Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Mechanistic Studies of Cp*Ir(III)/Cp*Rh(III)-Catalyzed *Branch*-Selective Allylic C–H Amidation: Why is Cp*Ir(III) Superior to Cp*Rh(III)?

Nan Ma,[a,b] Zheyuan Liu,[c,*] Jianhui Huang,[b,*] and Yanfeng Dang[a,*]

[a]Department of Chemistry, School of Science, Tianjin University, Tianjin 300072, China. yanfeng.dang@tju.edu.cn

[b]School of Pharmaceutical Science and Technology, Tianjin University, Tianjin 300072, China. jhuang@tju.edu.cn

[c]College of Materials Science and Engineering, Fuzhou University, Fuzhou 350108, China. zheyuan.liu@fzu.edu.cn

Energies and Cartesian Coordinates of All the Structures

All energies are given in Hartree.

1cat

SCF energy in gas phase: -722.823697
Free energy in gas phase: -722.596479
Free energy in solution: -722.596479

C	-1.494571	-0.617055	-1.054853
C	-1.502725	0.844368	-0.886316
C	-1.499998	1.128898	0.515553
C	-1.466315	-0.149798	1.221361
C	-1.499951	-1.223922	0.245771
C	-1.530721	-1.331162	-2.366734
H	-1.112107	-2.336237	-2.292854
H	-0.984915	-0.785928	-3.139709
C	-1.554259	1.840662	-1.999815
H	-1.006781	1.493985	-2.878829
H	-2.598040	1.998907	-2.299130
H	-1.141784	2.804954	-1.698516
C	-1.549185	2.480931	1.156405
H	-1.133079	3.250419	0.503824
H	-2.590566	2.748749	1.372498
H	-0.996852	2.502469	2.098139
C	-1.466503	-0.320373	2.704177
H	-0.965162	0.507859	3.208683
H	-2.505085	-0.347868	3.059732
H	-0.987041	-1.253856	3.004515
C	-1.545682	-2.689448	0.550520
H	-1.005135	-2.926679	1.469004
H	-2.586757	-3.008095	0.681291
H	-1.112444	-3.282300	-0.256968
Ir	0.304109	0.002609	-0.006658
O	2.119630	1.089786	0.013507
C	2.809405	0.001436	0.006672
O	2.121573	-1.086743	0.003298
C	4.294964	0.004009	-0.024124
H	4.681698	0.887654	0.486245
H	4.685267	-0.913393	0.418676
H	4.618832	0.046717	-1.071162
H	-2.572791	-1.423886	-2.698896

IM1

SCF energy in gas phase:-919.40521
Free energy in gas phase: -919.046462
Free energy in solution: -919.25299

C	1.253035	-1.810017	-0.472962
C	0.793671	-1.728810	0.907670
C	1.511327	-0.647414	1.553345
C	2.337629	-0.009879	0.574750
C	2.179729	-0.735480	-0.690856
C	0.920246	-2.895188	-1.451510
H	0.974978	-2.544398	-2.483983
H	-0.073215	-3.315621	-1.283495
C	-0.072227	-2.728671	1.613866
H	-0.763350	-3.227724	0.932217
H	0.555239	-3.504854	2.068680
H	-0.655905	-2.265182	2.412232
C	1.376057	-0.264075	2.992674
H	0.350447	-0.388582	3.346710
H	2.019742	-0.908797	3.603966
H	1.675152	0.770200	3.168466
C	3.288348	1.126544	0.797573
H	3.010149	1.725025	1.667208
H	4.298631	0.736903	0.971005
H	3.330701	1.786730	-0.071320
C	2.949641	-0.453094	-1.943630
H	3.067201	0.620347	-2.107862
H	3.951998	-0.892184	-1.866636
H	2.464523	-0.880954	-2.822519
Ir	0.232273	0.132592	-0.175506
O	-0.826960	1.777069	0.768923
C	-0.332266	2.634294	-0.042342
O	0.437815	2.159547	-0.947028
C	-0.617958	4.096504	0.072258
H	-1.612177	4.256784	0.492901
H	0.114383	4.550604	0.749153
H	-0.527895	4.578486	-0.902513
H	1.640955	-3.714437	-1.342456
C	-1.329758	-0.002585	-1.754363

C	-1.847519	-0.747529	-0.690283
H	-0.875991	-0.494616	-2.609632
H	-1.701914	1.001320	-1.941234
H	-1.691005	-1.823924	-0.716777
C	-2.974833	-0.302710	0.203757
H	-2.818611	-0.675539	1.223358
H	-3.009878	0.787799	0.263148
C	-4.325462	-0.844616	-0.323482
H	-4.486892	-0.473074	-1.342752
H	-4.279794	-1.939013	-0.395169
C	-5.497449	-0.433980	0.573291
H	-5.586273	0.655650	0.636804
H	-6.440931	-0.822824	0.179985
H	-5.375392	-0.820373	1.590802

TS1

SCF energy in gas phase: -919.366257

Free energy in gas phase: -919.011927

Free energy in solution: -919.226441

C	2.343277	-0.096877	-0.156531
C	1.752642	-1.093257	0.716491
C	0.993944	-0.400490	1.741698
C	1.041525	0.998393	1.456854
C	1.875713	1.198160	0.266904
C	3.326766	-0.365818	-1.254436
H	3.305927	0.414274	-2.017483
H	3.148327	-1.327911	-1.739952
C	2.063153	-2.560888	0.703712
H	2.301916	-2.918734	-0.300262
H	2.934816	-2.761443	1.338314
H	1.233572	-3.156310	1.090780
C	0.304904	-1.049192	2.902144
H	-0.082576	-2.036740	2.642471
H	1.017080	-1.180655	3.726221
H	-0.523589	-0.442424	3.271293
C	0.440063	2.100043	2.274323
H	-0.420980	1.755324	2.849678
H	1.184874	2.486907	2.980104
H	0.121178	2.931957	1.643064
C	2.293186	2.528683	-0.283065
H	1.474104	3.249737	-0.245624
H	3.125847	2.933041	0.305167
H	2.622832	2.450370	-1.320708
Ir	0.125632	0.029549	-0.359099
O	-2.637129	0.687436	0.584624
C	-2.259895	1.683360	-0.079630
O	-1.136407	1.700785	-0.727398
C	-3.125233	2.913130	-0.181310
H	-4.038600	2.657327	-0.727290
H	-3.426370	3.227935	0.821088
H	-2.608235	3.722769	-0.695178
H	4.339973	-0.393402	-0.835369
C	-0.113419	-0.321522	-2.531658
C	-0.469822	-1.467608	-1.784820
H	0.790113	-0.345676	-3.132811
H	-0.865626	0.398823	-2.838734
H	0.156411	-2.356772	-1.788592
C	-1.639358	-1.425845	-0.907526
H	-1.695942	-0.358594	0.076854
H	-2.494517	-0.924380	-1.369927
C	-2.006165	-2.694737	-0.144362
H	-2.359734	-3.418879	-0.891132
H	-1.097703	-3.127747	0.291432
C	-3.080165	-2.517266	0.933414
H	-3.997876	-2.094041	0.514533
H	-3.330380	-3.484354	1.377474
H	-2.746977	-1.851043	1.734173

IM2

SCF energy in gas phase:-919.401329

Free energy in gas phase: -919.041548

Free energy in solution: -919.25064

C	1.870629	-1.158292	0.290622
C	1.249677	-0.676362	1.518004
C	1.232356	0.750373	1.461147
C	1.913949	1.162502	0.224773
C	2.353015	-0.004031	-0.459491
C	2.221148	-2.587926	-0.001598
H	2.294850	-2.777137	-1.074919
H	1.487355	-3.279780	0.417536
C	0.822299	-1.529130	2.673380
H	0.470724	-2.510464	2.349694
H	1.675747	-1.692300	3.343237
H	0.029026	-1.060120	3.259025
C	0.828544	1.685122	2.565653
H	0.101307	1.231632	3.242861

