Os.acac^{-}

A
Gas phase Energy: -934.54904035172 hartrees
Solvation Energy:-934.59032087478 hartrees
Zero Point Energy: 163.014 kcal/mol
Coordinates:

Os1	-0.3106208466	0.0336233993	-0.1420981385
O2	-1.9820476306	-0.1442655498	-1.3771971440
O3	0.8184823543	0.2248433298	-1.9424363798
C4	2.0845814858	0.3528372938	-1.8958653438
C5	2.9336211465	0.3676126936	-0.7840515807
C6	2.5503317597	0.2575476835	0.5641021963
O7	1.3799806631	0.1465778998	1.0465914459
H8	3.3574230511	0.2741082014	1.3118512297
H9	3.9964241832	0.4771137746	-0.9817273437
H10	2.5734359388	0.4616025883	-2.8778227035
C11	-0.4468867651	2.1220751412	-0.2632935135
C12	-1.0462668543	2.7342067568	-1.3870772862
C13	-1.0808514288	4.1217304619	-1.5576022156
C14	-0.5091543690	4.9691853050	-0.6055925205
C15	0.0971309521	4.3978930364	0.5166033255
C16	0.1219229508	3.0103127396	0.6774125831
H17	0.6041048239	2.5975042234	1.5608513295
H18	0.5557909085	5.0375724657	1.2708807223
H19	-0.5328830845	6.0498028596	-0.7357140575
H20	-1.5588333949	4.5445332756	-2.4415236953
H21	-1.5003312349	2.0991717298	-2.1424283697
O22	0.2567586635	-2.0772777821	-0.5046373232
C23	-0.4314949180	-2.7856398830	-1.2953579139
C24	-2.2786014552	-1.2220061508	-1.9819378444
C25	-1.6169918965	-2.4612723325	-1.9758185051
H26	-0.0464698462	-3.8066027454	-1.4748213473
H27	-3.1816230751	-1.1580588119	-2.6096709721
H28	-2.0508703977	-3.2416016318	-2.5958271872
C29	-1.4173453949	0.4731264921	1.6664125133
C30	-1.4912358026	-0.9159255123	1.3832786010
H31	-0.7463778652	0.8281099482	2.4472032839
H32	-0.8837574165	-1.6196589839	1.9500696465
H33	-2.4112037372	-1.3388752472	0.9778944327
H34	-2.2802065341	1.1116258065	1.4946869129

B
Gas phase Energy: -855.90904507400 hartrees
Solvation Energy:-855.95519206800 hartrees
Zero Point Energy: 128.240 kcal/mol
Coordinates:

Os1	0.0484452205	0.4240472726	0.2799925790
O2	0.0554742526	-0.7733212015	1.9753220072
C3	0.1876834875	-2.0399404530	1.8857946886
C4	0.3720912942	-2.8193790951	0.7333375901
C5	0.4784337315	-2.3565606638	-0.5873088315
O6	0.4074638919	-1.1564799453	-1.0166513885
H7	0.6659093315	-3.1148500926	-1.3632005899

H8	0.4631327461	-3.8926735790	0.8814596093
H9	0.1711457437	-2.5756610238	2.8474936619
O10	0.2561285900	1.6354834383	-1.3911140039
C11	0.1928010160	2.9071266310	-1.2947142108
C12	0.0162562839	3.6874152472	-0.1417592424
C13	-0.0982218285	3.2241938699	1.1779878889
O14	-0.0957203580	2.0187763507	1.5989590498
H15	-0.1837301056	3.9886080408	1.9654662883
H16	-0.0090964924	4.7652045037	-0.2830286276
H17	0.3119136872	3.4489973045	-2.2455277514
C18	-1.9285670636	0.2831293866	0.0665155121
C19	-2.5356350151	0.0781962752	-1.2011338908
C20	-3.9198612445	-0.0204814149	-1.3474681202
C21	-4.7695642908	0.0792801189	-0.2402687666
C22	-4.1971405802	0.2808326656	1.0204508346
C23	-2.8136730728	0.3804355204	1.1730296601
H24	-2.3938831485	0.5367654671	2.1628176659
H25	-4.8380346396	0.3618237494	1.8988565950
H26	-5.8488016357	0.0022310106	-0.3567882403
H27	-4.3416443292	-0.1775373207	-2.3406154139
H28	-1.8973951639	-0.0030107455	-2.0765739513

