-3.422025	-2.289105
N	-0.762821	-3.166026	-1.711781
C	0.364349	-4.027311	-2.040689
H	0.324031	-4.944211	-1.446259
H	1.281394	-3.473800	-1.827594
H	0.318256	-4.273153	-3.103491
H	0.734307	-0.365946	-1.379954
H	1.296212	0.311223	-1.313143
C	2.709778	4.946812	0.316724
C	3.807294	4.470594	-0.360665
C	3.725285	3.262270	-1.095378
C	2.493262	2.551789	-1.116695
C	1.369034	3.076307	-0.441365
C	1.480151	4.248336	0.268176
H	5.766619	3.241683	-1.816160
H	2.778444	5.872184	0.883803
H	4.753074	5.009952	-0.343546
C	4.815580	2.711199	-1.808179
H	0.425768	2.537330	-0.507749
H	0.614164	4.648503	0.792425
C	4.664788	1.517248	-2.472171
H	5.482261	1.067042	-3.027723
N	2.381520	1.355888	-1.760284
C	3.420766	0.859610	-2.401481
H	3.278936	-0.111855	-2.878745
O	-5.129948	1.931710	0.411494
C	-5.365399	3.192588	-0.078031
O	-4.519143	3.816875	-0.670485
C	-6.758107	3.609241	0.214668
H	-6.922476	3.609742	1.297809
H	-6.942106	4.604524	-0.192190
H	-7.459917	2.889838	-0.220718

$1_{Rh\text{-OCH3-isopropanol}}$ Gsolv= -1642.173668

Rh	-0.944676	-0.270220	-0.200036
Cl	-0.799948	-0.082940	-2.651280
C	-2.226590	-0.177488	1.527006
C	-3.029286	-0.344592	0.344081
C	-2.700171	-1.633456	-0.226099
C	-1.677266	-2.228943	0.548626
C	-1.354145	-1.311713	1.626882
C	-2.303742	0.937941	2.507413
H	-2.743830	1.839370	2.069007
H	-1.317128	1.196947	2.907895
H	-2.934781	0.640118	3.356011

C	-4.145325	0.526088	-0.115381
H	-5.110572	0.073313	0.151201
H	-4.136618	0.655546	-1.204336
H	-4.105349	1.517166	0.347247
C	-3.352817	-2.228143	-1.418202
H	-2.694089	-2.932989	-1.936004
H	-3.670806	-1.462455	-2.132914
H	-4.249905	-2.779305	-1.101783
C	-1.095981	-3.579646	0.318994
H	-1.799370	-4.355930	0.649799
H	-0.163687	-3.727999	0.873216
H	-0.894768	-3.757210	-0.745237
C	-0.351039	-1.532334	2.701826
H	0.116290	-0.588806	3.008717
H	0.443502	-2.216667	2.386080
H	-0.832481	-1.967048	3.588689
N	1.229395	-0.552732	-0.197931
C	1.841047	-1.727411	-0.356186
H	1.200518	-2.582738	-0.563616
C	3.216010	-1.894096	-0.273952
H	3.641212	-2.882576	-0.412005
C	4.000789	-0.767498	-0.014373
C	3.376206	0.479806	0.119549
H	3.985940	1.360343	0.298913
C	2.000149	0.549605	0.016382
C	1.176467	1.741111	0.064602
C	-0.201279	1.634771	-0.085444
N	1.477779	3.064083	0.121155
C	2.770003	3.723846	0.255347
H	2.591682	4.799491	0.284286
H	3.395471	3.473437	-0.606100
H	3.249992	3.398971	1.182006
N	0.398234	3.804528	0.009361
N	-0.597157	2.930730	-0.120455
C	-1.941561	3.453920	-0.314757
H	-2.444059	3.571109	0.649465
H	-2.490454	2.752600	-0.946808
H	-1.867313	4.422635	-0.812305
O	5.330889	-0.777078	0.113388
C	6.016922	-2.023266	-0.009667
H	7.071746	-1.800915	0.158059
H	5.667626	-2.735915	0.746523
H	5.885544	-2.441250	-1.014530