H	1.707912	1.955149	3.163245
H	0.401744	2.614913	2.182714
C	2.195476	2.582650	-0.165307
H	1.387699	3.253204	0.136698
H	3.111663	2.931784	0.326364
H	2.334064	2.686703	-1.243202
C	3.187418	-0.053735	-1.704161
H	3.033313	0.827080	-2.330491
H	4.250715	-0.092128	-1.437426
H	2.970201	-0.939481	-2.305125
Ir	0.076004	-0.050676	-0.318396
O	-2.220433	1.695808	1.118947
C	-2.003410	2.197964	-0.080596
O	-1.178417	1.693525	-0.865461
C	-2.821524	3.397834	-0.433375
H	-3.878557	3.114113	-0.466231
H	-2.715841	4.160045	0.343692
H	-2.513351	3.791838	-1.400356
H	3.194169	-2.831595	0.441789
C	-0.490816	-0.690285	-2.341787
C	-0.957209	-1.642186	-1.392604
H	0.300504	-0.982440	-3.025334
H	-1.157538	0.083068	-2.713143
H	-0.471362	-2.612685	-1.311777
C	-1.848630	-1.220849	-0.361876
H	-1.637634	0.899089	1.199466
H	-2.594282	-0.480845	-0.655745
C	-2.309066	-2.177146	0.717572
H	-1.503295	-2.881545	0.956615
H	-2.522702	-1.624082	1.640334
C	-3.568465	-2.957477	0.299796
H	-3.382939	-3.560028	-0.594921
H	-3.886776	-3.630650	1.100941
H	-4.400586	-2.280081	0.082131

IM3

SCF energy in gas phase:-1086.81984

Free energy in gas phase: -1086.456322

Free energy in solution: -1086.708308

C	-2.461543	-0.354033	0.347712
C	-1.724273	-0.139558	1.585637
C	-0.729424	-1.152546	1.671602
C	-0.889930	-2.060399	0.526267
C	-1.987828	-1.588976	-0.256021
C	-3.690364	0.401273	-0.069515
H	-3.861695	0.337475	-1.146527
H	-3.631327	1.457322	0.203920
C	-2.020449	0.911522	2.611535
H	-2.419449	1.821697	2.160088
H	-2.772901	0.538277	3.317276
H	-1.132345	1.180800	3.186540
C	0.218367	-1.372148	2.814082
H	0.425722	-0.447299	3.355364
H	-0.216339	-2.084741	3.525674
H	1.171368	-1.790142	2.481127
C	-0.164250	-3.363344	0.354639
H	0.865345	-3.306849	0.716990
H	-0.663116	-4.151542	0.931639
H	-0.143647	-3.684648	-0.689192
C	-2.596964	-2.267352	-1.446337
H	-1.881116	-2.915920	-1.955407
H	-3.440845	-2.890949	-1.126814
H	-2.981164	-1.548269	-2.173564
Ir	-0.355206	-0.013676	-0.264208
H	-4.573488	-0.017303	0.427974
C	-0.173681	0.502462	-2.385880
C	-0.734371	1.605488	-1.666747
H	-0.805546	-0.028288	-3.092338
H	0.875336	0.547610	-2.667963
H	-1.791632	1.843103	-1.764541
C	0.021071	2.201814	-0.623408
H	1.100825	2.238984	-0.755952
C	-0.533736	3.306115	0.243601
H	-1.617383	3.183528	0.357700
H	-0.097057	3.237222	1.246382
C	-0.231410	4.698855	-0.340467
H	-0.683984	4.822903	-1.329387
H	-0.626127	5.481880	0.313250
H	0.846744	4.860160	-0.440648
N	1.757159	-0.168156	-0.205615
C	2.679324	-0.866283	-0.792509
C	3.774126	0.327191	0.711650
O	2.437037	0.619478	0.775735
O	4.642608	0.779780	1.374167
O	3.908570	-0.624801	-0.300198
C	2.526783	-1.850102	-1.888040
H	1.477965	-1.941213	-2.165761

H	3.116413	-1.528758	-2.752585
H	2.915812	-2.820463	-1.564350

TS2

SCF energy in gas phase:-1086.791679

Free energy in gas phase: -1086.433823

Free energy in solution: -1086.708878

C	-2.415928	0.205647	0.730074
C	-1.392096	0.087092	1.744613
C	-0.766587	-1.205111	1.587388
C	-1.420057	-1.895083	0.489274
C	-2.436625	-1.018211	-0.037712
C	-3.411180	1.324087	0.623329
H	-3.815020	1.421668	-0.386643
H	-2.981321	2.284248	0.916750
C	-1.110759	1.062563	2.846069
H	-1.359447	2.084827	2.556540
H	-1.716812	0.811446	3.725461
H	-0.061460	1.037861	3.146419
C	0.292472	-1.769005	2.484696
H	1.023439	-1.008486	2.765467
H	-0.170430	-2.153621	3.401423
H	0.826729	-2.595417	2.013082
C	-1.177419	-3.312764	0.067686
H	-0.140463	-3.613323	0.228460
H	-1.810522	-3.986853	0.657663
H	-1.420351	-3.468547	-0.985454
C	-3.426106	-1.370363	-1.107595
H	-3.001511	-2.054186	-1.845387
H	-4.293734	-1.867312	-0.656876
H	-3.794837	-0.486459	-1.632113
Ir	-0.390021	-0.028457	-0.307180
H	-4.256729	1.126735	1.293107
C	-0.493962	0.519730	-2.448634
C	-0.664038	1.697822	-1.662086
H	-1.343777	0.137329	-3.005297
H	0.478278	0.300899	-2.878024
H	-1.648185	2.153223	-1.570780
C	0.374952	2.129910	-0.807407
H	1.394813	1.860324	-1.068003
C	0.244961	3.285999	0.141968
H	-0.807338	3.465361	0.391358
H	0.773316	3.044911	1.070069
C	0.862400	4.563029	-0.468084
H	0.350814	4.853515	-1.390586
H	0.780205	5.390586	0.241530
H	1.922921	4.419098	-0.694492
N	1.421881	-0.542808	-0.542259
C	2.458750	-1.260995	-0.859196
C	3.767650	0.054677	0.838203
O	2.643558	0.566487	0.896326
O	4.866233	0.074622	1.277352
O	3.633020	-1.164796	-0.367549
C	2.260472	-2.310982	-1.944363
H	1.234530	-2.346266	-2.309235
H	2.944413	-2.078605	-2.764968
H	2.547023	-3.280855	-1.529163

IM4

SCF energy in gas phase: -898.242264

Free energy in gas phase: -897.894549

Free energy in solution: -898.109719

C	1.747874	-1.408991	-0.142652
C	1.418161	-1.047511	1.222524
C	1.684742	0.362373	1.385972
C	2.165527	0.870568	0.120518
C	2.198979	-0.228623	-0.823120
C	1.775877	-2.804722	-0.693156
H	1.634720	-2.823060	-1.776287
H	1.015756	-3.441249	-0.235800
C	1.037996	-1.999722	2.315476
H	0.471833	-2.851682	1.935487
H	1.944782	-2.392119	2.792235
H	0.441867	-1.512224	3.089257
C	1.569678	1.163379	2.645527
H	1.010882	0.627503	3.414068
H	2.566479	1.384852	3.043433
H	1.058974	2.111946	2.459659
C	2.661145	2.261981	-0.125637
H	2.151547	2.986546	0.511594
H	3.733517	2.312515	0.101868
H	2.529734	2.564325	-1.166497
C	2.743624	-0.161208	-2.218634
H	2.578705	0.818985	-2.670784
H	3.825683	-0.339659	-2.204125
H	2.297686	-0.917360	-2.868644

Ir	0.011317	0.152657	-0.157361
H	2.750515	-3.262805	-0.485746
C	-1.026885	0.230389	-2.093744
C	-1.270552	-1.039435	-1.490479
H	-0.402111	0.273440	-2.980539
H	-1.780337	1.009152	-2.029601
H	-0.779824	-1.929483	-1.878721
C	-1.954392	-1.109808	-0.253258
H	-2.656181	-0.317509	0.000420
C	-2.146933	-2.394685	0.500678
H	-1.365613	-3.119229	0.244315
H	-2.077897	-2.196679	1.575688
C	-3.536362	-2.994410	0.192727
H	-3.640027	-3.235689	-0.869440
H	-3.678639	-3.914654	0.765635
H	-4.335457	-2.299245	0.465517
N	-0.924090	1.637937	0.501792
C	-2.166907	2.185943	0.303187
O	-3.159862	1.643108	0.788186
C	-2.195821	3.529631	-0.393567
H	-3.112401	3.597067	-0.985117
H	-2.222451	4.319100	0.364695
H	-1.320127	3.691303	-1.027974

