

Supplementary Information

Mechanistic insights into iridium catalysed hydrogenation of ethyl acetate to ethanol: A DFT Study

Xiuli Yan,^{a, b} and Xinzheng Yang^{*a, b}

^aBeijing 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

^bUniversity of Chinese Academy of Sciences, Beijing 100049, People's Republic of China

1. Cartesian coordinates (Ångström) of all structures optimized in gas-phase and the corresponding absolute free energies with solvent effect corrections in ethyl acetate

H ₂ O G _{solv} = -76.380102	C	2.120813	-0.883642	-0.000067
O 0.000000 0.000000 0.117659	H	2.029382	-1.526749	-0.880826
H 0.000000 0.758304 -0.470638	H	3.092339	-0.388402	0.000850
H 0.000000 -0.758304 -0.470638	H	2.028339	-1.528269	0.879453
	O	-0.178198	-0.444583	0.000341
H ₂ G _{solv} = -1.170934	C	-1.299340	0.448915	0.000250
H 0.000000 0.000000 0.371073	H	-1.236609	1.100012	-0.880772
H 0.000000 0.000000 -0.371073	H	-1.237088	1.099554	0.881656
	C	-2.546152	-0.395089	-0.000280
HOTf G _{solv} = -961.773450	H	-3.436456	0.241641	-0.000266
S -0.841192 -0.141073 0.081289	H	-2.581864	-1.036414	-0.886835
F 1.402225 -0.228178 -1.229163	H	-2.582242	-1.036978	0.885851
F 1.511675 -0.870989 0.830332				
F 1.339264 1.231894 0.361556	EtOH G _{solv} = -154.882956			
O -1.225584 1.031043 -0.951391	O	1.227650	-0.258939	-0.105782
O -1.194135 -1.396588 -0.522085	H	1.218083	-0.912812	0.599931
O -1.242386 0.264112 1.409154	C	0.086949	0.554342	0.046527
C 0.991717 0.009124 -0.001493	H	0.126884	1.134689	0.985175
H -1.472869 1.819334 -0.441615	H	0.128796	1.283478	-0.771784
	C	-1.202609	-0.237055	-0.022131
EtOAc G _{solv} = -307.432921	H	-1.266972	-0.955679	0.805710
C 1.030489 0.145685 0.000036	H	-2.079134	0.417424	0.041317
O 1.189366 1.342131 -0.000183	H	-1.254894	-0.799311	-0.960475

MeCHO Gsolv= -153.701205

C	0.231320	0.397955	-0.000005
H	0.292353	1.514118	-0.000032
O	1.231701	-0.275134	0.000001
C	-1.162699	-0.148870	0.000013
H	-1.707799	0.217469	0.878544
H	-1.707414	0.216190	-0.879281
H	-1.142473	-1.241213	0.000716

OTf⁻ Gsolv= -961.281045

S	-0.911342	-0.000176	0.000046
F	1.420386	-0.543511	1.118827
F	1.418882	1.241195	-0.088591
F	1.419908	-0.696970	-1.030461
O	-1.221290	-1.433018	0.100378
O	-1.221493	0.803115	1.190719
O	-1.221424	0.629470	-1.290938
C	0.927091	-0.000026	0.000003

[(EtO)(Me)COH(OTf)]⁻ Gsolv= -1269.876774

H	-2.349882	-1.064909	-1.096778
C	-2.853169	-0.806923	-0.141896
O	-2.132550	-1.326422	0.919733
C	-4.255522	-1.362969	-0.092682
H	-4.873277	-0.933725	-0.888049
H	-4.233105	-2.452503	-0.190332
H	-4.697174	-1.105722	0.876599
O	-2.988289	0.598689	-0.087650
C	-1.746109	1.264050	-0.151021
H	-1.160388	0.900619	-1.012870
H	-1.142638	1.038669	0.741293
C	-1.998409	2.747238	-0.257123
H	-1.045894	3.287661	-0.295705
H	-2.572806	2.982841	-1.160903
H	-2.569361	3.104834	0.607892
H	-1.189396	-1.347381	0.660298
O	2.459767	-1.028557	-1.540725
C	1.868117	0.763820	0.234195
S	1.761622	-1.004542	-0.254456
O	0.297216	-1.207275	-0.348731
O	2.411860	-1.687495	0.865440
F	3.137231	1.152197	0.362073
F	1.291511	1.559847	-0.674397
F	1.257312	0.981229	1.403045

[(EtO)(Me)COH]⁺ Gsolv= -307.749259

C	0.995453	0.011599	0.000028
O	1.301880	1.263877	-0.000223
C	2.108658	-0.946663	-0.000102
H	1.736917	-1.970865	0.000208
H	2.737297	-0.764791	-0.879329
H	2.737941	-0.764308	0.878540
O	-0.197057	-0.426553	0.000484
C	-1.383893	0.463859	0.000058
H	-1.316500	1.082661	-0.903857
H	-1.316803	1.082674	0.903975
C	-2.594114	-0.420772	-0.000227
H	-3.490122	0.206526	-0.000511
H	-2.618617	-1.052289	-0.891809
H	-2.619087	-1.052180	0.891412
H	0.553763	1.885837	0.000753

I Gsolv= -1064.823348

Ir	-0.453723	0.001795	-0.181470
O	0.292245	-0.066541	-2.383889
N	1.218895	1.322888	-0.066028
N	1.222652	-1.299179	-0.036432
C	-1.637295	0.441768	1.529598
C	-2.167266	1.220861	0.424004
C	-2.584891	0.306607	-0.585381
C	-2.356449	-1.047856	-0.119112
C	-1.816349	-0.957493	1.206721
C	-1.141340	0.983349	2.822521
C	-2.344870	2.698173	0.396255
C	-3.166506	0.671826	-1.902808
C	-2.743181	-2.285566	-0.853819
C	-1.491253	-2.082281	2.121194
C	1.125059	2.660756	-0.118408
C	2.235144	3.488579	-0.056236
C	3.491716	2.908343	0.065084
C	3.594408	1.523657	0.108288
C	2.442968	0.748205	0.036104
C	2.445612	-0.720009	0.048075
C	3.597791	-1.495430	0.121517
C	3.495030	-2.880212	0.095083
C	2.238039	-3.464853	-0.012470
C	1.127766	-2.638959	-0.074826
H	-0.054706	0.581573	-3.010912