D
Gas phase Energy: -934.52165920360 hartrees
Solvation Energy:-934.56358255354 hartrees
Zero Point Energy: 163.376 kcal/mol
Coordinates:

Os1	-0.4963476716	0.1758966433	-0.3168010290
O2	-1.1902508566	-0.0303391280	-2.2898141824
O3	1.3093179598	-0.0761075511	-1.3037477007
C4	2.4448649799	-0.1450618956	-0.7239875471
C5	2.7197607020	-0.0635298315	0.6433346522
C6	1.7554227346	0.1492124323	1.6401755341
O7	0.5008377127	0.3100009187	1.4988187863
H8	2.1096063645	0.2005158508	2.6806593061
H9	3.7557464140	-0.1579445659	0.9567857291
H10	3.2986195800	-0.2848582212	-1.4039232532
O11	-0.3946648334	-2.0388741767	-0.0505571976
C12	-0.7158492868	-2.8000956422	-1.0000932173
C13	-1.3437335896	-1.1760780573	-2.8268001468
C14	-1.1764524433	-2.4586197096	-2.2912734567
H15	-0.6250920922	-3.8863275623	-0.8051376919
H16	-1.6583663477	-1.1381576287	-3.8830345185
H17	-1.3807480874	-3.2874349458	-2.9652270445
C18	-0.6534912281	2.2712351019	-0.5546187169
H19	0.2757157339	2.8498693751	-0.4382010848
H20	-1.0799941843	2.5273184406	-1.5359992048
C21	-1.6484714259	2.5248399737	0.5986577950
H22	-1.1429766900	2.9676830734	1.4669526560
H23	-2.5045207342	3.1847099047	0.3634546255
C24	-3.4254420943	-1.2957739209	1.7421849620
C25	-3.4130129833	-0.9181078416	0.4272616077
C26	-2.7362062524	0.2755168476	-0.0093406985
C27	-2.0896859223	1.1107192713	0.9753696322
C28	-2.1867417682	0.6990042237	2.3550525704
C29	-2.8107272514	-0.4599990639	2.7260264719

H30	-3.9211616236	-2.2145336496	2.0485738079
H31	-3.9261710844	-1.5202812520	-0.3197490386
H32	-3.0578966839	0.7095307184	-0.9530936666
H33	-1.7445865027	1.3441708919	3.1110476909
H34	-2.8507498742	-0.7477809360	3.7749333930

E
Gas phase Energy: -1166.79085103865 hartrees
Solvation Energy:-1166.82999829231 hartrees
Zero Point Energy: 227.961 kcal/mol
Coordinates:

Os1	0.4370511869	-0.9005309634	-0.0663273750
O2	2.1171155403	-1.2157868674	1.3788707897
C3	1.9316568606	-1.9177117556	2.4162204837
C4	0.7549511275	-2.5270342275	2.8801158589
C5	-0.5063109037	-2.5103091610	2.2596603916
O6	-0.8678347169	-1.9392565561	1.1873008508
H7	-1.3060181615	-3.0696636258	2.7712174459
H8	0.8309653590	-3.0905708806	3.8066286160
H9	2.8257272722	-2.0769303094	3.0480611676
O10	1.7935363456	0.0459105856	-1.3005217753
C11	-1.9404476463	1.2235223140	0.1735619118
C12	-0.5104808027	1.1081638341	-0.0374487788
H13	-2.5750619299	1.4143719335	-0.6896966887
H14	-0.1070519436	1.5925140526	-0.9244354960
C15	-2.4940802861	1.1199837012	1.4159841795
C16	0.3328883291	0.9628263951	1.1311064646
C17	-1.6547107700	0.9622820963	2.5718083794
C18	-0.2977292513	0.9235239868	2.4341167484
H19	-2.1097663355	0.9119263260	3.5590632847
H20	0.3387752785	0.8680657463	3.3146742253
H21	-3.5724286918	1.1905938381	1.5449842867
H22	1.3572969261	1.3266305447	1.0947019238
O23	1.0652505823	-2.8193788169	-0.6508727451
C24	2.0238967217	-2.9610364885	-1.4837889405
C25	2.6286746280	-0.5902639445	-2.0167356993
C26	2.7756047795	-1.9850910115	-2.1424242694
H27	2.2812729780	-4.0079230602	-1.7079321773
H28	3.3126102369	0.0407217700	-2.6029356951
H29	3.5522457599	-2.3369065276	-2.8159999667
C30	-0.9009279845	-1.1263841125	-1.7250518165
H31	-0.3459840051	-1.6921410199	-2.4914411688
H32	-1.1711298753	-0.1746630820	-2.2045565961
C33	-2.2032600670	-1.9050939113	-1.4204075766
H34	-2.7581834211	-1.3928966010	-0.6273489893
H35	-1.9358886925	-2.8901492963	-1.0214205504
C36	-4.6959936056	-2.3372442928	-4.9509016873
C37	-4.9573325156	-1.3284380885	-4.0212327775
C38	-4.1638420870	-1.2019723625	-2.8792925855
C39	-3.0903999356	-2.0723792495	-2.6320436215
C40	-2.8446449766	-3.0809025283	-3.5788340849
C41	-3.6324388793	-3.2142730115	-4.7215485248
H42	-5.3127759708	-2.4401265658	-5.8405844487
H43	-5.7839489587	-0.6395831779	-4.1837067301
H44	-4.3749755784	-0.4153662682	-2.1578050244
H45	-2.0175019398	-3.7661446772	-3.4074237060