TS3A

SCF energy in gas phase: -898.231532

Free energy in gas phase: -897.881945

Free energy in solution: -898.095738

C	1.458577	-1.203803	1.152209
C	1.016199	0.059320	1.728050
C	1.518749	1.120740	0.904554
C	2.271742	0.505907	-0.192624
C	2.259395	-0.928578	0.000500
C	1.204079	-2.555766	1.748596
H	1.295799	-3.353278	1.008406
H	0.214192	-2.621144	2.206418
C	0.225507	0.236232	2.987446
H	-0.250941	-0.694315	3.300688
H	0.890438	0.556664	3.799067
H	-0.551806	0.994137	2.862364
C	1.425382	2.586009	1.208416
H	0.491369	2.826151	1.720886
H	2.253817	2.883379	1.862481
H	1.487372	3.193309	0.302942
C	3.070043	1.247450	-1.220719
H	2.619375	2.211774	-1.463242
H	4.078974	1.439356	-0.834156
H	3.171707	0.676656	-2.145907
C	2.999784	-1.932231	-0.832625
H	3.135254	-1.583845	-1.858626
H	3.996294	-2.107474	-0.410058
H	2.485520	-2.895641	-0.865820
Ir	0.159900	-0.075689	-0.372271
H	1.940591	-2.754956	2.536343
C	-0.414674	-1.218179	-2.220361
C	-1.185953	-1.673033	-1.126448
H	0.383322	-1.846467	-2.601212
H	-0.829705	-0.499166	-2.917576
H	-0.922291	-2.588579	-0.600068
C	-2.328880	-0.945746	-0.640437
H	-2.910737	-0.387838	-1.363516
C	-3.011797	-1.257926	0.648476
H	-2.364028	-1.864889	1.290703
H	-3.201315	-0.311180	1.166678
C	-4.354388	-1.980313	0.388975
H	-4.208730	-2.937120	-0.120704
H	-4.849360	-2.176131	1.343508
H	-5.025435	-1.365075	-0.217461
N	-1.311781	1.060091	-0.846179
C	-1.740285	2.145152	-0.105664
O	-2.223403	2.021218	1.019202
C	-1.680529	3.468928	-0.845210
H	-2.665079	3.670105	-1.280981
H	-1.458035	4.264614	-0.130616
H	-0.946864	3.463643	-1.654865

TS3B

SCF energy in gas phase:-898.221545

Free energy in gas phase: -897.872714

Free energy in solution: -898.089256

C	-0.647289	-2.045912	-0.546495
C	-0.603868	-1.833111	0.874632
C	0.758304	-1.480143	1.242647
C	1.555269	-1.461664	0.040259
C	0.672533	-1.799032	-1.068373
C	-1.829088	-2.533985	-1.332467

H	-1.814555	-2.169297	-2.362356
H	-2.774110	-2.229673	-0.877392
C	-1.722252	-2.078372	1.839873
H	-2.700235	-1.933432	1.378502
H	-1.673514	-3.115501	2.194123
H	-1.655158	-1.429478	2.715288
C	1.272173	-1.251827	2.630274
H	0.465089	-1.008261	3.323367
H	1.760596	-2.165428	2.992052
H	1.997040	-0.435573	2.652389
C	3.042176	-1.288474	-0.021129
H	3.390318	-0.566179	0.720593
H	3.535562	-2.245940	0.185278
H	3.369948	-0.955577	-1.008446
C	1.100208	-1.981315	-2.492499
H	1.940213	-1.333080	-2.750541
H	1.424956	-3.017561	-2.648692
H	0.284294	-1.786214	-3.191872
	-0.009184	0.113018	-0.100739
H	-1.824830	-3.629637	-1.375048
C	-0.318420	1.975927	-1.700452
C	-1.510945	1.328440	-1.217455
H	-2.038095	0.656002	-1.892685
C	-1.962736	1.498385	0.099407
H	-1.532379	2.308499	0.680256
C	-3.268644	0.941860	0.594364
H	-3.552011	0.058735	0.010005
H	-3.158872	0.622680	1.636251
C	-4.386398	2.002510	0.511170
H	-4.556895	2.319779	-0.521991
H	-5.322505	1.592373	0.899861
H	-4.136969	2.888624	1.102564
N	0.800734	1.827756	0.212342
C	2.144871	2.041223	0.479235
O	2.570232	1.720863	1.585631
C	2.967083	2.768618	-0.560965
H	3.993740	2.851263	-0.201200
H	2.953704	2.240809	-1.520113
H	2.563435	3.772642	-0.726901
H	0.128020	1.626734	-2.626869
H	-0.104489	3.000319	-1.433120

IM5A

SCF energy in gas phase:-898.299266

Free energy in gas phase: -897.945557

Free energy in solution: -898.153611

C	1.856332	-0.427148	1.331129
C	1.634904	1.006731	1.105014
C	1.890687	1.277941	-0.271097
C	2.255268	0.009964	-0.911388
C	2.290989	-1.015883	0.096284
C	1.786182	-1.109890	2.660796
H	1.604967	-2.181400	2.557195
H	1.001625	-0.686928	3.291613
C	1.290430	2.012627	2.157601
H	0.749682	1.554896	2.988531
H	2.213153	2.448598	2.561161
H	0.673184	2.811789	1.747384
C	1.849505	2.619076	-0.928162
H	0.990465	3.194453	-0.576614
H	2.762862	3.176600	-0.685509
H	1.791266	2.534212	-2.014867
C	2.669151	-0.141189	-2.341989
H	2.108667	0.528888	-2.997572
H	3.732921	0.105618	-2.447642
H	2.531567	-1.164294	-2.697077
C	2.745023	-2.433571	-0.091885
H	2.603261	-2.775734	-1.119216
H	3.815122	-2.513009	0.132895
H	2.220002	-3.122590	0.574042
H	2.739643	-0.983234	3.189525
C	-0.595361	-1.907870	-1.399232
C	-1.471056	-1.706798	-0.343166
H	0.084501	-2.753358	-1.393450
H	-0.764224	-1.437913	-2.365855
H	-1.477207	-2.392072	0.500684
C	-2.536448	-0.600609	-0.381568
H	-3.033557	-0.561367	-1.362528
C	-3.592789	-0.788036	0.719519
H	-3.077302	-0.888480	1.683263
H	-4.207974	0.113002	0.787533
C	-4.497958	-1.999009	0.461819
H	-3.930999	-2.934978	0.412693
H	-5.232712	-2.103800	1.264166
H	-5.047520	-1.891923	-0.479198
N	-1.627966	0.548557	-0.193762
C	-2.002723	1.904777	-0.163764

O	-1.186689	2.752586	0.165259
C	-3.409121	2.284964	-0.581198
H	-4.043906	2.370105	0.307266
H	-3.364935	3.270832	-1.046589
H	-3.872088	1.573664	-1.268043
Ir	0.186243	-0.195696	-0.106777

IM5B

SCF energy in gas phase:-898.300823

Free energy in gas phase: -897.948405

Free energy in solution: -898.156914

C	-1.339921	-1.784395	-0.229138
C	-0.778061	-1.684675	1.087820
C	0.679695	-1.800191	0.981607
C	1.005648	-1.909047	-0.405150
C	-0.249146	-1.856892	-1.162255
C	-2.792682	-1.900088	-0.582130
H	-3.029389	-1.395346	-1.521627
H	-3.440620	-1.495186	0.195844
C	-1.532796	-1.637289	2.379895
H	-2.548423	-1.260908	2.246558
H	-1.607913	-2.647759	2.800575
H	-1.027668	-1.011339	3.119223
C	1.642147	-1.867778	2.123312
H	1.219581	-1.433864	3.031719
H	1.884830	-2.916626	2.336683
H	2.565866	-1.338544	1.882314
C	2.366668	-2.140290	-0.981105
H	3.125413	-1.590963	-0.423004
H	2.601966	-3.211205	-0.937590
H	2.417814	-1.833053	-2.027717
C	-0.366396	-2.015876	-2.645414
H	0.465183	-1.539002	-3.168689
H	-0.351820	-3.082452	-2.904103
H	-1.299208	-1.595304	-3.025913
Ir	0.016977	0.050957	-0.080427
H	-3.051831	-2.958548	-0.705068
C	0.569067	2.711021	-0.538941
C	-0.802559	2.082932	-0.774027
H	-1.179503	2.011385	-1.792105
C	-1.629982	1.778026	0.290682
H	-1.304171	2.076761	1.289029
C	-3.095332	1.465065	0.155840
H	-3.301615	1.045682	-0.834046
H	-3.389633	0.719079	0.900478
C	-3.937618	2.740430	0.368223
H	-3.703128	3.498934	-0.384273
H	-5.001761	2.502018	0.290434
H	-3.763131	3.175701	1.357078
N	1.306964	1.531969	-0.083328
C	2.682252	1.533932	0.195493
O	3.241254	0.507412	0.551463
C	3.414818	2.850977	0.047704
H	4.451817	2.706620	0.348352
H	3.388037	3.201262	-0.989991
H	2.962862	3.630754	0.669887
H	0.971291	3.123187	-1.471115
H	0.544319	3.516795	0.207014