H	0.293761	-0.920591	-2.836090	C	-2.480108	0.735323	0.021127
H	-1.980996	1.142998	3.511028	C	-3.628913	1.512028	0.024381
H	-0.635816	1.945457	2.692847	C	-3.517004	2.899215	0.008436
H	-0.441644	0.296716	3.307979	C	-2.254635	3.480083	-0.011899
H	-3.368075	2.948627	0.703604	C	-1.145095	2.651489	-0.010595
H	-1.674261	3.209549	1.093434	H	3.239754	0.001960	3.028675
H	-2.202586	3.118386	-0.605554	H	1.717127	-0.890664	3.094222
H	-2.810249	1.645339	-2.255515	H	1.713672	0.888538	3.094119
H	-4.258663	0.741962	-1.814727	H	3.327893	-2.770468	1.204722
H	-2.958270	-0.081698	-2.668958	H	1.636602	-2.764094	1.702198
H	-2.514616	-2.214127	-1.922987	H	2.097856	-3.312030	0.072262
H	-3.822142	-2.462336	-0.765320	H	1.867988	-2.603949	-2.015293
H	-2.241511	-3.174781	-0.460110	H	3.167772	-1.593245	-2.655504
H	-1.420785	-3.041764	1.601891	H	1.487376	-1.166092	-2.982910
H	-0.559501	-1.910662	2.670047	H	1.487838	1.166720	-2.982807
H	-2.292302	-2.179179	2.865336	H	3.168224	1.593574	-2.654942
H	0.123783	3.072160	-0.213859	H	1.868426	2.604318	-2.014798
H	2.108181	4.565522	-0.101342	H	2.098354	3.311923	0.073025
H	4.569976	1.056309	0.195967	H	1.636279	2.763583	1.702617
H	4.573992	-1.026965	0.194862	H	3.327783	2.769912	1.205941
H	2.113081	-4.542457	-0.045809	H	-0.137101	-3.056586	-0.021281
H	0.123668	-3.048131	-0.158136	H	-2.124996	-4.557326	-0.027417
H	4.384258	3.524947	0.122443	H	-4.610193	-1.048462	0.037723
H	4.388516	-3.495469	0.153076	H	-4.610173	1.048591	0.037409
				H	-2.124881	4.557386	-0.027528
2 Gsolv= -988.425090				H	-0.137010	3.056584	-0.021164
Ir	0.391548	-0.000002	0.004986	H	-4.410434	-3.517609	0.010596
N	-1.247715	-1.310319	0.007533	H	-4.410335	3.517728	0.010259
N	-1.247686	1.310351	0.007615				
C	2.185064	-0.000188	1.198408	3 Gsolv= -989.586720			
C	2.204751	-1.177516	0.357469	Ir	-0.465677	0.001094	-0.363094
C	2.166852	-0.733455	-0.994154	N	1.225306	1.307109	-0.256242
C	2.166897	0.733569	-0.994003	N	1.211703	-1.312782	-0.250469
C	2.204838	1.177315	0.357715	C	-1.486571	0.583623	1.478356
C	2.197397	-0.000166	2.678207	C	-2.144080	1.217847	0.346716
C	2.306157	-2.576725	0.855216	C	-2.655604	0.177363	-0.493057
C	2.160059	-1.570322	-2.219221	C	-2.306237	-1.100192	0.085769
C	2.160410	1.570699	-2.218890	C	-1.623633	-0.837683	1.330023
C	2.306195	2.576380	0.855878	C	-0.869450	1.286380	2.634178
C	-1.145168	-2.651453	-0.010634	C	-2.390103	2.676249	0.172935
C	-2.254734	-3.480021	-0.011811	C	-3.432786	0.371482	-1.744701
C	-3.517083	-2.899124	0.008645	C	-2.749433	-2.428417	-0.425315
C	-3.628950	-1.511930	0.024560	C	-1.137458	-1.852345	2.298592
C	-2.480128	-0.735259	0.021146	C	1.140493	2.645189	-0.339350

C	2.249377	3.466091	-0.213365	C	-3.669634	-1.790277	1.248622
C	3.491115	2.880740	0.006000	C	-2.333820	-3.273911	-1.275472
C	3.583573	1.496768	0.074487	C	0.813558	-3.137841	-0.903694
C	2.435638	0.724304	-0.066176	C	1.453662	-1.773310	1.875943
C	2.428545	-0.742870	-0.066224	C	-1.333359	-0.854533	3.176842
C	3.568169	-1.528811	0.068759	C	-3.450109	0.250993	-1.692478
C	3.459128	-2.911502	-0.000394	C	-4.421180	1.075131	-2.237556
C	2.209852	-3.483437	-0.214469	C	-4.393760	2.431729	-1.932766
C	1.110147	-2.650027	-0.334175	C	-3.398676	2.919020	-1.096995
H	-1.630881	1.480045	3.400431	C	-2.451975	2.040152	-0.578738
H	-0.445167	2.253253	2.347402	C	-1.341654	2.449654	0.287495
H	-0.078896	0.690952	3.100653	C	-1.106696	3.760492	0.686025
H	-3.403679	2.922150	0.513804	C	0.004061	4.041218	1.472962
H	-1.702663	3.285134	0.767480	C	0.854057	3.006975	1.842525
H	-2.320289	2.987345	-0.875088	C	0.561447	1.717794	1.421151
H	-3.191195	1.316520	-2.239846	H	-4.031654	-2.613935	1.877636
H	-4.503161	0.393874	-1.501550	H	-4.250611	-1.805265	0.321440
H	-3.280330	-0.444245	-2.457698	H	-3.883871	-0.853225	1.774064
H	-2.682313	-2.493275	-1.516008	H	-2.408379	-4.350232	-1.072275
H	-3.797304	-2.604269	-0.152176	H	-3.354254	-2.896219	-1.399921
H	-2.169635	-3.251534	0.002743	H	-1.807184	-3.153506	-2.228585
H	-0.973560	-2.829044	1.835249	H	0.476658	-3.095914	-1.944398
H	-0.211959	-1.540139	2.792267	H	0.984147	-4.193350	-0.651881
H	-1.893613	-1.991220	3.082298	H	1.773795	-2.618756	-0.824171
H	0.150854	3.057549	-0.519104	H	2.199578	-1.408156	1.161884
H	2.134020	4.542581	-0.290191	H	1.790407	-2.751310	2.244385
H	4.548488	1.024947	0.230504	H	1.447748	-1.087342	2.728749
H	4.539396	-1.068480	0.219832	H	-0.491625	-0.192755	3.406367
H	2.082680	-4.558498	-0.292413	H	-2.254367	-0.262846	3.204455
H	0.114440	-3.049202	-0.513044	H	-1.391079	-1.602613	3.978438
H	-0.216966	0.382612	-2.125036	H	-3.421002	-0.812835	-1.913551
H	-0.278604	-0.455215	-2.112617	H	-5.176145	0.653695	-2.893774
H	4.381366	3.493949	0.113679	H	-3.356022	3.976696	-0.857044
H	4.342907	-3.534877	0.102149	H	-1.771780	4.560123	0.375893
				H	1.745023	3.183180	2.437539
				H	1.218629	0.886828	1.662982
4 Gsolv=	-1951.227862			H	-0.221563	-0.046648	-1.687229
Ir	-0.964673	-0.509799	-0.039959	H	0.402097	0.120263	-1.167195
N	-2.492327	0.719502	-0.877818	O	2.322485	0.692109	-0.937466
N	-0.514644	1.447223	0.669947	C	4.700619	-0.375723	-0.891289
C	-2.215697	-1.958189	0.993971	H	-5.136670	3.107907	-2.346654
C	-1.616996	-2.591352	-0.163392	H	0.206620	5.062513	1.783346
C	-0.193121	-2.573864	0.029405	S	3.602288	0.971796	-0.251415
C	0.104746	-1.907770	1.264003	O	4.284198	2.197336	-0.676257
C	-1.159571	-1.536942	1.868786				