H46	-3.4182657348	-4.0066800246	-5.4357631323

G
Gas phase Energy: -1013.17351868591 hartrees
Solvation Energy:-1013.21407156666 hartrees
Zero Point Energy: 198.570 kcal/mol
Coordinates:

Os1	-0.3263644884	0.0159405481	-0.3582119887
O2	-0.5617456768	0.0027613678	-2.4302963729
O3	1.7769611259	-0.0547913865	-0.7509551091
C4	2.6093311072	-0.1157185747	0.2124705539
C5	2.3690206024	-0.1466518654	1.5897502080
C6	1.1116738399	-0.1055437549	2.2213548321
O7	-0.0367805857	-0.0186968663	1.6847967826
H8	1.1057628800	-0.1467395915	3.3210708203
H9	3.2394558088	-0.2070469115	2.2376750308
H10	3.6686468412	-0.1465612714	-0.0924013881
O11	0.0425243775	-2.1763967260	-0.3256732265
C12	0.0509265238	-2.8247691547	-1.4118875616
C13	-0.4679090023	-1.0564759757	-3.1265598360
C14	-0.2042483923	-2.3744992712	-2.7182038022
H15	0.2940230666	-3.8999061777	-1.3217765976
H16	-0.6020495299	-0.9031342251	-4.2094212238
H17	-0.1538678075	-3.1209257460	-3.5069304411
C18	-0.0131971766	2.1343452787	-0.3697940531
H19	-0.5321949952	2.6324135673	0.4625396097
H20	1.0628516546	2.2836445268	-0.1886863499
C21	-0.3675602903	2.8735999052	-1.6810865091
H22	0.1731343816	2.4049282765	-2.5099597769
H23	-1.4348401715	2.7434194954	-1.8996088124
C24	0.5808277975	7.1062959472	-1.4678292144
C25	-0.6860692001	6.6464014829	-1.1007395292
C26	-0.9919977320	5.2875911870	-1.1853135427
C27	-0.0488610373	4.3500818911	-1.6355904765
C28	1.2192642762	4.8314734830	-1.9987349899
C29	1.5336226512	6.1884268297	-1.9172520292
H30	0.8219167754	8.1647490910	-1.4053244625
H31	-1.4390250808	7.3490863831	-0.7506702444
H32	-1.9806471669	4.9366025373	-0.8968612863
H33	1.9659464720	4.1217788225	-2.3482655580
H34	2.5243908026	6.5316580650	-2.2074912520
C35	-2.3039772553	0.7051033807	0.1127277759
C36	-2.3498713929	-0.6711462625	-0.2513207240
H37	-2.3696128809	0.9858751554	1.1641680112
H38	-2.4620567121	-1.4334217189	0.5188270829
H39	-2.7428977561	-0.9609344532	-1.2271676760
H40	-2.6936961483	1.4577036355	-0.5713905836