IM6

SCF energy in gas phase: -1127.404197

Free energy in gas phase: -1126.992722

Free energy in solution: -1127.238315

C	0.855624	-2.142046	0.428888
C	0.832002	-1.319554	1.619417
C	1.797351	-0.275682	1.449363
C	2.515446	-0.523824	0.188902
C	1.940767	-1.665751	-0.432572
C	0.128371	-3.440566	0.246883
H	-0.029883	-3.678598	-0.807373
H	-0.839799	-3.443939	0.750214
C	-0.017224	-1.539422	2.830079
H	-0.905166	-2.132075	2.601046
H	0.565060	-2.090558	3.579400
H	-0.335448	-0.591183	3.263960
C	2.137795	0.781569	2.454214
H	1.242490	1.120295	2.977614
H	2.849346	0.386453	3.189678
H	2.600609	1.646319	1.974893
C	3.677663	0.282446	-0.298643
H	3.482009	1.352651	-0.202595
H	4.565822	0.047369	0.299826
H	3.909573	0.069294	-1.343488
C	2.404652	-2.340149	-1.688919
H	2.941944	-1.652538	-2.344537
H	3.085550	-3.162614	-1.439214

H	1.573052	-2.768934	-2.254118
H	0.726089	-4.254187	0.676203
C	-0.399092	0.000013	-2.370068
C	-1.280771	-0.789803	-1.631137
H	0.304074	-0.465243	-3.053678
H	-0.630568	1.040106	-2.578453
H	-1.252866	-1.869602	-1.741463
C	-2.428160	-0.192882	-0.804518
H	-3.079133	0.437902	-1.429847
C	-3.280059	-1.303552	-0.169084
H	-2.616577	-1.972445	0.393766
H	-3.968307	-0.866645	0.556955
C	-4.091557	-2.093175	-1.204201
H	-3.457345	-2.581176	-1.952051
H	-4.678661	-2.874850	-0.714895
H	-4.789792	-1.440675	-1.738527
N	-1.616001	0.622160	0.138867
C	-2.036285	1.098416	1.377123
O	-1.220196	1.363654	2.254203
C	-3.508136	1.434832	1.568069
H	-3.957996	0.728464	2.272774
H	-3.560719	2.424134	2.028436
H	-4.090518	1.434824	0.644798
Ir	0.346646	-0.086906	-0.247481
C	0.296834	3.030858	-0.766897
O	0.982128	2.000265	-0.576597
O	-1.005119	3.022644	-0.802927
C	0.949097	4.364717	-0.965533
H	0.473146	4.889130	-1.797690
H	0.791266	4.968483	-0.065329
H	2.017229	4.249388	-1.143583
H	-1.334628	2.095922	-0.504407

TS4

SCF energy in gas phase: -1127.40174

Free energy in gas phase: -1126.993651

Free energy in solution: -1127.23753

C	1.037383	-2.088412	0.365134
C	0.944893	-1.323203	1.585060
C	1.809791	-0.184230	1.460781
C	2.542203	-0.314144	0.194552
C	2.063783	-1.476146	-0.478599
C	0.419652	-3.433814	0.125819
H	0.266949	-3.633729	-0.937280
H	-0.538542	-3.542168	0.637159
C	0.141064	-1.689791	2.791107
H	-0.711156	-2.323336	2.536674
H	0.778976	-2.258268	3.480166
H	-0.226949	-0.805964	3.310732
C	2.066031	0.853080	2.510770
H	1.168494	1.041054	3.101664
H	2.865068	0.520201	3.184621
H	2.380725	1.796986	2.061194
C	3.624820	0.613405	-0.258281
H	3.312137	1.655393	-0.158955
H	4.517533	0.465561	0.360636
H	3.902492	0.437088	-1.298675
C	2.583356	-2.051653	-1.762140
H	3.042727	-1.288927	-2.393424
H	3.345759	-2.809483	-1.545820
H	1.794346	-2.541238	-2.338636
H	1.087389	-4.215377	0.508900
C	-0.360208	0.055899	-2.369744
C	-1.189617	-0.813028	-1.658279
H	0.387060	-0.343605	-3.047815
H	-0.661365	1.081410	-2.556408
H	-1.089784	-1.885793	-1.792896
C	-2.392201	-0.318015	-0.846207
H	-3.084772	0.265418	-1.469545
C	-3.149871	-1.493676	-0.213323
H	-2.437338	-2.102152	0.358429
H	-3.885074	-1.119277	0.502203
C	-3.879366	-2.353532	-1.253834
H	-3.197947	-2.795566	-1.988245
H	-4.408417	-3.175394	-0.764322
H	-4.620414	-1.763641	-1.802929
N	-1.671632	0.571387	0.126368
C	-2.175611	0.876775	1.426442
O	-1.407633	1.019357	2.357752
C	-3.653934	1.193114	1.557878
H	-4.120636	0.488976	2.253163
H	-3.735098	2.187007	2.006663
H	-4.196764	1.183837	0.611786
Ir	0.362988	-0.034773	-0.239222
C	0.006603	3.010081	-0.721560
O	0.829706	2.058468	-0.517726
O	-1.255448	2.849185	-0.777524

C	0.558629	4.399206	-0.894900
H	0.032421	4.902666	-1.709012
H	0.367166	4.968620	0.020864
H	1.630973	4.376930	-1.086452
H	-1.531995	1.723013	-0.373013

IM7

SCF energy in gas phase: -1127.41142

Free energy in gas phase: -1127.000321

Free energy in solution: -1127.249596

C	0.602266	-2.124780	0.537470
C	1.187793	-1.262294	1.552551
C	2.220764	-0.492810	0.943497
C	2.332175	-0.895671	-0.459207
C	1.365919	-1.945833	-0.682366
C	-0.432229	-3.177612	0.802994
H	-0.875012	-3.551465	-0.122695
H	-1.233669	-2.788989	1.434921
C	0.798421	-1.261366	2.995833
H	-0.278902	-1.384038	3.123935
H	1.287441	-2.108184	3.493940
H	1.116786	-0.351223	3.507066
C	3.100086	0.527907	1.592322
H	2.751539	0.792697	2.591721
H	4.119832	0.135900	1.682854
H	3.140807	1.437490	0.987122
C	3.395277	-0.419874	-1.401936
H	3.540741	0.658843	-1.311902
H	4.348750	-0.911983	-1.175262
H	3.144655	-0.641758	-2.440897
C	1.245602	-2.778813	-1.921188
H	1.597506	-2.249580	-2.808574
H	1.866630	-3.675477	-1.806763
H	0.221952	-3.115574	-2.098342
H	0.026071	-4.031971	1.315741
C	-0.488398	0.271781	-2.305630
C	-1.429061	-0.448604	-1.560027
H	0.137446	-0.230093	-3.036250
H	-0.603038	1.342217	-2.443669
H	-1.557720	-1.517629	-1.705959
C	-2.470114	0.290589	-0.723419
H	-2.768273	1.203102	-1.252635
C	-3.734739	-0.511197	-0.415300
H	-3.478216	-1.459508	0.062920
H	-4.340573	0.046026	0.307033
C	-4.554466	-0.750188	-1.691046
H	-3.994028	-1.318227	-2.441841
H	-5.456108	-1.321953	-1.457602
H	-4.867546	0.192857	-2.151137
N	-1.648077	0.781375	0.453551
C	-1.947948	0.419598	1.809549
O	-2.311791	-0.697963	2.111241
C	-1.763014	1.545970	2.798641
H	-1.674517	1.138214	3.805660
H	-0.902747	2.174602	2.554529
H	-2.649168	2.191405	2.761469
Ir	0.324716	-0.042232	-0.255779
C	0.430424	3.073050	-0.396407
O	1.071776	1.938453	-0.457034
O	-0.783042	3.197372	-0.157682
C	1.302538	4.286663	-0.648067
H	0.697728	5.192225	-0.609380
H	2.093918	4.340422	0.105541
H	1.787502	4.202964	-1.624710
H	-1.449714	1.808951	0.331463