O	3.578933	0.710776	1.196925	H	0.142901	3.033800	-0.329613
F	4.213888	-1.579463	-0.567194	H	2.114944	4.541455	-0.155221
F	4.804051	-0.321460	-2.220049	H	4.593302	1.044618	0.144987
F	5.924636	-0.275301	-0.374269	H	4.593693	-1.043502	0.144642
				H	2.116618	-4.541238	-0.155544
				H	0.144019	-3.034339	-0.329613
5 Gsolv= -989.340089				H	-0.021579	-0.000494	-1.858778
Ir	-0.411831	-0.000218	-0.294918	H	4.397497	3.516308	0.089274
N	1.243072	1.295835	-0.152536	H	4.398817	-3.515263	0.088844
N	1.243486	-1.295959	-0.152363				
C	-1.833357	0.706943	1.346199				
C	-2.225919	1.158196	0.016412	6 Gsolv= -2258.547023			
C	-2.535337	-0.001884	-0.767831	Ir	-1.452396	-0.476021	-0.064884
C	-2.225172	-1.159244	0.020033	N	-0.157869	0.419076	-1.463402
C	-1.832931	-0.703708	1.348458	N	-2.104474	1.524151	-0.159206
C	-1.488423	1.614664	2.475913	C	-2.294679	-2.298324	-1.144374
C	-2.500715	2.571413	-0.376445	C	-1.202525	-2.635782	-0.240036
C	-3.106482	-0.004189	-2.143795	C	-1.616106	-2.310863	1.092261
C	-2.498859	-2.573855	-0.368441	C	-2.903959	-1.679682	1.012723
C	-1.487930	-1.607684	2.481177	C	-3.330747	-1.718175	-0.380392
C	1.145556	2.634359	-0.201794	C	-2.272966	-2.534811	-2.615069
C	2.248851	3.465308	-0.113021	C	0.026929	-3.398828	-0.602778
C	3.510137	2.894055	0.019842	C	-0.845820	-2.599547	2.334622
C	3.618500	1.513266	0.053254	C	-3.763573	-1.295507	2.170312
C	2.469348	0.731325	-0.035077	C	-4.640930	-1.207406	-0.872034
C	2.469588	-0.731016	-0.035073	C	0.859959	-0.231194	-2.048994
C	3.619054	-1.512520	0.053049	C	1.732896	0.390837	-2.926873
C	3.511209	-2.893346	0.019562	C	1.548745	1.738099	-3.215092
C	2.250121	-3.465046	-0.113230	C	0.502521	2.416849	-2.607050
C	1.146505	-2.634504	-0.201795	C	-0.336400	1.737524	-1.727122
H	-2.393596	2.066627	2.900788	C	-1.436454	2.359956	-0.991349
H	-0.840288	2.438197	2.152418	C	-1.783921	3.706036	-1.091084
H	-0.971185	1.085720	3.281500	C	-2.828753	4.202225	-0.328664
H	-3.565403	2.808843	-0.255878	C	-3.502340	3.339243	0.530128
H	-1.948122	3.282307	0.248356	C	-3.107013	2.014441	0.588532
H	-2.237530	2.760135	-1.423253	H	-2.416702	-3.599261	-2.839383
H	-2.795480	0.878378	-2.710663	H	-1.313855	-2.239961	-3.057815
H	-4.202908	-0.004562	-2.095503	H	-3.059997	-1.976449	-3.130141
H	-2.794782	-0.888208	-2.708017	H	-0.103543	-4.465414	-0.380089
H	-2.237418	-2.765104	-1.415228	H	0.257034	-3.324690	-1.671272
H	-3.563030	-2.812268	-0.245256	H	0.902257	-3.048562	-0.045678
H	-1.944263	-3.282362	0.257301	H	0.232797	-2.569617	2.152033
H	-0.839515	-2.432086	2.160534	H	-1.095974	-3.599660	2.710817
H	-0.971032	-1.075983	3.285168	H	-1.068866	-1.877465	3.126524
H	-2.393067	-2.058500	2.907364	H	-3.174970	-0.874255	2.992841

H	-4.299558	-2.168482	2.564402	C	-0.866176	-2.515623	0.769491
H	-4.526855	-0.561600	1.886504	C	-2.203819	-2.074081	1.136243
H	-4.888504	-0.233836	-0.431065	C	-2.966682	-1.947575	-0.063743
H	-4.650978	-1.089075	-1.959318	C	-2.488468	-2.270529	-2.616851
H	-5.451176	-1.896893	-0.603330	C	0.316376	-3.203705	-1.441246
H	0.996433	-1.272546	-1.774500	C	0.213235	-2.809475	1.745812
H	2.549562	-0.185289	-3.350879	C	-2.696500	-1.931448	2.534417
H	0.344472	3.471992	-2.809911	C	-4.411791	-1.612894	-0.176866
H	-1.240787	4.361175	-1.765706	C	0.968645	0.136877	-2.063829
H	-4.322833	3.683216	1.151725	C	1.821935	0.956715	-2.791039
H	-3.591425	1.305163	1.255683	C	1.529652	2.308280	-2.884174
H	-0.405312	0.137624	0.991139	C	0.393725	2.801515	-2.248237
H	2.213504	2.256563	-3.900117	C	-0.408257	1.934335	-1.520790
H	-3.112045	5.248250	-0.399843	C	-1.610819	2.342983	-0.792088
C	0.870930	1.332546	2.786320	C	-2.066468	3.655638	-0.711376
O	1.610948	0.362850	2.720071	C	-3.227710	3.933724	-0.008726
C	-0.233743	1.462542	3.780457	C	-3.917312	2.890902	0.603190
H	-1.162789	1.156814	3.280210	C	-3.403083	1.611341	0.502677
H	-0.052798	0.797433	4.626100	H	-2.771481	-3.288251	-2.915824
H	-0.353834	2.495709	4.113664	H	-1.663566	-1.954876	-3.264334
O	0.935763	2.379646	1.972136	H	-3.341361	-1.613853	-2.813673
C	1.958583	2.371080	0.956225	H	0.259070	-4.299282	-1.411790
H	1.707083	1.597398	0.217161	H	0.260387	-2.909933	-2.494298
H	2.912293	2.097329	1.421747	H	1.303010	-2.921340	-1.061484
C	2.004515	3.741791	0.340232	H	1.186086	-2.963272	1.272220
H	2.755768	3.760075	-0.456747	H	-0.051079	-3.715596	2.307398
H	1.032663	4.009781	-0.092431	H	0.331719	-1.993629	2.469773
H	2.269045	4.501667	1.081334	H	-1.880726	-1.670295	3.216089
H	2.186619	-0.466043	1.439350	H	-3.122464	-2.880063	2.885168
O	3.404826	-2.020616	-1.248330	H	-3.475371	-1.166820	2.628060
C	4.673703	-0.037846	-0.020793	H	-4.825766	-1.248741	0.768498
S	3.605722	-1.532910	0.097630	H	-4.603353	-0.867378	-0.956920
O	2.242693	-0.844724	0.510576	H	-4.974620	-2.515595	-0.445672
O	4.138108	-2.344750	1.162503	H	1.198409	-0.915478	-1.951998
F	5.868829	-0.387186	-0.433595	H	2.704845	0.515444	-3.242263
F	4.137424	0.829102	-0.872791	H	0.145353	3.856359	-2.314574
F	4.747172	0.524312	1.176710	H	-1.511552	4.456248	-1.189964
				H	-4.832264	3.063096	1.160457
				H	-3.890273	0.767052	0.982981
7 Gsolv= -2258.519870				H	-0.351847	0.494217	1.194755
Ir	-1.309995	-0.551625	-0.136281	H	2.175242	2.979648	-3.443376
N	-0.117479	0.610811	-1.440228	H	-3.592631	4.954366	0.061889
N	-2.276926	1.336144	-0.177045	C	0.104552	1.171240	2.070321
C	-2.094442	-2.241246	-1.183213	O	1.064648	0.428864	2.662896
C	-0.809011	-2.645002	-0.646396				