TS1
Gas phase Energy: -934.48329610313 hartrees
Solvation Energy: -934.52555638494 hartrees
Zero Point Energy: 162.465 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-223.26 cm^{-1})
Coordinates:

Os1	-0.0866677046	0.1860356218	0.0400270728

O2	-0.2166157393	0.2521670900	2.0949560691
O3	2.0956950013	-0.1831453753	0.3059368756
C4	2.8382788619	-0.2697666987	-0.7109240147
C5	2.5006347069	-0.1274388126	-2.0717244630
C6	1.2304067980	0.0988645609	-2.6177490405
O7	0.0972304018	0.1951910402	-2.0422305636
H8	1.1896162708	0.1914067308	-3.7155176060
H9	3.3190466846	-0.2108733233	-2.7829405402
H10	3.9066668319	-0.4798263553	-0.5114961426
C11	-0.4517841687	-2.0681985697	-0.0678231874
C12	0.1536361523	-2.7533258533	1.0224117131
C13	0.8968678755	-3.9139702537	0.8331342254
C14	1.0332736652	-4.4780266705	-0.4406426658
C15	0.3961703670	-3.8547957000	-1.5256256829
C16	-0.3444786229	-2.6972159972	-1.3429615524
H17	-0.8380794061	-2.2297763725	-2.1899223245
H18	0.4809695739	-4.2845529025	-2.5225695345
H19	1.6107624677	-5.3878227579	-0.5860211859
H20	1.3790356620	-4.3839777335	1.6889250529
H21	0.0635743517	-2.3187359387	2.0130843802
O22	0.6371219534	2.0904247523	-0.1348158266
C23	0.8545861125	2.8135693998	0.9004489194
C24	0.1631127718	1.2789348371	2.7539110830
C25	0.6553645450	2.4924614816	2.2489156185
H26	1.2462717224	3.8160142700	0.6763386935
H27	0.0850488307	1.1824754338	3.8464925033
H28	0.9173936695	3.2558125026	2.9772127324
C29	-1.9261427653	-1.3074083021	0.2598657673
C30	-2.1360644612	0.1606488781	-0.1072115141
H31	-2.5595787105	-1.9825432685	-0.3205648797
H32	-2.5643737858	0.2982618930	-1.1085900318
H33	-2.7424671901	0.6871598255	0.6416027062
H34	-2.0932285872	-1.4816821993	1.3239173790

TS2.Ph-H
Gas phase Energy: -1166.78605031901 hartrees
Solvation Energy: -1166.82476995532 hartrees
Zero Point Energy: 225.422 kcal/mol
Number and Magnitude of negative Eigen values: 1 (209.61 cm^{-1})
Coordinates:

Os1	-0.0018485256	-0.0623686205	-0.0044733579
O2	0.0492687010	0.0323912569	2.2004349263
C3	1.1549815156	-0.0845119884	2.8041008659
C4	2.4408273278	-0.2826109895	2.2710474576
C5	2.7990188123	-0.3621906957	0.9179036729
O6	2.0659052755	-0.3172892121	-0.1213468124
H7	3.8742459007	-0.4729746537	0.7079436920
H8	3.2553508235	-0.3509358627	2.9872228621
H9	-0.8404630434	1.1057838075	-2.2755024083
O10	-2.0335173017	0.3200286579	0.1716494945
O11	0.4830767289	1.9945434264	0.1931127362
C12	-0.4255228462	2.8758247095	0.3408567842
C13	-2.5051833040	1.4857124365	0.3474861921
C14	-1.8103679543	2.7069559324	0.4267142056
H15	-0.0563618495	3.9120297475	0.4088740603
H16	-3.6003729244	1.5303914214	0.4409027790