2cat

SCF energy in gas phase: -729.023436

Free energy in gas phase: -728.79914

Free energy in solution: -728.999417

C	1.563275	0.733534	-0.847489
C	1.562844	-0.735879	-0.846078
C	1.372011	-1.182748	0.494021
C	1.211807	0.001101	1.328256
C	1.372740	1.183138	0.491757
C	1.762401	1.586842	-2.057874
H	1.366701	2.593634	-1.915538
H	1.290239	1.152326	-2.942217
C	1.761215	-1.591619	-2.054891
H	1.286402	-1.160051	-2.939286
H	2.834546	-1.677630	-2.268443
H	1.367603	-2.598766	-1.909419
C	1.336107	-2.598610	0.976931
H	1.072611	-3.291861	0.176642
H	2.324571	-2.883637	1.357643
H	0.616538	-2.730144	1.787962

C	1.011120	0.002534	2.806137
H	0.471912	-0.884340	3.144476
H	1.993097	0.001820	3.299090
H	0.473864	0.891121	3.143051
C	1.337689	2.599996	0.971830
H	0.617584	2.733795	1.782021
H	2.326099	2.884923	1.352744
H	1.075436	3.291846	0.169927
O	-2.157409	-1.092614	-0.088421
C	-2.834929	0.000808	-0.119777
O	-2.157225	1.093835	-0.088599
C	-4.321187	0.000235	-0.216396
H	-4.730644	-0.885667	0.272206
H	-4.729513	0.914416	0.217246
H	-4.602662	-0.034374	-1.275566
H	2.836022	1.674353	-2.269407
Rh	-0.359642	0.000055	-0.118346

IM1'

SCF energy in gas phase: -925.601381

Free energy in gas phase: -925.245353

Free energy in solution: -925.454294

C	1.424077	-1.731668	-0.511705
C	0.922884	-1.709127	0.853276
C	1.529708	-0.588199	1.528554
C	2.346676	0.118787	0.583700
C	2.290428	-0.604707	-0.682638
C	1.162337	-2.809796	-1.518321
H	1.314908	-2.460506	-2.541171
H	0.149679	-3.212361	-1.439934
C	0.099192	-2.775066	1.510254
H	-0.508531	-3.327406	0.790966
H	0.759291	-3.500652	2.001732
H	-0.563115	-2.363732	2.275341
C	1.322543	-0.222234	2.963273
H	0.329307	-0.509254	3.314116
H	2.059869	-0.746911	3.584036
H	1.446745	0.848869	3.130822
C	3.206947	1.313652	0.856757
H	2.858506	1.872533	1.727206
H	4.236327	0.993028	1.058652
H	3.231977	1.991978	0.001050
C	3.055246	-0.229536	-1.912188
H	3.036170	0.850629	-2.077423
H	4.104196	-0.531022	-1.800111
H	2.661129	-0.718928	-2.804071
O	-0.771702	1.748470	0.767365
C	-0.371892	2.586390	-0.112435
O	0.360224	2.122394	-1.051911
C	-0.726858	4.038631	-0.034345
H	-1.679353	4.170617	0.481641
H	0.046501	4.563605	0.537416
H	-0.764379	4.474423	-1.034250
H	1.855359	-3.642811	-1.348365
C	-1.296803	-0.177193	-1.809333
C	-1.860046	-0.804115	-0.718631
H	-0.752948	-0.737692	-2.563280
H	-1.611230	0.821453	-2.097010
H	-1.669603	-1.868826	-0.594152
C	-2.985013	-0.259087	0.115350
H	-2.801746	-0.459791	1.177926
H	-3.052613	0.826182	0.003725
C	-4.325296	-0.918063	-0.292636
H	-4.517804	-0.711565	-1.352399
H	-4.240906	-2.008500	-0.198893
C	-5.495124	-0.415651	0.558859
H	-5.623169	0.667331	0.459448
H	-6.430299	-0.891208	0.250177
H	-5.340584	-0.639516	1.619788
Rh	0.288091	0.142333	-0.190075

TS1'

SCF energy in gas phase: -925.562576

Free energy in gas phase: -925.20749

Free energy in solution: -925.42279

C	2.377555	-0.181502	-0.208090
C	1.730168	-1.161001	0.639571
C	0.992608	-0.451317	1.667189
C	1.107040	0.944012	1.404581
C	1.962793	1.120330	0.230698
C	3.355220	-0.479707	-1.302839
H	3.380418	0.313324	-2.052214
H	3.132311	-1.422841	-1.806894
C	1.967130	-2.641127	0.603448
H	2.219362	-2.989696	-0.400529
H	2.808238	-2.898736	1.258869

H	1.098318	-3.203512	0.953108
C	0.261319	-1.086235	2.808469
H	-0.161119	-2.054748	2.531578
H	0.954247	-1.258089	3.641858
H	-0.547921	-0.452107	3.175002
C	0.545343	2.062678	2.225957
H	-0.324892	1.746925	2.804481
H	1.304219	2.421044	2.932347
H	0.256358	2.909302	1.599400
C	2.410004	2.440862	-0.315652
H	1.584123	3.154841	-0.353254
H	3.192824	2.865362	0.325084
H	2.818980	2.344535	-1.322867
O	-2.580352	0.731764	0.378847
C	-2.124430	1.765380	-0.203020
O	-0.996398	1.762837	-0.808500
C	-2.944218	3.028147	-0.209979
H	-3.860408	2.852144	-0.782209
H	-3.245580	3.272827	0.812018
H	-2.388945	3.854724	-0.651889
H	4.362955	-0.566831	-0.877903
C	-0.081163	-0.432813	-2.588661
C	-0.544971	-1.468322	-1.768561
H	0.819450	-0.576399	-3.176721
H	-0.735224	0.374695	-2.902115
H	0.014086	-2.399830	-1.703053
C	-1.711877	-1.283216	-0.898889
H	-1.902891	-0.257770	-0.123019
H	-2.528201	-0.836816	-1.484169
C	-2.164134	-2.515865	-0.103565
H	-2.442692	-3.292580	-0.828373
H	-1.307196	-2.916373	0.452736
C	-3.339667	-2.281144	0.851136
H	-4.210865	-1.887087	0.318663
H	-3.636292	-3.223612	1.319380
H	-3.090159	-1.571758	1.644831
Rh	0.183515	0.032607	-0.419060

IM2’

SCF energy in gas phase: -925.600181

Free energy in gas phase: -925.239741

Free energy in solution: -925.449302

C	1.716305	-1.234932	0.496049
C	1.171574	-0.453769	1.594974
C	1.329860	0.914397	1.251941
C	2.057848	0.999157	-0.024075
C	2.341898	-0.321313	-0.452943
C	1.880156	-2.725773	0.498502
H	1.970952	-3.129973	-0.512209
H	1.047049	-3.227352	0.996514
C	0.628274	-1.011478	2.876443
H	0.043702	-1.919189	2.710368
H	1.452353	-1.273240	3.551591
H	-0.005036	-0.291680	3.400098
C	0.994000	2.101685	2.104864
H	0.207566	1.884958	2.830399
H	1.883604	2.412944	2.666487
H	0.682287	2.958721	1.502937
C	2.510626	2.277360	-0.663887
H	1.723714	3.035909	-0.651806
H	3.373082	2.688570	-0.125040
H	2.809450	2.123909	-1.702354
C	3.164204	-0.730000	-1.638201
H	3.178734	0.042580	-2.409372
H	4.200748	-0.909783	-1.327605
H	2.797582	-1.654366	-2.091402
O	-2.250974	1.685646	1.015707
C	-1.935587	2.241540	-0.145051
O	-1.084164	1.749432	-0.900487
C	-2.695461	3.488628	-0.468631
H	-3.756626	3.243666	-0.581707
H	-2.615078	4.198717	0.359175
H	-2.317384	3.929424	-1.389522
H	2.795186	-2.996832	1.040048
C	-0.439027	-0.721997	-2.390526
C	-0.934551	-1.650543	-1.443174
H	0.364320	-1.024300	-3.054971
H	-1.068916	0.084254	-2.755220
H	-0.448757	-2.618906	-1.337076
C	-1.847615	-1.233628	-0.444728
H	-1.717376	0.862073	1.098453
H	-2.554377	-0.455650	-0.733915
C	-2.335966	-2.171403	0.635240
H	-1.548169	-2.891674	0.887206
H	-2.552331	-1.609838	1.552572
C	-3.607282	-2.929477	0.206718
H	-3.421328	-3.542700	-0.680347