$TS_{4,5\text{-Rh-OCH3-isopropanol}}$ Gsolv= -1584.482889

Rh	-0.186653	-0.821824	0.378818
C	-0.451401	-2.357158	1.902126
C	0.862322	-2.464752	1.326449
C	1.594169	-1.264762	1.678337
C	0.725605	-0.396694	2.373859
C	-0.564852	-1.059255	2.489891
C	-1.510038	-3.400709	1.928273
H	-1.304930	-4.212606	1.224444
H	-2.499820	-2.986411	1.704621
H	-1.560659	-3.838529	2.934405
C	1.470321	-3.661499	0.684934
H	2.096858	-4.200199	1.409664
H	2.115588	-3.381256	-0.156542
H	0.713472	-4.361489	0.316981
C	3.042125	-1.051930	1.428870
H	3.321335	0.006301	1.485900
H	3.359994	-1.452673	0.459288
H	3.616075	-1.586128	2.199567
C	1.096710	0.912079	2.975942
H	1.668404	0.744747	3.899170
H	0.217272	1.506610	3.243029
H	1.732277	1.507965	2.307852
C	-1.768256	-0.528733	3.182421
H	-2.689493	-0.903317	2.720025
H	-1.799325	0.566213	3.164133
H	-1.772962	-0.843877	4.234988
N	-1.373392	1.011620	0.094962
C	-1.072938	2.211664	0.598156
H	-0.118571	2.297732	1.114641
C	-1.902399	3.318302	0.499087
H	-1.583652	4.259912	0.933393
C	-3.125423	3.168253	-0.160021
C	-3.456199	1.916923	-0.698106
H	-4.405207	1.799118	-1.212596
C	-2.565310	0.871367	-0.553955
C	-2.715722	-0.478611	-1.059986
C	-1.725931	-1.424278	-0.823238
N	-3.645146	-1.061365	-1.860406
C	-4.880001	-0.515615	-2.409221
H	-5.348289	-1.296614	-3.009140
H	-4.646017	0.347791	-3.037701
H	-5.543925	-0.225631	-1.590782
N	-3.313983	-2.297614	-2.155679

N	-2.155962	-2.496054	-1.532287	H	6.572709	2.171116	-0.649542
C	-1.498547	-3.783629	-1.704073	C	5.374924	0.058205	-1.885054
H	-1.866779	-4.497492	-0.961949	H	1.588842	2.181074	-0.411400
H	-0.423443	-3.631113	-1.585686	H	2.902720	3.999934	0.666030
H	-1.713000	-4.152324	-2.708974	C	4.604837	-0.941953	-2.430054
H	0.414526	-0.592956	-1.242881	H	5.049141	-1.776069	-2.964907
H	1.235955	-0.215038	-1.203127	N	2.609840	0.111402	-1.634961
C	4.824367	3.183382	0.081725	C	3.209119	-0.881567	-2.260991
C	5.485941	2.178754	-0.583335	H	2.561816	-1.676778	-2.636602
C	4.759143	1.128241	-1.195041	O	-4.027387	4.137514	-0.324752
C	3.339903	1.132557	-1.106133	C	-3.730732	5.439200	0.183968
C	2.677169	2.186756	-0.440481	H	-4.595392	6.058491	-0.058648
C	3.411039	3.189849	0.147015	H	-3.594142	5.410100	1.271083
H	6.460293	0.038257	-1.970927	H	-2.837861	5.849465	-0.301514
H	5.385522	3.985423	0.555318				

References

1 J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.

2 A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.

3 C. Lee, W. Yang and R. G. Parr, *Phys. Rev. B*, 1988, **37**, 785-789.

4 J. P. Perdew, J. A. Chevary, S. H. Vosko, K. A. Jackson, M. R. Pederson, D. J. Singh and C. Fiolhais, *Phys. Rev. B*, 1992, **46**, 6671-6687.

5 J. M. Shi, F. M. Peeters, G. Q. Hai and J. T. Devreese, *Phys. Rev. B*, 1993, **48**, 4978-4978.

6 J. P. Perdew, K. Burke and Y. Wang, *Phys. Rev. B*, 1996, **54**, 16533-16539.

7 T. M. Henderson, A. F. Izmaylov, G. Scalmani and G. E. Scuseria, *J. Chem. Phys.*, 2009, **131**, 044108.

8 A. V. Krukau, O. A. Vydrov, A. F. Izmaylov and G. E. Scuseria, *J. Chem. Phys.*, 2006, **125**, 224106.

9 M. Ernzerhof and J. P. Perdew, *J. Chem. Phys.*, 1998, **109**, 3313-3320.
10 J. Tao, J. P. Perdew, V. N. Staroverov and G. E. Scuseria, *Phys. Rev. Lett.*, 2003, **91**, 146401.
11 Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
12 Á. Vivancos, M. Beller and M. Albrecht, *ACS Catal.*, 2018, **8**, 17-21.