H17	-2.4086677514	3.6037970239	0.5607210704
C18	-0.1005757066	-2.1619442950	0.3649249698
H19	-0.3546398278	-0.5049678203	-2.7481718076
C20	1.2710579945	0.9063062437	-2.6923586131
H21	2.0441740354	0.1339048670	-2.6277752937
H22	1.6069879185	1.7347924506	-2.0609396421
C23	-1.0893921321	-2.6823579021	1.2358114868
C24	-1.0533092325	-4.0052547040	1.6746219606
C25	-0.0465899874	-4.8748811689	1.2430879301
C26	0.9164217669	-4.3954234212	0.3497670177
C27	0.8841936284	-3.0724690617	-0.0880340205
H28	-1.8862753773	-2.0238566095	1.5671762727
H29	-1.8221708881	-4.3630734092	2.3581339064
H30	-0.0251374580	-5.9090502236	1.5794650966
H31	1.6996630970	-5.0601633904	-0.0121329764
H32	1.6310935080	-2.7172682062	-0.7919517209
H33	1.1054034006	-0.0082716359	3.9052897310
H34	-0.6046645814	-1.3917280129	-0.7389867381
C35	-0.0549895766	0.3462019718	-2.1195742432
C36	0.8415895710	2.2557686223	-6.7983615078
C37	1.2497895309	0.9486266618	-6.5242321065
C38	1.3982571960	0.5207643555	-5.2040484769
C39	1.1465904826	1.3794488955	-4.1224310456
C40	0.7390070340	2.6904404696	-4.4185786411
C41	0.5860444966	3.1255306337	-5.7353125093
H42	0.7263903187	2.5927491483	-7.8257574580
H43	1.4564135078	0.2610279724	-7.3416389020
H44	1.7183286002	-0.4987308160	-4.9993416944
H45	0.5373163846	3.3722662288	-3.5954703810
H46	0.2703951440	4.1474918355	-5.9331746805

TS2 – intermediate
Gas phase Energy: -1166.79174488470 hartrees
Solvation Energy:-1166.83105403785 hartrees
Zero Point Energy: 226.488 kcal/mol
Coordinates:

Os1	-0.1174070943	-0.1508245405	-0.2161956263
O2	-0.1484379921	-0.0352545412	1.9792353070
C3	0.9403602041	-0.0739300157	2.6270781200
C4	2.2538475295	-0.2018288867	2.1520683092
C5	2.6656076290	-0.2802372876	0.8125151484
O6	1.9633124088	-0.2919725100	-0.2468061597
H7	3.7514110367	-0.3300474640	0.6387091649
H8	3.0419160044	-0.2104741854	2.9000349758
H9	0.2216658073	1.6013668139	-2.1754313691
O10	-2.1829438852	0.1149157477	-0.1136323722
O11	0.2267703290	1.9844911079	0.1719167078
C12	-0.7561852210	2.7659605855	0.3520766396
C13	-2.7289020440	1.2302428686	0.1419676717
C14	-2.1281413644	2.4837399036	0.3557297015
H15	-0.4876783023	3.8221370025	0.5317892490
H16	-3.8284160648	1.2003000427	0.1922018687
H17	-2.7983399963	3.3180708547	0.5430582889
C18	-0.1830380811	-2.2051754368	0.2501159092
H19	-1.0093015971	0.4748206779	-2.7503064274
C20	1.0267417023	-0.1354718319	-3.1684687786

H21	0.7560613249	-1.1875116328	-3.3250816468
H22	1.9893743799	-0.1329906593	-2.6476807037
C23	-1.2243179119	-2.7177133619	1.0511735368
C24	-1.2544559612	-4.0551008760	1.4567831859
C25	-0.2450043243	-4.9388952809	1.0680332463
C26	0.7918284679	-4.4592439849	0.2629012387
C27	0.8153636066	-3.1220334260	-0.1390656578
H28	-2.0227192956	-2.0496342791	1.3606081606
H29	-2.0754751816	-4.4094835692	2.0793712037
H30	-0.2688197702	-5.9812289320	1.3799493159
H31	1.5876816353	-5.1315953446	-0.0558938916
H32	1.6279369282	-2.7710001968	-0.7699468602
H33	0.8378573601	0.0125258684	3.7231145685
H34	-0.5089259744	-1.2164667085	-1.3259772418
C35	-0.0268212811	0.5350680868	-2.2594996916
C36	1.3775577312	1.8776901069	-6.9988403810
C37	0.5230703024	0.7829022968	-6.8530495410
C38	0.4234147641	0.1285297574	-5.6241020363
C39	1.1693865384	0.5456889146	-4.5110517859
C40	2.0228471109	1.6481703897	-4.6764540880
C41	2.1276313575	2.3078010873	-5.9012118401
H42	1.4591416680	2.3885434448	-7.9552370172
H43	-0.0658659101	0.4356725768	-7.6993084431
H44	-0.2439604507	-0.7241149500	-5.5180097302
H45	2.6082274717	1.9882061219	-3.8250638636
H46	2.7985595547	3.1583188026	-6.0009313576