H	-3.948597	-3.588567	1.010054
H	-4.421766	-2.236567	-0.027340
Rh	0.100688	-0.057921	-0.380197

IM3'

SCF energy in gas phase: -1093.016688

Free energy in gas phase: -1092.653877

Free energy in solution: -1092.904691

C	-2.503917	-0.415025	0.288813
C	-1.789383	-0.153396	1.529464
C	-0.768276	-1.127530	1.641395
C	-0.894518	-2.064463	0.512926
C	-1.996425	-1.651862	-0.281266
C	-3.749419	0.293441	-0.156528
H	-3.901812	0.214741	-1.235521
H	-3.735605	1.352333	0.111526
C	-2.129287	0.909022	2.530203
H	-2.548628	1.798963	2.056797
H	-2.879860	0.530364	3.235169
H	-1.256997	1.214930	3.111554
C	0.185229	-1.295052	2.786774
H	0.356674	-0.355972	3.316038
H	-0.222701	-2.013968	3.508235
H	1.153786	-1.681638	2.460867
C	-0.108651	-3.334058	0.368132
H	0.928446	-3.211218	0.690861
H	-0.545687	-4.120516	0.995878
H	-0.108711	-3.699981	-0.661016
C	-2.584940	-2.374958	-1.455686
H	-1.855241	-3.025831	-1.941825
H	-3.420874	-3.004397	-1.126303
H	-2.976649	-1.684507	-2.206494
H	-4.625174	-0.154153	0.329581
C	-0.295096	0.494889	-2.432428
C	-0.845853	1.589553	-1.710865
H	-0.930153	-0.048841	-3.125632
H	0.758392	0.513767	-2.696270
H	-1.910150	1.802461	-1.788617
C	-0.101324	2.214692	-0.689350
H	0.981892	2.224789	-0.790352
C	-0.663765	3.311683	0.177066
H	-1.751993	3.204980	0.257248
H	-0.256694	3.224444	1.191086
C	-0.321916	4.708336	-0.378659
H	-0.744954	4.853280	-1.377497
H	-0.723051	5.486836	0.276478
H	0.761011	4.853249	-0.445807
N	1.726471	-0.163990	-0.250853
C	2.669199	-0.835578	-0.832096
C	3.722295	0.364383	0.692467
O	2.377422	0.625298	0.742213
O	4.571601	0.831044	1.370400
O	3.889913	-0.574479	-0.325984
C	2.545687	-1.809478	-1.940706
H	1.499788	-1.930402	-2.219876
H	3.122950	-1.459394	-2.802453
H	2.963591	-2.772218	-1.631076
Rh	-0.425471	-0.021481	-0.309501

TS2'

SCF energy in gas phase: -1092.979146

Free energy in gas phase: -1092.62168

Free energy in solution: -1092.896462

C	-2.598317	-0.289644	0.284604
C	-1.868377	-0.007716	1.512318
C	-0.902430	-1.034706	1.676034
C	-1.076928	-2.010408	0.592706
C	-2.150558	-1.574984	-0.231847
C	-3.803652	0.460994	-0.196360
H	-3.955523	0.348463	-1.272240
H	-3.741169	1.526619	0.034754
C	-2.143224	1.117716	2.462217
H	-2.549422	1.993673	1.953108
H	-2.882843	0.800836	3.207996
H	-1.243689	1.424713	2.999967
C	0.059834	-1.178918	2.814518
H	0.294581	-0.215962	3.271042
H	-0.376640	-1.821355	3.589818
H	0.998586	-1.637390	2.498088
C	-0.344776	-3.314280	0.493597
H	0.689747	-3.224711	0.832226
H	-0.830346	-4.061902	1.133215
H	-0.344036	-3.705253	-0.525996
C	-2.774383	-2.324180	-1.370224
H	-2.071183	-3.016888	-1.836767
H	-3.625472	-2.912562	-1.005204

H	-3.153258	-1.651789	-2.143248
H	-4.700459	0.071703	0.301751
C	-0.394869	0.479363	-2.459109
C	-0.831161	1.620146	-1.733512
H	-1.090466	-0.016571	-3.129199
H	0.652044	0.386884	-2.727993
H	-1.873590	1.926572	-1.795856
C	-0.017021	2.190586	-0.737010
H	1.059360	2.056716	-0.818516
C	-0.454717	3.339242	0.129004
H	-1.548407	3.365421	0.203016
H	-0.061995	3.202979	1.142889
C	0.059935	4.684020	-0.426114
H	-0.336551	4.878651	-1.427154
H	-0.249223	5.503859	0.228075
H	1.152593	4.694955	-0.484380
N	1.693291	-0.393622	-0.382423
C	2.745241	-0.990323	-0.820064
C	3.911177	0.274766	0.719961
O	2.689314	0.679586	0.915144
O	4.929049	0.597426	1.251339
O	3.944824	-0.734633	-0.332207
C	2.681130	-2.014031	-1.917976
H	1.659671	-2.156511	-2.267720
H	3.316620	-1.677777	-2.742578
H	3.084867	-2.958009	-1.540618
Rh	-0.515861	-0.028331	-0.320715

IM4’

SCF energy in gas phase: -904.426116

Free energy in gas phase: -904.078146

Free energy in solution: -904.294728

C	1.710347	-1.422109	-0.121080
C	1.393317	-1.018838	1.234321
C	1.686242	0.382778	1.357657
C	2.181058	0.846830	0.079857
C	2.197999	-0.275507	-0.829834
C	1.700902	-2.831827	-0.633620
H	1.573851	-2.875596	-1.717827
H	0.916054	-3.432519	-0.169241
C	0.973069	-1.933393	2.343746
H	0.376507	-2.771404	1.978259
H	1.861336	-2.352765	2.832946
H	0.393896	-1.408572	3.105917
C	1.572682	1.229193	2.586249
H	1.068882	0.700389	3.396532
H	2.568930	1.519415	2.938612
H	1.006984	2.141810	2.376412
C	2.707859	2.220162	-0.197730
H	2.213064	2.970966	0.420660
H	3.780843	2.253760	0.031583
H	2.587132	2.500405	-1.246181
C	2.755994	-0.263021	-2.221276
H	2.633290	0.710769	-2.700347
H	3.830850	-0.480704	-2.192341
H	2.289800	-1.019165	-2.857165
H	2.657971	-3.314803	-0.401046
C	-0.968592	0.222141	-2.151092
C	-1.273432	-1.008698	-1.514949
H	-0.320603	0.218431	-3.021882
H	-1.661512	1.054103	-2.091954
H	-0.795743	-1.921727	-1.864756
C	-1.992665	-1.042942	-0.304469
H	-2.639245	-0.205271	-0.048518
C	-2.246279	-2.303354	0.466562
H	-1.512864	-3.076537	0.211186
H	-2.157337	-2.096899	1.538911
C	-3.675004	-2.822949	0.183386
H	-3.806742	-3.070025	-0.874061
H	-3.861438	-3.726263	0.770334
H	-4.426962	-2.078212	0.458824
N	-0.882759	1.672093	0.440396
C	-2.101911	2.248340	0.254634
O	-3.103137	1.723994	0.754472
C	-2.116353	3.587211	-0.452207
H	-2.991252	3.627231	-1.107028
H	-2.218772	4.378397	0.297407
H	-1.204377	3.768227	-1.027525
Rh	0.040233	0.169019	-0.191937

TS3A’