C	-1.014376	1.471679	3.033705	C	-0.163112	-1.987607	3.500446
H	-1.757333	2.131802	2.575432	C	0.538642	-1.163723	2.641674
H	-1.492197	0.546796	3.371045	H	3.809635	-2.006487	-3.016598
H	-0.585841	1.980872	3.902443	H	2.414396	-1.029514	-3.476484
O	0.489412	2.357568	1.473099	H	2.192072	-2.488145	-2.491020
C	1.834307	2.491300	0.997656	H	4.161244	1.770782	-2.820369
H	1.976849	1.865491	0.105887	H	2.565044	1.211708	-3.322803
H	2.532353	2.128936	1.762350	H	2.711198	2.540054	-2.163164
C	2.060987	3.948534	0.697016	H	3.855251	2.334537	1.623347
H	3.065319	4.090737	0.284814	H	2.859829	2.968266	0.303621
H	1.332733	4.315861	-0.037256	H	4.598172	2.723080	0.063607
H	1.966780	4.558088	1.600695	H	3.567769	0.452124	2.827612
H	1.640447	0.019622	1.966737	H	4.976801	-0.476315	2.312222
O	3.293413	-1.593684	-1.399866	H	3.472639	-1.315199	2.681562
C	4.545867	-0.034444	0.299876	H	2.860200	-2.986624	1.276256
S	3.258357	-1.314333	0.041256	H	2.505359	-3.383382	-0.408489
O	2.020812	-0.557661	0.427170	H	4.186031	-3.266433	0.138362
O	3.579600	-2.407250	0.948584	H	0.351257	0.177049	-2.980549
F	5.744642	-0.506365	0.031265	H	-2.618045	-3.041873	-0.797585
F	4.298692	1.010090	-0.498122	H	-2.152729	-3.428164	1.177122
F	4.504728	0.389452	1.559651	H	1.309099	-0.492558	3.011230
				H	-2.949975	-2.559322	-3.205806
				H	-1.694885	-3.504192	3.611628
8 Gsolv=	-2258.524427			C	-0.349026	2.054352	1.568887
Ir	1.507988	-0.093350	-0.105429	H	-0.898227	1.120645	1.769354
N	-0.104206	-0.850005	-1.244369	O	0.346354	1.783993	0.241667
N	0.309573	-1.138353	1.317373	O	-1.168464	3.119607	1.478074
C	3.053722	-0.826831	-1.428326	C	-0.146094	2.542539	-0.893988
C	3.152238	0.605644	-1.338282	H	0.168071	1.970562	-1.774407
C	3.459637	0.930245	0.040645	H	-1.240565	2.530225	-0.893410
C	3.499974	-0.274434	0.796377	C	0.413265	3.943525	-0.932603
C	3.204021	-1.378135	-0.106994	H	0.025248	4.466028	-1.814201
C	2.842783	-1.624815	-2.665263	H	0.113453	4.508095	-0.046182
C	3.140257	1.579285	-2.466629	H	1.509212	3.949686	-1.000311
C	3.701775	2.308950	0.541501	C	0.748844	2.349109	2.555659
C	3.884939	-0.408232	2.228714	H	0.333143	2.368426	3.567882
C	3.186851	-2.826006	0.243634	H	1.553987	1.607270	2.512572
C	-0.311393	-0.561971	-2.537289	H	1.166744	3.338264	2.336824
C	-1.309787	-1.162230	-3.282351	H	-1.441216	-0.889753	-4.324121
C	-2.141807	-2.082675	-2.658979	H	0.049141	-1.962770	4.564269
C	-1.946997	-2.365817	-1.316803	H	-2.080921	2.830270	1.228437
C	-0.920373	-1.733531	-0.626780	O	-2.692044	0.696775	-1.243880
C	-0.663607	-1.920884	0.802801	C	-4.989530	0.085494	-0.164280
C	-1.378439	-2.803015	1.608272	S	-3.291581	0.717114	0.098413
C	-1.130154	-2.836084	2.968048				

O	-2.701572	-0.253524	1.044407	H	-2.929721	2.288051	-2.586966
O	-3.485516	2.065778	0.666937	H	0.290590	-2.843948	-0.902331
F	-5.647905	0.865592	-1.001491	H	2.392638	-4.113634	-1.308494
F	-4.907186	-1.140164	-0.691729	H	4.556334	-0.445776	-0.733381
F	-5.642198	0.011947	0.981643	H	4.380983	1.579799	-0.330986
				H	1.627279	4.756307	0.555675
				H	-0.218305	3.096146	0.384445
9 Gsolv= -1143.035250				H	4.578079	-2.875844	-1.216578
Ir	-0.490835	0.025478	0.003776	H	3.985388	3.970517	0.185686
N	1.240366	-1.031240	-0.630122	O	0.494239	-0.213949	1.781106
N	1.022310	1.516488	-0.088378	C	0.455676	-1.466024	2.395772
C	-1.994810	-0.529673	-1.474256	H	0.367610	-2.291147	1.656327
C	-2.234212	-1.234845	-0.221331	H	-0.420647	-1.568007	3.066687
C	-2.515131	-0.247483	0.781200	C	1.729622	-1.676084	3.188660
C	-2.390025	1.048815	0.189830	H	1.711683	-2.628525	3.730669
C	-2.093385	0.868647	-1.222773	H	2.597522	-1.674443	2.515658
C	-1.732766	-1.172612	-2.792089	H	1.864635	-0.866473	3.913425
C	-2.343770	-2.711572	-0.042828				
C	-2.853404	-0.488010	2.210088				
C	-2.680541	2.332640	0.890843	10 Gsolv= -2104.813744			
C	-1.947374	1.965892	-2.219778	Ir	-1.550794	-0.074966	0.095690
C	1.257228	-2.346025	-0.885761	N	-0.115957	-1.278464	-0.864413
C	2.431055	-3.048330	-1.105744	N	-0.476399	1.277696	-1.113023
C	3.636828	-2.359327	-1.052068	C	-3.511106	-1.136201	-0.361340
C	3.624174	-0.999171	-0.782968	C	-3.036511	-1.384705	0.994172
C	2.409228	-0.354816	-0.566538	C	-3.025670	-0.130994	1.690628
C	2.285978	1.075149	-0.268253	C	-3.384627	0.896293	0.756667
C	3.369930	1.944129	-0.179969	C	-3.722722	0.252347	-0.506178
C	3.149144	3.281367	0.111326	C	-3.706718	-2.192848	-1.392901
C	1.846796	3.721503	0.313847	C	-2.837163	-2.726381	1.617164
C	0.814094	2.803879	0.212060	C	-2.727770	0.060814	3.138241
H	-2.676119	-1.422085	-3.293455	C	-3.622757	2.332204	1.085316
H	-1.166495	-2.104317	-2.687111	C	-4.194856	0.976782	-1.719258
H	-1.164073	-0.514424	-3.456024	C	-0.005808	-2.601808	-0.663735
H	-3.395150	-3.024396	-0.031434	C	0.935378	-3.375866	-1.318661
H	-1.862444	-3.256794	-0.862185	C	1.810757	-2.757871	-2.205912
H	-1.888575	-3.042583	0.897634	C	1.718485	-1.389362	-2.396251
H	-2.735369	-1.538690	2.487992	C	0.745914	-0.665768	-1.709656
H	-3.897233	-0.205419	2.396431	C	0.560756	0.780113	-1.827812
H	-2.218479	0.113063	2.870773	C	1.367993	1.609769	-2.601661
H	-2.177244	2.382495	1.863749	C	1.093762	2.966033	-2.659629
H	-3.757860	2.435927	1.072347	C	0.018324	3.467284	-1.934972
H	-2.376910	3.201759	0.297461	C	-0.732295	2.594141	-1.168084
H	-1.457764	2.845975	-1.787744	H	-4.614816	-2.773359	-1.187685
H	-1.354677	1.651229	-3.083987	H	-2.868721	-2.900436	-1.411983

H	-3.801295	-1.769168	-2.396758	C	-2.793325	-1.757637	0.570775
H	-3.726126	-3.027684	2.185829	C	-2.973715	-0.697641	1.523758
H	-2.669154	-3.503275	0.863032	C	-3.441974	0.475296	0.843144
H	-1.985824	-2.732528	2.307383	C	-3.570091	0.138535	-0.555843
H	-2.013481	-0.684113	3.503457	C	-3.213305	-1.993064	-2.005565
H	-3.645878	-0.037176	3.731447	C	-2.399190	-3.157018	0.906962
H	-2.310748	1.054051	3.335634	C	-2.733851	-0.802219	2.986063
H	-2.887230	2.716809	1.800903	C	-3.853179	1.750325	1.497480
H	-4.615890	2.468549	1.532267	C	-4.067576	1.034777	-1.632937
H	-3.591878	2.965747	0.191727	C	0.287553	-2.160663	-1.357765
H	-3.597301	1.876111	-1.912935	C	1.305054	-2.626274	-2.167889
H	-4.144588	0.350175	-2.614192	C	2.133845	-1.702085	-2.794960
H	-5.235941	1.301246	-1.597010	C	1.919640	-0.348945	-2.589290
H	-0.696494	-3.034613	0.055107	C	0.876571	0.057876	-1.764405
H	2.407580	-0.880148	-3.060943	C	0.562411	1.455572	-1.458413
H	2.218663	1.198628	-3.133854	C	1.354620	2.533708	-1.835353
H	-1.564080	2.943822	-0.561255	C	0.962888	3.816020	-1.483944
H	-0.336400	0.179592	1.131888	C	-0.207236	3.996817	-0.755359
H	2.565546	-3.333960	-2.733124	C	-0.939524	2.882232	-0.391994
H	1.716042	3.625100	-3.257729	H	-4.226868	-2.372415	-2.185856
C	1.029918	2.235230	1.843991	H	-2.538051	-2.853467	-1.999646
O	1.729609	2.401731	0.857972	H	-2.939769	-1.358335	-2.854411
H	-0.023250	2.588083	1.813970	H	-3.206543	-3.664688	1.448441
H	0.981261	-4.443042	-1.126408	H	-2.197697	-3.751084	0.010216
H	-0.232903	4.523037	-1.948410	H	-1.504728	-3.186887	1.540430
C	1.462227	1.608802	3.120079	H	-2.051557	-1.621411	3.231238
H	1.342837	2.333806	3.934814	H	-3.685972	-1.000031	3.495868
H	0.790403	0.770885	3.347288	H	-2.329621	0.124979	3.406774
H	2.497883	1.260993	3.086464	H	-3.137345	2.074024	2.261587
O	4.161946	1.425733	1.124090	H	-4.823551	1.626734	1.994074
C	3.490815	-1.092136	1.001503	H	-3.968979	2.562662	0.772970
S	4.426524	0.231624	0.132666	H	-3.831688	2.084517	-1.432847
O	3.714108	0.448527	-1.112990	H	-3.639355	0.774272	-2.605444
O	5.815464	-0.129363	0.186687	H	-5.158755	0.952295	-1.715743
F	3.943303	-1.252211	2.225732	H	-0.365765	-2.841459	-0.819360
F	2.201750	-0.748417	1.054379	H	2.577264	0.386123	-3.037274
F	3.606854	-2.217531	0.320693	H	2.296068	2.362419	-2.344030
H	3.280885	1.869816	0.928774	H	-1.839163	2.967743	0.212541
				H	-0.071014	0.139876	1.278899
				H	2.954916	-2.032697	-3.423926
11 Gsolv= -2104.796911				H	1.578339	4.666854	-1.760869
Ir	-1.501856	-0.092006	0.011201	C	0.311614	0.900568	2.143001
N	0.064969	-0.848720	-1.172036	O	1.097516	1.852301	1.610782
N	-0.573868	1.639706	-0.744479	H	-0.626389	1.352758	2.503287
C	-3.174827	-1.240454	-0.723171				