TS2.CH_2-H
Gas phase Energy: -1166.78141538231 hartrees
Solvation Energy: -1166.82143996003 hartrees
Zero Point Energy: 225.377 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-602.54 cm^{-1})
Coordinates:

Os1	-.0874679790	-.0894361105	-.0836408348
O2	-.0725145238	.0213351957	2.0128018824
C3	1.0231280872	-.0360772967	2.6622989575
C4	2.3293349199	-.1664526187	2.1776090522
C5	2.7160633571	-.2331164118	.8292859987
O6	1.9729908975	-.2195221138	-.2046401508
H7	3.7941824739	-.2919257971	.6210321646
H8	3.1252906301	-.1942885929	2.9167452205
H9	.0856409297	1.4356952380	-2.1781370736
O10	-2.1645619080	.1255887733	.0911659666
O11	.1820394110	2.1213456666	.0711380586
C12	-.8234928588	2.8718478154	.2375176797
C13	-2.7380250261	1.2414681372	.2730775356
C14	-2.1818368432	2.5311133851	.3366582522
H15	-.6029410779	3.9532137267	.3166146781
H16	-3.8322531829	1.1794544306	.3880394389
H17	-2.8791951555	3.3507980781	.4884692615
C18	-.2049634142	-2.1543457487	.1555497424
H19	-1.0399702484	.2784819589	-2.8717015473
C20	1.0535158357	-.2390773726	-3.1678389338
H21	.8851760107	-1.3155904150	-3.2948823850
H22	1.9823754059	-.1328121558	-2.6002636110
C23	-1.1875222758	-2.7325998028	.9946326117

C24	-1.2584031128	-4.1080868774	1.2312041084
C25	-.3448479262	-4.9819481900	.6350758044
C26	.6393131796	-4.4466001267	-.2009587800
C27	.7013659481	-3.0701998973	-.4312593742
H28	-1.9151539134	-2.0786859329	1.4686861265
H29	-2.0357090443	-4.5021696360	1.8861632300
H30	-.3990641883	-6.0539144079	.8161905991
H31	1.3656945207	-5.1063072647	-.6764174164
H32	1.4862093822	-2.6846318640	-1.0795904275
H33	.9128132965	.0349298274	3.7556872418
H34	-.4419095203	-.7556395612	-1.5226244117
C35	-.0897976815	.3668174512	-2.3261796154
C36	1.3697076492	1.6669703102	-7.0494318947
C37	.6750851970	.4641849070	-6.9102493800
C38	.5858675135	-.1536208728	-5.6615148154
C39	1.1840767085	.4108122076	-4.5255687966
C40	1.8781034276	1.6205046019	-4.6826823838
C41	1.9713009148	2.2429172106	-5.9273980265
H42	1.4430443288	2.1496726480	-8.0207433497
H43	.2037989284	.0035949829	-7.7754874573
H44	.0452173840	-1.0921061929	-5.5597107574
H45	2.3475675540	2.0726303648	-3.8121402014
H46	2.5170543540	3.1786330192	-6.0231508087

TS3
Gas phase Energy: -1013.09394429093 hartrees
Solvation Energy: -1013.13645621781 hartrees
Zero Point Energy: 198.187 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-540.36 cm^{-1})
Coordinates:

Os1	.0593937414	.1722629554	.0489361768
O2	-.2112214827	.2982190808	2.0911993169
O3	2.2295208548	.1713448674	.4347476732
C4	3.0438988377	.1285025326	-.5360337957
C5	2.7692094604	.0949289885	-1.9178957177
C6	1.5093146122	.1053690306	-2.5402302674
O7	.3482645994	.0845500155	-2.0131734044
H8	1.5121525891	.1142683721	-3.6420965069
H9	3.6312554069	.0943593533	-2.5814422222
H10	4.1157759814	.1161537472	-.2648637606
O11	.3048055936	2.1833492663	-.2003846530
C12	.2410126780	2.9914091902	.7908059028
C13	-.1693193652	1.4223222295	2.6984684233
C14	.0259464951	2.6962826753	2.1440142113
H15	.3749195420	4.0493130651	.5228268362
H16	-.3039179779	1.3647732986	3.7889326072
H17	.0190153955	3.5372773808	2.8333417107
C18	.0333936073	-2.2740569296	.1472218268
H19	1.0242692662	-1.9129360372	.4375172560
H20	-.2602099340	-2.9443474609	.9606495481
C21	.1189936834	-3.0423101719	-1.1770096805
H22	-.8639230220	-3.4695453979	-1.4229980197
H23	.3703144111	-2.3439870194	-1.9788340627
C24	-1.7002839157	-1.4200927436	.2593698343
C25	-1.9963772326	-.0665635339	-.2408060679
H26	-2.1043890963	-2.2632522045	-.3121469797