SCF energy in gas phase: -904.42113

Free energy in gas phase: -904.072005

Free energy in solution: -904.286251

C	2.246056	-0.954002	-0.047159
C	1.418416	-1.230604	1.085151

C	0.983937	0.032306	1.663262	Rh	0.182353	-0.090984	-0.445020
C	1.521519	1.088422	0.863159				
C	2.290786	0.478428	-0.217544	**TS3B'**			
C	2.988285	-1.960892	-0.874745	SCF energy in gas phase: -904.41682			
H	3.154602	-1.604738	-1.893645	Free energy in gas phase: -904.067595			
H	2.459492	-2.915495	-0.929869	Free energy in solution: -904.283857			
C	1.142927	-2.584136	1.666378				
H	1.229663	-3.377071	0.920430	C	-0.068042	-1.983753	-0.856004
H	1.872661	-2.800172	2.456516	C	-0.626732	-2.018431	0.461598
H	0.150732	-2.641745	2.120114	C	0.367865	-1.516894	1.376803
C	0.168859	0.213330	2.905590	C	1.575607	-1.222389	0.618550
H	-0.307457	-0.717320	3.218676	C	1.303469	-1.508095	-0.760709
H	0.814999	0.546222	3.727472	C	-0.727492	-2.474731	-2.109503
H	-0.609685	0.966369	2.757846	H	-0.406308	-1.911491	-2.988848
C	1.429187	2.551127	1.173268	H	-1.816633	-2.423952	-2.046772
H	0.478196	2.795880	1.651393	C	-1.973779	-2.551904	0.844370
H	2.233164	2.832910	1.864235	H	-2.693433	-2.475854	0.026728
H	1.536091	3.166372	0.277529	H	-1.889521	-3.613516	1.107615
C	3.108446	1.220014	-1.228518	H	-2.386187	-2.032669	1.711993
H	2.668430	2.188577	-1.474051	C	0.233925	-1.445828	2.866306
H	4.112022	1.405448	-0.824020	H	-0.799870	-1.274829	3.173530
H	3.225926	0.652547	-2.153956	H	0.558061	-2.395559	3.311175
H	3.971615	-2.158303	-0.431084	H	0.853731	-0.654229	3.292070
C	-0.390898	-1.256772	-2.322874	C	2.910063	-0.842336	1.181972
C	-1.140239	-1.692180	-1.222521	H	2.817273	-0.336515	2.145248
H	0.415151	-1.874970	-2.703007	H	3.510388	-1.746559	1.341549
H	-0.775276	-0.492380	-2.987719	H	3.461103	-0.193189	0.498092
H	-0.861688	-2.601144	-0.692281	C	2.290564	-1.393164	-1.879995
C	-2.240994	-0.933290	-0.695416	H	2.860525	-0.463509	-1.806329
H	-2.820832	-0.351541	-1.400893	H	2.995041	-2.233423	-1.837029
C	-2.919719	-1.255955	0.595424	H	1.803876	-1.423044	-2.856733
H	-2.275485	-1.879360	1.225513	H	-0.460008	-3.524379	-2.282369
H	-3.099643	-0.315390	1.127377	C	-0.436772	1.642769	-1.805843
C	-4.268578	-1.965550	0.333687	C	-1.647295	1.054603	-1.289914
H	-4.132046	-2.916190	-0.190048	H	-2.108914	0.250112	-1.859837
H	-4.761074	-2.171014	1.287578	C	-2.172575	1.394855	-0.047264
H	-4.937753	-1.337392	-0.261487	H	-1.763528	2.266226	0.456448
N	-1.238932	1.091991	-0.944029	C	-3.452394	0.835348	0.500058
C	-1.657553	2.154857	-0.183509	H	-3.719392	-0.090192	-0.021749
O	-2.143909	2.019812	0.942392	H	-3.321075	0.587551	1.560210
C	-1.577377	3.494825	-0.895803	C	-4.601384	1.859578	0.371288
H	-2.580134	3.762770	-1.244801	H	-4.796173	2.106348	-0.676355
H	-1.254394	4.255669	-0.180858	H	-5.518242	1.447143	0.800940
H	-0.907744	3.473771	-1.758944	H	-4.367754	2.787048	0.902532

N	0.663184	1.904221	0.100168
C	2.007618	2.182474	0.036151
O	2.712050	1.917171	-0.937392
C	2.515787	2.948869	1.248699
H	3.504731	2.567136	1.513736
H	2.621586	4.002458	0.970182
H	1.840888	2.885187	2.105530
H	0.045996	1.190578	-2.666617
H	-0.254033	2.700488	-1.685481
Rh	-0.042254	0.123775	-0.042908

IM5A'

SCF energy in gas phase: -904.489346

Free energy in gas phase: -904.136854

Free energy in solution: -904.34413

C	1.900695	-0.449330	1.302622
C	1.660416	0.975710	1.069791
C	1.901915	1.237241	-0.311018
C	2.280497	-0.026302	-0.942265
C	2.322730	-1.044991	0.067580
C	1.829617	-1.127863	2.633010
H	1.666416	-2.202759	2.534018
H	1.035935	-0.711908	3.257485
C	1.328307	1.990599	2.116706
H	0.858564	1.531552	2.988895
H	2.251381	2.478650	2.455511
H	0.653705	2.750024	1.720748
C	1.841206	2.573644	-0.974921
H	0.947245	3.118288	-0.660083
H	2.720469	3.165812	-0.691061
H	1.836428	2.486552	-2.062915
C	2.671994	-0.185668	-2.377069
H	2.087333	0.465662	-3.030769
H	3.728012	0.085528	-2.503384
H	2.554715	-1.215582	-2.719608
C	2.778425	-2.462729	-0.115471
H	2.636039	-2.809584	-1.141060
H	3.849048	-2.539859	0.108734
H	2.256409	-3.150363	0.554332
H	2.777212	-0.985119	3.169005
C	-0.619979	-2.024688	-1.375789
C	-1.475388	-1.760218	-0.339190
H	0.058203	-2.870761	-1.336387
H	-0.741780	-1.544293	-2.344230
H	-1.466051	-2.389528	0.548422
C	-2.494112	-0.614225	-0.384403
H	-2.975724	-0.568254	-1.373226
C	-3.574357	-0.785138	0.698940
H	-3.077203	-0.891602	1.671739
H	-4.176198	0.125168	0.755956
C	-4.493132	-1.982637	0.427557
H	-3.940390	-2.927745	0.390379
H	-5.243905	-2.074391	1.216639
H	-5.023819	-1.869203	-0.523558
N	-1.578548	0.518785	-0.182093
C	-1.946303	1.867531	-0.169770
O	-1.131876	2.721661	0.159714
C	-3.345567	2.260880	-0.607637
H	-3.984940	2.378344	0.273683
H	-3.280026	3.235025	-1.094895
H	-3.817022	1.543700	-1.282462
Rh	0.233622	-0.237090	-0.115489

IM5B'

SCF energy in gas phase: -904.4924

Free energy in gas phase: -904.139807

Free energy in solution: -904.346954

C	-1.164762	-1.892070	-0.206076
C	-0.576707	-1.751743	1.092150
C	0.877282	-1.719045	0.941097
C	1.170197	-1.791057	-0.456363
C	-0.102443	-1.864618	-1.170913
C	-2.612554	-2.129638	-0.513758
H	-2.920986	-1.648530	-1.444647
H	-3.267801	-1.780600	0.285276
C	-1.299371	-1.756279	2.401942
H	-2.336666	-1.432322	2.297983
H	-1.310676	-2.773291	2.814465
H	-0.807882	-1.112801	3.135399
C	1.877509	-1.706934	2.051095
H	1.436472	-1.367515	2.990318
H	2.257880	-2.724218	2.210610
H	2.718946	-1.057257	1.803056
C	2.528587	-1.892589	-1.071974
H	3.237182	-1.241526	-0.558116
H	2.883901	-2.928430	-0.997136

H	2.512803	-1.624574	-2.130285
C	-0.254009	-2.014523	-2.650880
H	0.521370	-1.470253	-3.194524
H	-0.164066	-3.074046	-2.924603
H	-1.229386	-1.667259	-2.997385
H	-2.786427	-3.206331	-0.630233
C	0.339135	2.743658	-0.475527
C	-0.995959	2.059619	-0.750929
H	-1.309380	1.938769	-1.786782
C	-1.843208	1.707252	0.263360
H	-1.558518	1.980526	1.281872
C	-3.267851	1.263843	0.080331
H	-3.416179	0.874620	-0.932549
H	-3.502947	0.457314	0.782783
C	-4.236950	2.437594	0.336073
H	-4.067953	3.251002	-0.375225
H	-5.270750	2.098940	0.227374
H	-4.120073	2.839378	1.347343
N	1.179932	1.618797	-0.078990
C	2.548947	1.739498	0.160842
O	3.214596	0.761375	0.479939
C	3.165085	3.118162	0.021093
H	4.214155	3.058881	0.308481
H	3.097592	3.474686	-1.012737
H	2.656241	3.851437	0.655558
H	0.704190	3.240729	-1.382131
H	0.251840	3.505037	0.311909
Rh	0.015183	0.040184	-0.081823