H	1.453622	-3.694554	-2.286489	H	-2.558586	-3.199195	-1.505515
H	-0.539761	4.983104	-0.448945	H	-0.971359	-3.184753	-2.295744
C	0.929028	-0.018476	3.172806	H	1.296230	-2.965343	-1.862163
H	1.220728	0.578444	4.044060	H	1.931876	-3.877773	-0.489371
H	0.212214	-0.782055	3.494990	H	2.449095	-2.199648	-0.746935
H	1.827409	-0.504452	2.786837	H	2.625029	-1.003911	1.264222
O	3.543570	0.988668	1.763912	H	2.349499	-2.355874	2.380545
C	3.646099	-1.287891	0.572303	H	1.778763	-0.747312	2.811681
S	4.158866	0.474075	0.510952	H	-0.307639	-0.157730	3.432880
O	3.464435	0.954303	-0.698324	H	-2.031462	-0.446745	3.142153
O	5.606461	0.430765	0.479466	H	-1.047023	-1.677422	3.941771
F	4.098826	-1.896676	1.651528	H	-2.902318	-0.949804	-2.028616
F	2.290838	-1.362409	0.604980	H	-4.926511	0.294111	-2.781199
F	4.047778	-1.950358	-0.507081	H	-3.600440	3.624731	-0.408717
H	2.063326	1.569678	1.622579	H	-2.050329	4.348138	0.804277
				H	1.819090	3.444023	2.441909
				H	1.628570	1.165356	1.437373
12 Gsolv= -1297.035708				H	0.126369	0.005095	-1.671493
Ir	-0.529376	-0.492432	-0.064005	H	0.820569	0.080495	-1.185740
N	-2.200268	0.590207	-0.838998	C	3.605625	0.763361	-1.540041
N	-0.258842	1.497114	0.661825	O	2.717758	0.318253	-0.813536
C	-1.658157	-2.108429	0.919598	C	3.383514	1.374607	-2.884046
C	-0.927223	-2.634435	-0.213623	H	3.848684	0.747955	-3.652059
C	0.475831	-2.441436	0.054825	H	2.317558	1.478047	-3.094365
C	0.615964	-1.750053	1.303014	H	3.873460	2.350841	-2.940116
C	-0.718023	-1.546857	1.843471	O	4.879737	0.742648	-1.214356
C	-3.132395	-2.147100	1.102064	C	5.259173	0.150143	0.048749
C	-1.493492	-3.402931	-1.358554	H	4.926547	-0.896862	0.048606
C	1.597566	-2.883764	-0.813514	H	4.722824	0.676645	0.849955
C	1.909238	-1.437573	1.972672	C	6.751544	0.276651	0.174953
C	-1.043337	-0.917093	3.150769	H	7.085671	-0.163149	1.118943
C	-3.102875	0.060807	-1.680406	H	7.257781	-0.243753	-0.642814
C	-4.223850	0.759948	-2.097683	H	7.057835	1.326372	0.158489
C	-4.415989	2.053735	-1.626110	H	-5.286512	2.629207	-1.927926
C	-3.472902	2.609905	-0.772089	H	-0.077950	5.057315	2.127477
C	-2.363631	1.860361	-0.394259				
C	-1.275586	2.368581	0.449979	13 Gsolv= -1297.035648			
C	-1.231042	3.656323	0.972807	Ir	-0.513277	-0.464490	0.032763
C	-0.123337	4.055592	1.709609	N	-1.855628	0.762040	-1.067900
C	0.927412	3.164134	1.890124	N	-0.327275	1.458307	0.925244
C	0.825031	1.892559	1.347398	C	-1.937463	-2.042303	0.750734
H	-3.406787	-3.052233	1.658571	C	-1.099126	-2.526811	-0.336758
H	-3.667896	-2.181558	0.148846	C	0.260085	-2.503390	0.120384
H	-3.499000	-1.288381	1.672901	C	0.282539	-1.929317	1.436356
H	-1.400236	-4.480271	-1.174342				

C	-1.095460	-1.680641	1.832517	H	2.336750	1.086839	-2.986919
C	-3.422629	-1.957765	0.705875	O	4.833815	0.500517	-1.356111
C	-1.580707	-3.153515	-1.601529	C	5.506291	0.627431	-0.036824
C	1.431667	-3.045499	-0.622587	H	5.265891	-0.282720	0.522225
C	1.471783	-1.838302	2.332426	H	5.049508	1.488593	0.461064
C	-1.517993	-1.143595	3.154621	C	6.969122	0.795894	-0.311625
C	-2.560292	0.324832	-2.122862	H	7.499336	0.892146	0.640377
C	-3.459787	1.131455	-2.801329	H	7.377081	-0.069754	-0.839997
C	-3.629842	2.445012	-2.379047	H	7.162375	1.697046	-0.899445
C	-2.887751	2.906298	-1.301150	H	-4.327287	3.105138	-2.886554
C	-2.002981	2.044739	-0.658730	H	-0.320806	4.943220	2.592439
C	-1.154979	2.431678	0.473034				
C	-1.165274	3.695073	1.058732				
C	-0.316369	3.964183	2.122027	14 Gsolv=	-1297.013360		
C	0.537231	2.962754	2.572711	Ir	0.730123	0.070714	0.027490
C	0.502824	1.728026	1.946480	N	-0.847429	1.372153	-0.546733
H	-3.864478	-2.942796	0.900470	N	-0.474450	-1.098983	-1.272732
H	-3.783714	-1.631874	-0.276077	C	2.561334	1.259714	-0.550616
H	-3.816880	-1.264833	1.454424	C	2.318259	1.284508	0.885370
H	-1.605637	-4.245904	-1.501803	C	2.435924	-0.059533	1.372579
H	-2.599366	-2.839701	-1.851731	C	2.649610	-0.923700	0.247309
H	-0.930681	-2.916404	-2.451115	C	2.763977	-0.086924	-0.939455
H	1.303632	-2.951671	-1.706081	C	2.591028	2.462298	-1.427404
H	1.548397	-4.113943	-0.401377	C	2.208613	2.510009	1.729121
H	2.365554	-2.553326	-0.330592	C	2.386786	-0.482344	2.799774
H	2.378413	-1.551077	1.788158	C	2.945292	-2.384217	0.317089
H	1.667444	-2.807904	2.807352	C	3.048722	-0.592795	-2.310091
H	1.317766	-1.118723	3.143570	C	-0.939413	2.651295	-0.143616
H	-0.835783	-0.366891	3.518557	C	-1.933238	3.505743	-0.591997
H	-2.523908	-0.715901	3.120766	C	-2.880902	3.019130	-1.487980
H	-1.523859	-1.943552	3.905347	C	-2.803860	1.693705	-1.890567
H	-2.381433	-0.703696	-2.426225	C	-1.775034	0.886203	-1.407327
H	-4.010979	0.731181	-3.646277	C	-1.582954	-0.515042	-1.790477
H	-2.998427	3.932492	-0.965100	C	-2.445195	-1.219484	-2.628260
H	-1.837267	4.464549	0.691924	C	-2.155146	-2.534739	-2.960352
H	1.219899	3.129579	3.399883	C	-1.005825	-3.121431	-2.439447
H	1.155931	0.915855	2.258957	C	-0.199261	-2.373873	-1.596539
H	0.539244	0.071429	-1.136580	H	3.545639	2.991668	-1.317550
H	1.872402	0.142971	-0.550426	H	1.798480	3.175138	-1.171148
C	3.578713	0.339194	-1.449971	H	2.476639	2.202771	-2.483453
O	2.873069	0.279571	-0.380908	H	3.183805	2.768701	2.160244
C	3.001014	0.233441	-2.806494	H	1.885218	3.380203	1.147921
H	3.793472	0.222439	-3.555251	H	1.509265	2.373587	2.562124
H	2.391306	-0.673467	-2.883918	H	1.783067	0.203708	3.403197
				H	3.398796	-0.487611	3.223853