IM6’

SCF energy in gas phase: -1133.599407

Free energy in gas phase: -1133.188754

Free energy in solution: -1133.435842

C	1.335277	-1.979136	0.104519
C	1.535608	-1.168281	1.280561
C	2.236645	0.024374	0.899502
C	2.555812	-0.080911	-0.517544
C	2.023722	-1.327747	-0.992326
C	0.711910	-3.342934	0.087083
H	0.477263	-3.665531	-0.929430
H	-0.210802	-3.366019	0.672125
C	1.151397	-1.561691	2.669410
H	0.247328	-2.172683	2.686597
H	1.963305	-2.166675	3.094130
H	1.016196	-0.697480	3.321912
C	2.700785	1.123183	1.804212
H	2.068379	1.218473	2.688902
H	3.724062	0.920515	2.144201
H	2.707375	2.083032	1.284124
C	3.357336	0.922446	-1.284970
H	2.930307	1.922573	-1.167532
H	4.387897	0.944128	-0.911997
H	3.391199	0.689609	-2.350385
C	2.231495	-1.916443	-2.352688
H	2.426354	-1.154272	-3.108983
H	3.105909	-2.578598	-2.319733
H	1.382624	-2.523171	-2.675462
H	1.403730	-4.080111	0.512707
C	-0.606123	0.040644	-2.433892
C	-1.447462	-0.624106	-1.578868
H	0.027651	-0.504118	-3.124867
H	-0.684901	1.112215	-2.585152
H	-1.481883	-1.711361	-1.559907
C	-2.413307	0.110293	-0.666199
H	-2.496619	1.144403	-1.017407
C	-3.817559	-0.492631	-0.578577
H	-3.755271	-1.537799	-0.264528
H	-4.372317	0.043864	0.201052
C	-4.564162	-0.377820	-1.913831
H	-4.049113	-0.917367	-2.716018
H	-5.566064	-0.805055	-1.824848
H	-4.673394	0.666115	-2.226443
N	-1.660141	0.228363	0.633060
C	-1.906914	-0.702144	1.688454
O	-2.064619	-1.886431	1.465697
C	-1.970642	-0.076744	3.061377
H	-1.837527	-0.842698	3.825338
H	-1.242765	0.730372	3.180950
H	-2.963500	0.371739	3.189325
C	-0.193168	2.995062	0.138055
O	0.385631	2.096526	-0.608802
O	-0.999161	2.756714	1.055306
C	0.203818	4.422809	-0.188728
H	-0.485657	5.119567	0.287865
H	1.215310	4.611828	0.186572
H	0.221030	4.580703	-1.269514
H	-1.567386	1.228080	0.946926

Rh	0.377570	0.001631	-0.294508

TS4'

SCF energy in gas phase: -1133.596142

Free energy in gas phase: -1133.188739

Free energy in solution: -1133.434225

C	1.049836	-2.125029	0.269740
C	0.921937	-1.395148	1.500613
C	1.814894	-0.268990	1.442814
C	2.589597	-0.378341	0.208443
C	2.106853	-1.498866	-0.521355
C	0.415332	-3.447219	-0.039208
H	0.306825	-3.611766	-1.113764
H	-0.566093	-3.552284	0.427108
C	0.073663	-1.783389	2.668920
H	-0.779165	-2.395905	2.368690
H	0.679358	-2.381322	3.362320
H	-0.296011	-0.908242	3.202458
C	2.054956	0.731364	2.529757
H	1.137998	0.936096	3.083385
H	2.809701	0.350265	3.229491
H	2.426008	1.673410	2.120699
C	3.691693	0.551447	-0.182611
H	3.348472	1.589144	-0.156068
H	4.524549	0.451437	0.523031
H	4.068901	0.339518	-1.184008
C	2.651066	-2.033655	-1.811910
H	3.135789	-1.255232	-2.403952
H	3.398958	-2.809020	-1.605423
H	1.871861	-2.493345	-2.424957
H	1.049599	-4.254981	0.347361
C	-0.367703	0.043488	-2.450142
C	-1.211681	-0.759833	-1.720839
H	0.375274	-0.392976	-3.109565
H	-0.570547	1.099872	-2.586021
H	-1.126503	-1.839017	-1.808779
C	-2.356592	-0.228474	-0.851304
H	-3.032942	0.405950	-1.442445
C	-3.157373	-1.392600	-0.248296
H	-2.462267	-2.059163	0.278836
H	-3.855268	-1.015414	0.501915
C	-3.951943	-2.170501	-1.305424
H	-3.310170	-2.605371	-2.078958
H	-4.503793	-2.991267	-0.839886
H	-4.679851	-1.523182	-1.805059
N	-1.588706	0.594807	0.134392
C	-2.079313	0.916468	1.432739
O	-1.302151	1.047793	2.359567
C	-3.549991	1.264184	1.581439
H	-4.028741	0.557494	2.266098
H	-3.602798	2.250165	2.051027
H	-4.100100	1.286821	0.639887
C	0.177521	2.978462	-0.777118
O	0.974509	2.000787	-0.605475
O	-1.090548	2.857591	-0.781569
C	0.763106	4.352259	-0.974680
H	0.201211	4.884032	-1.745524
H	0.654292	4.915448	-0.041568
H	1.819270	4.297200	-1.237486
H	-1.391229	1.728560	-0.355265
Rh	0.425527	-0.049416	-0.259866

IM7'

SCF energy in gas phase: -1133.609226

Free energy in gas phase: -1133.196793

Free energy in solution: -1133.448597

C	0.871526	-2.175877	0.354778
C	0.852435	-1.370128	1.550149
C	1.837440	-0.341507	1.398186
C	2.560181	-0.589877	0.145827
C	1.965237	-1.704214	-0.495505
C	0.114154	-3.452074	0.146768
H	-0.026376	-3.680099	-0.912204
H	-0.864078	-3.433475	0.630530
C	0.004176	-1.599551	2.759277
H	-0.897685	-2.167280	2.521558
H	0.578263	-2.181510	3.491841
H	-0.289644	-0.655228	3.218076
C	2.185903	0.700867	2.413465
H	1.283668	1.091427	2.886830
H	2.832202	0.267973	3.187541
H	2.725892	1.532520	1.957015
C	3.729266	0.212156	-0.327496
H	3.506195	1.281575	-0.297525
H	4.590124	0.029874	0.326600
H	4.018332	-0.050484	-1.346280

C	2.414264	-2.363088	-1.765123	H	-4.824791	-1.170882	-1.788918
H	2.965221	-1.675030	-2.408824	N	-1.534765	0.609413	0.166798
H	3.078656	-3.204288	-1.532668	C	-1.921331	1.088002	1.410449
H	1.574218	-2.765798	-2.337089	O	-1.084828	1.327894	2.278172
H	0.680132	-4.284820	0.583405	C	-3.381366	1.457841	1.637411
C	-0.420152	-0.029057	-2.439592	H	-3.847347	0.725481	2.304325
C	-1.308294	-0.751596	-1.677947	H	-3.397239	2.419896	2.154072
H	0.276232	-0.531285	-3.103330	H	-3.972324	1.528744	0.722159
H	-0.555880	1.034163	-2.607753	C	0.435053	2.997934	-0.816481
H	-1.294981	-1.836145	-1.737057	O	1.095297	1.947757	-0.674395
C	-2.394017	-0.117005	-0.798995	O	-0.869741	3.025809	-0.767003
H	-3.008049	0.579795	-1.391479	C	1.102175	4.318999	-1.053988
C	-3.313581	-1.203613	-0.215122	H	0.586580	4.857614	-1.852783
H	-2.693900	-1.940253	0.312396	H	1.015852	4.923244	-0.144483
H	-3.974317	-0.762647	0.533148	H	2.153988	4.180311	-1.299953
C	-4.169345	-1.890429	-1.287269	H	-1.199594	2.107280	-0.460264
H	-3.563831	-2.378686	-2.058589	Rh	0.399643	-0.110849	-0.271283
H	-4.804278	-2.658057	-0.837094				