H	1.978148	-1.492277	2.910343	C	2.873545	-2.109829	1.247571
H	2.306716	-2.897410	1.045597	C	2.943370	-1.552693	-1.923079
H	3.985891	-2.552126	0.621882	C	-0.958469	2.616242	-0.519290
H	2.823579	-2.874652	-0.654735	C	-2.053846	3.365297	-0.915962
H	2.510306	-1.523783	-2.522887	C	-3.127310	2.712169	-1.512009
H	2.775608	0.133447	-3.080582	C	-3.068983	1.335091	-1.682848
H	4.118471	-0.808877	-2.422171	C	-1.944780	0.637295	-1.254079
H	-0.180829	2.984355	0.561149	C	-1.782130	-0.814739	-1.387879
H	-1.953926	4.535371	-0.248578	C	-2.775365	-1.668593	-1.851598
H	-3.530963	1.295642	-2.591727	C	-2.510466	-3.027578	-1.964456
H	-3.334518	-0.742008	-3.027998	C	-1.253273	-3.504600	-1.610288
H	-0.732447	-4.144193	-2.679767	C	-0.313421	-2.605497	-1.134293
H	0.698757	-2.795993	-1.150729	H	3.561541	1.889375	-2.596030
H	-0.313505	-0.431436	1.187334	H	1.897370	2.443609	-2.383789
H	-3.667506	3.663781	-1.869671	H	2.221795	0.898813	-3.188487
H	-2.812887	-3.091969	-3.621205	H	3.377408	3.317971	0.731240
C	-1.920024	-1.712515	2.281159	H	2.026442	3.528037	-0.372369
O	-1.260281	-1.605500	3.384286	H	1.734635	3.217395	1.357636
C	-1.755977	-2.966510	1.531890	H	2.038383	1.652411	2.966341
H	-2.142034	-2.857649	0.516668	H	3.379364	0.514412	3.139755
H	-0.699548	-3.251021	1.529951	H	1.713024	-0.080188	3.164493
H	-2.313130	-3.759006	2.048911	H	2.417936	-2.128489	2.242297
O	-2.768988	-0.855644	1.867917	H	3.950121	-2.274382	1.382312
C	-2.938228	0.448563	2.532807	H	2.487476	-2.962901	0.679860
H	-1.952432	0.936992	2.491246	H	2.848501	-2.582504	-1.567705
H	-3.243139	0.257463	3.570205	H	2.272651	-1.409846	-2.777283
C	-3.988229	1.202358	1.772044	H	3.969570	-1.436422	-2.295000
H	-4.132959	2.181338	2.238333	H	-0.098589	3.083846	-0.048317
H	-3.682594	1.356808	0.731040	H	-2.055818	4.440011	-0.764180
H	-4.944730	0.673624	1.791086	H	-3.893686	0.810938	-2.156245
H	-1.390943	-0.775095	3.872957	H	-3.753055	-1.281720	-2.121555
				H	-1.001658	-4.557323	-1.690053
				H	0.673954	-2.934314	-0.820600
15 Gsolv= -1297.016320				H	-0.489040	-0.354202	1.389577
Ir	0.757669	0.082855	-0.100115	H	-3.998757	3.268379	-1.846019
N	-0.897406	1.283548	-0.683777	H	-3.277515	-3.705713	-2.327620
N	-0.566853	-1.291076	-1.018899	C	-1.161116	-0.840861	2.236900
C	2.505117	0.863175	-1.061081	O	-0.754661	-0.283652	3.424833
C	2.404886	1.495634	0.239645	C	-0.893119	-2.318732	2.273364
C	2.467747	0.469038	1.226170	H	-1.268213	-2.797066	1.364101
C	2.641521	-0.809582	0.559747	H	0.176561	-2.518490	2.389132
C	2.700329	-0.558308	-0.846277	H	-1.423052	-2.741883	3.131963
C	2.538909	1.556586	-2.374085	O	-2.467441	-0.631641	1.865346
C	2.366025	2.961070	0.499859	C	-3.034873	0.653373	2.106340
C	2.383796	0.650159	2.696855				

H	-2.418936	1.424548	1.602454	H	1.704290	-0.565868	-3.470349
H	-3.039693	0.864352	3.185505	H	3.160159	-0.008637	-2.623878
C	-4.444558	0.637702	1.575418	H	3.131531	-1.605068	-3.390123
H	-4.916469	1.615644	1.707850	H	2.457542	0.045982	2.609006
H	-4.456124	0.384611	0.508751	H	3.396813	1.992822	3.846942
H	-5.043634	-0.106217	2.107560	H	1.727531	4.556403	0.821709
H	-0.947556	0.661576	3.462689	H	0.451988	4.605937	-0.841269
TS _{4,5} Gsolv= -1951.228074				H	-1.555794	2.186777	-3.778901
Ir	0.895855	-0.462766	-0.014034	H	-0.744093	0.171977	-2.562299
N	1.647372	1.197880	1.094907	H	-0.465826	-0.238765	1.086798
N	0.269749	1.253165	-1.122207	H	-1.159443	0.318611	0.730784
C	2.758443	-1.570157	-0.329843	O	-2.209140	1.066367	0.612795
C	1.933054	-2.267368	0.638155	C	-4.164596	-0.542066	1.245961
C	0.722612	-2.656208	-0.031808	H	3.030066	4.300027	2.917146
C	0.759883	-2.162887	-1.376503	H	-0.951043	4.457061	-2.882462
C	2.040195	-1.502493	-1.564514	S	-3.363996	0.407153	-0.126476
C	4.122407	-1.027843	-0.091563	O	-4.358688	1.373185	-0.562778
C	2.326743	-2.669217	2.016963	O	-2.912438	-0.620457	-1.060055
C	-0.398624	-3.424569	0.569167	F	-3.275464	-1.367749	1.796781
C	-0.272482	-2.429672	-2.416584	F	-4.619738	0.279598	2.183155
C	2.529616	-0.882053	-2.823915	F	-5.176167	-1.257739	0.769939
C	2.332373	1.060741	2.239207	TS _{6,7} Gsolv= -2258.519942			
C	2.845935	2.150088	2.924832	Ir	-1.339388	-0.517506	-0.095650
C	2.636675	3.424453	2.408091	N	-0.135986	0.674069	-1.371200
C	1.909141	3.568991	1.235011	N	-2.284624	1.376677	-0.085381
C	1.415934	2.434653	0.595658	C	-2.134487	-2.172582	-1.321283
C	0.612975	2.466985	-0.631816	C	-0.877244	-2.584051	-0.730108
C	0.186587	3.637020	-1.252265	C	-1.007525	-2.534718	0.689692
C	-0.601144	3.552501	-2.392793	C	-2.352300	-2.087764	1.001020
C	-0.938398	2.300211	-2.893264	C	-3.042996	-1.897270	-0.248702
C	-0.484002	1.172379	-2.227445	C	-2.437207	-2.135867	-2.778907
H	4.874612	-1.767589	-0.395948	C	0.294835	-3.109246	-1.480783
H	4.298507	-0.799532	0.965091	C	0.037816	-2.918953	1.676333
H	4.300908	-0.116528	-0.673050	C	-2.959436	-2.032060	2.362085
H	2.681754	-3.708301	2.022818	C	-4.470502	-1.505856	-0.409989
H	3.140388	-2.048957	2.407596	C	0.964056	0.218221	-1.986951
H	1.483342	-2.604685	2.713821	C	1.789266	1.043108	-2.739247
H	-0.473533	-3.257715	1.648735	C	1.452848	2.382384	-2.876248
H	-0.234955	-4.498506	0.406670	C	0.306261	2.856140	-2.248883
H	-1.356686	-3.160114	0.108987	C	-0.466351	1.984366	-1.490161
H	-1.285848	-2.291423	-2.022577	C	-1.662636	2.382371	-0.746709
H	-0.188991	-3.464950	-2.773299	C	-2.142957	3.688414	-0.680651
H	-0.155487	-1.778391	-3.289565	C	-3.278747	3.963661	0.063142

C	-3.915506	2.923447	0.733680	O	2.151208	-0.640069	0.458937
C	-3.383877	1.650019	0.637104	O	3.859880	-2.377761	0.897795
H	-2.645270	-3.143915	-3.160019	F	5.840310	-0.331414	-0.122533
H	-1.593460	-1.737304	-3.353531	F	4.267525	1.086225	-0.557251
H	-3.310365	-1.511999	-2.993330	F	4.622920	0.462269	1.478762
H	0.243994	-4.205296	-1.503457				
H	0.304929	-2.768872	-2.521217				
H	1.252240	-2.840239	-1.024632	TS _{8,9} G _{solv} =	-2258.506185		
H	1.046151	-2.798549	1.268590	Ir	-1.833732	-0.044799	-0.138826
H	-0.092277	-3.969621	1.965585	N	-0.339650	-1.281488	-0.982642
H	-0.018327	-2.310079	2.584933	N	-0.470783	1.318966	-1.051557
H	-2.189658	-1.952280	3.136217	C	-3.621505	-1.032454	-0.874166
H	-3.532055	-2.944889	2.568731	C	-3.511996	-1.203811	0.560731
H	-3.644039	-1.184053	2.481792	C	-3.600979	0.106981	1.156046
H	-4.893633	-1.101786	0.515110	C	-3.697462	1.074247	0.113504
H	-4.605988	-0.765959	-1.206826	C	-3.704622	0.367244	-1.157598
H	-5.067879	-2.386752	-0.675885	C	-3.672895	-2.118005	-1.891913
H	1.225492	-0.823151	-1.844391	C	-3.494838	-2.483931	1.324519
H	2.687854	0.617105	-3.175155	C	-3.540078	0.381411	2.616951
H	0.023250	3.900276	-2.344169	C	-3.907302	2.538431	0.303370
H	-1.627516	4.486477	-1.206005	C	-3.870265	0.986123	-2.502387
H	-4.807905	3.091764	1.327810	C	-0.370867	-2.620130	-0.931567
H	-3.833609	0.806776	1.155488	C	0.699109	-3.405855	-1.327260
H	-0.457165	0.255285	1.159811	C	1.853216	-2.779981	-1.776591
H	2.073478	3.055706	-3.460753	C	1.883724	-1.395046	-1.851680
H	-3.662862	4.977931	0.121906	C	0.773952	-0.665676	-1.449345
C	0.263497	0.986551	2.292682	C	0.696680	0.795133	-1.490040
O	1.167585	0.110773	2.612249	C	1.729656	1.616407	-1.938039
C	-0.879292	1.126177	3.246765	C	1.539668	2.987816	-1.973927
H	-1.652981	1.777456	2.831552	C	0.320026	3.516398	-1.559120
H	-1.291530	0.144039	3.488374	C	-0.652230	2.649614	-1.093765
H	-0.494855	1.582235	4.166836	H	-4.711859	-2.286583	-2.200796
O	0.572459	2.138027	1.704347	H	-3.296117	-3.068614	-1.503065
C	1.867523	2.313549	1.080798	H	-3.097005	-1.864453	-2.788224
H	1.901602	1.692072	0.179174	H	-4.508764	-2.764156	1.636803
H	2.641640	1.948575	1.766096	H	-3.101231	-3.316570	0.731575
C	2.023356	3.776809	0.778070	H	-2.881258	-2.397834	2.228487
H	2.971562	3.935365	0.253955	H	-3.747401	1.431733	2.840917
H	1.210297	4.131944	0.133146	H	-2.543072	0.140044	3.007324
H	2.027928	4.378338	1.691623	H	-4.276392	-0.229763	3.151056
H	1.742027	-0.204500	1.815484	H	-3.260348	2.953396	1.084856
O	3.385382	-1.570831	-1.434335	H	-4.944641	2.734315	0.602188
C	4.628155	0.051594	0.212041	H	-3.737380	3.099172	-0.621592
S	3.423619	-1.317801	0.006675	H	-3.358524	1.952098	-2.573111
				H	-3.468215	0.342662	-3.290836

H	-4.931281	1.160005	-2.721540	C	-2.437338	-3.165337	0.853036
H	-1.280816	-3.065964	-0.538750	C	-2.774037	-0.843431	2.983453
H	2.790615	-0.893948	-2.170851	C	-3.864437	1.738131	1.515402
H	2.683697	1.186439	-2.221212	C	-4.114928	1.067820	-1.605824
H	-1.603301	3.017494	-0.718184	C	0.264797	-2.127249	-1.406252
H	2.734727	-3.353679	-2.044591	C	1.263922	-2.576381	-2.249612
H	2.337573	3.639831	-2.317410	C	2.080082	-1.640286	-2.875342
C	0.769264	1.572347	1.985332	C	1.873493	-0.292658	-2.630718
H	0.800687	1.844202	0.923244	C	0.847348	0.096327	-1.775237
O	-0.515372	0.026493	1.524490	C	0.539207	1.487216	-1.437580
O	1.789849	1.030333	2.481382	C	1.325752	2.571816	-1.811570
C	0.044156	-1.186953	1.996425	C	0.942247	3.848406	-1.433872
H	-0.523625	-2.037261	1.583436	C	-0.217317	4.016009	-0.685131
H	1.082155	-1.304662	1.630415	C	-0.943602	2.895031	-0.327172
C	0.011652	-1.281734	3.508781	H	-4.223373	-2.480737	-2.139442
H	0.417319	-2.247394	3.830807	H	-2.480115	-2.745114	-2.067162
H	0.616540	-0.500005	3.976170	H	-3.119634	-1.314473	-2.884086
H	-1.016064	-1.205480	3.888129	H	-3.264700	-3.689389	1.347067
C	-0.190285	2.294956	2.854002	H	-2.203518	-3.730892	-0.054738
H	0.233502	3.281201	3.084596	H	-1.566582	-3.218043	1.517079
H	-1.148467	2.433157	2.344024	H	-2.092329	-1.665805	3.221064
H	-0.339718	1.758504	3.794666	H	-3.729774	-1.053337	3.480959
H	0.628564	-4.486278	-1.255486	H	-2.375920	0.076676	3.425661
H	0.127540	4.584344	-1.576623	H	-3.157264	2.043563	2.295364
H	2.469337	0.669259	1.623865	H	-4.844164	1.618803	1.994693
O	4.008115	-1.877093	0.041879	H	-3.960407	2.561890	0.800462
C	5.385690	0.297668	-0.388279	H	-3.791071	2.099061	-1.430002
S	4.212544	-0.596526	0.704429	H	-3.770318	0.776851	-2.602335
O	2.986210	0.314761	0.549027	H	-5.212146	1.067389	-1.618423
O	4.757694	-0.546222	2.044878	H	-0.377913	-2.819379	-0.868919
F	6.529051	-0.351215	-0.439660	H	2.519229	0.452601	-3.080242
F	4.874357	0.365047	-1.628885	H	2.254077	2.409655	-2.347270
F	5.583496	1.527612	0.048624	H	-1.836197	2.971611	0.289083
				H	-0.211542	0.081688	1.215811
				H	2.882954	-1.957607	-3.534078
TS _{10,11} Gsolv=	-2104.796853			H	1.551921	4.704013	-1.708818
Ir	-1.506298	-0.089626	0.038288	H	1.551921	4.704013	-1.708818
N	0.046009	-0.821021	-1.186348	C	0.403201	0.921281	2.180511
N	-0.582379	1.657264	-0.699018	O	1.224421	1.718871	1.583983
C	-3.222028	-1.221966	-0.739360	H	-0.533785	1.406451	2.500908
C	-2.814736	-1.754335	0.546382	H	1.404912	-3.642101	-2.397754
C	-2.993679	-0.712596	1.518419	H	-0.548167	4.997613	-0.361891
C	-3.452528	0.469133	0.848952	C	0.914992	-0.141731	3.113263
C	-3.609971	0.142968	-0.555125	H	1.327062	0.360377	3.997991
C	-3.256937	-1.974991	-2.022534	H	0.107974	-0.807077	3.434163

H	1.719399	-0.725578	2.661511	H	2.591697	-1.091975	1.612450
O	3.492091	0.948455	1.752259	H	2.199177	-2.485766	2.633591
C	3.708657	-1.309192	0.534904	H	1.610688	-0.889998	3.079404
S	4.191298	0.461304	0.501969	H	-0.514410	-0.325545	3.565586
O	3.544356	0.965208	-0.712458	H	-2.210095	-0.619771	3.147793
O	5.632138	0.469075	0.595438	H	-1.260639	-1.876868	3.948497
F	4.127902	-1.904209	1.633829	H	-2.435210	-0.963015	-2.306489
F	2.360101	-1.399556	0.506693	H	-4.286527	0.266440	-3.432454
F	4.178597	-1.947316	-0.525654	H	-3.454101	3.608423	-0.862007
H	2.293753	1.370830	1.609640	H	-2.199487	4.325234	0.649181
TS _{12,13} Gsolv= -1297.032559				H	1.202066	3.408084	3.109940
Ir	-0.454125	-0.482372	0.039693	H	1.253384	1.145872	2.062855
N	-1.980569	0.580590	-1.008093	H	0.483067	0.160770	-1.285635
N	-0.394937	1.485929	0.862855	H	1.337936	0.236347	-0.852972
C	-1.668531	-2.123354	0.859683	C	3.395858	0.631146	-1.563131
C	-0.849300	-2.604541	-0.239859	O	2.631557	0.427922	-0.592618
C	0.523834	-2.437738	0.141661	C	2.920993	0.771877	-2.966701
C	0.569777	-1.806474	1.431527	H	3.758464	0.907640	-3.651307
C	-0.800334	-1.640133	1.884842	H	2.353529	-0.120063	-3.255019
C	-3.154767	-2.160034	0.908545	H	2.246566	1.631507	-3.042112
C	-1.332053	-3.319365	-1.455711	O	4.674852	0.732523	-1.410523
C	1.701614	-2.866730	-0.659746	C	5.258579	0.594465	-0.075361
C	1.805255	-1.546813	2.225628	H	4.999101	-0.406734	0.289982
C	-1.218140	-1.078642	3.197014	H	4.779896	1.337421	0.572082
C	-2.702733	0.047122	-2.005686	C	6.738468	0.800112	-0.217629
C	-3.727712	0.738868	-2.630929	H	7.216707	0.700417	0.760852
C	-4.012315	2.033017	-2.210504	H	7.177237	0.056544	-0.888508
C	-3.253345	2.594309	-1.192745	H	6.961633	1.797694	-0.605681
C	-2.235477	1.848872	-0.605794	H	-4.811775	2.603325	-2.674753
C	-1.347621	2.355806	0.447089	H	-0.578081	5.025861	2.387254
C	-1.430463	3.636560	0.984496	TS _{14,15} Gsolv= -1297.008742			
C	-0.520626	4.030643	1.955735	Ir	-0.711525	-0.031108	-0.072251
C	0.465016	3.137572	2.360591	N	0.944083	-0.884364	-1.092481
C	0.495777	1.876081	1.788135	N	0.633073	1.595558	-0.349787
H	-3.492949	-3.134574	1.281996	C	-2.377601	-0.699390	-1.384349
H	-3.600987	-2.021301	-0.081608	C	-2.367716	-1.433314	-0.131668
H	-3.561944	-1.392776	1.573579	C	-2.606153	-0.489032	0.925381
H	-1.239245	-4.403976	-1.319181	C	-2.675349	0.822386	0.352683
H	-2.388959	-3.118748	-1.657515	C	-2.556130	0.683225	-1.089643
H	-0.753935	-3.052193	-2.347034	C	-2.237421	-1.299175	-2.738274
H	1.519509	-2.772744	-1.735502	C	-2.341396	-2.915412	0.032265
H	1.914677	-3.923980	-0.456628	C	-2.792496	-0.837367	2.359815
H	2.597408	-2.293817	-0.402116	C	-3.014060	2.078225	1.081681

C	-2.642930	1.798628	-2.070542	O	0.644555	-1.548035	3.216188
C	1.022632	-2.186969	-1.416660	C	0.514730	0.801864	3.444804
C	2.096632	-2.717619	-2.111629	H	0.736898	1.695750	2.858977
C	3.133441	-1.868635	-2.488730	H	-0.561254	0.670301	3.570970
C	3.059497	-0.525293	-2.150296	H	0.972285	0.907185	4.437540
C	1.952757	-0.051965	-1.447734	O	2.304470	-0.251231	2.318162
C	1.783184	1.341128	-1.020334	C	3.045431	-1.391592	1.804503
C	2.718787	2.345503	-1.253650	H	2.436802	-1.839519	1.001882
C	2.470044	3.632100	-0.796681	H	3.187003	-2.114450	2.620081
C	1.290300	3.883899	-0.105108	C	4.366370	-0.878884	1.303722
C	0.401988	2.840030	0.099411	H	4.945542	-1.705990	0.883045
H	-3.221223	-1.602931	-3.117290	H	4.219488	-0.123739	0.524064
H	-1.608785	-2.195873	-2.729554	H	4.946580	-0.435160	2.116932
H	-1.810555	-0.593946	-3.457602	H	1.128086	-2.315989	2.874682
H	-3.359357	-3.308474	0.147197				
H	-1.908812	-3.420350	-0.837906				
H	-1.774514	-3.213958	0.921790				
H	-2.072571	-1.589587	2.700012				
H	-3.796623	-1.255582	2.506966				
H	-2.714983	0.041018	3.008021				
H	-2.517558	2.138087	2.056909				
H	-4.094478	2.133197	1.263909				
H	-2.749019	2.970461	0.505061				
H	-2.166114	2.710944	-1.696052				
H	-2.173692	1.542466	-3.024630				
H	-3.692923	2.043958	-2.274014				
H	0.192810	-2.810973	-1.092186				
H	2.112259	-3.775241	-2.355759				
H	3.858140	0.151949	-2.438020				
H	3.635666	2.129516	-1.793778				
H	1.054055	4.874086	0.271655				
H	-0.531374	2.989284	0.637982				
H	0.210771	-0.300318	1.320689				
H	3.987267	-2.248052	-3.042988				
H	3.187790	4.426978	-0.977889				
C	1.105050	-0.393007	2.799983				