H27	-2.3283981242	-.0169992200	-1.2841577213
H28	-2.6442167020	.5271026864	.4167899933
H29	-1.8912895021	-1.5444015672	1.3253354052
C31	3.0596543949	-6.2203529448	-.9391961918
C32	3.4423710806	-4.9257719289	-1.3007233733
C33	2.4930336379	-3.9079150714	-1.3909601900
C34	1.1381730599	-4.1589894159	-1.1212637649
C35	.7691111233	-5.4627872845	-.7605238427
C36	1.7163623920	-6.4845685964	-.6682994658
H37	3.8003166175	-7.0134087966	-.8698652802
H38	4.4860784589	-4.7079206052	-1.5137257380
H39	2.7939792651	-2.8993588248	-1.6646442011
H40	-.2770174269	-5.6752441088	-.5497996216
H41	1.4041783677	-7.4876576928	-.3868801831

Ru.acac^{-}

A
Gas phase Energy: -937.38379311112 hartrees
Solvation Energy:-937.42510633720 hartrees
Zero Point Energy: 162.676 kcal/mol
Coordinates:

Ru1	-0.2940299594	0.0421907793	-0.1743133975
O2	-2.0029762151	-0.1511386578	-1.4112046477
O3	0.8993752733	0.2434026023	-1.9416864220
C4	2.1551811577	0.3548725623	-1.8589795332
C5	2.9770158782	0.3722173869	-0.7196868002
C6	2.5569384469	0.2609663143	0.6153579005
O7	1.3844253210	0.1453278686	1.0780940877
H8	3.3581644607	0.2763875730	1.3745003415
H9	4.0456655738	0.4724805868	-0.8887712996
H10	2.6841617365	0.4468868321	-2.8248840217
C11	-0.4328851296	2.1168188398	-0.2409558581
C12	-1.1374813490	2.7454235263	-1.2884403489
C13	-1.1868735775	4.1371157396	-1.4218282598
C14	-0.5285707811	4.9631430625	-0.5070757320
C15	0.1789943380	4.3685836679	0.5409485869
C16	0.2199080543	2.9764181620	0.6671097115
H17	0.7775955488	2.5421083214	1.4939604263
H18	0.7019181812	4.9925846067	1.2660695072
H19	-0.5657450066	6.0464538267	-0.6085724168
H20	-1.7455253317	4.5799849673	-2.2466753910
H21	-1.6628082719	2.1249847304	-2.0088499213
O22	0.1995697294	-2.1433300181	-0.5158120183
C23	-0.5249148030	-2.8435492888	-1.2650542876
C24	-2.3262216550	-1.2337187781	-1.9809484877
C25	-1.7059373277	-2.4924837018	-1.9520334550
H26	-0.2017314819	-3.8950604403	-1.4105993905
H27	-3.2414193902	-1.1745407059	-2.5977557837
H28	-2.1778581243	-3.2760358107	-2.5395322970
C29	-1.6304843963	0.5044368285	1.5083603244
C30	-1.3899717858	-0.8711975018	1.4661496864
H31	-1.1088625941	1.1340927581	2.2224610362

H32	-0.6585514657	-1.3238884942	2.1306349404
H33	-2.1245148524	-1.5527521225	1.0434832470
H34	-2.5545292494	0.9192978806	1.1159224713

B
Gas phase Energy: -937.36873819117 hartrees
Solvation Energy:-937.41140945350 hartrees
Zero Point Energy: 163.155 kcal/mol
Coordinates:

Ru1	-0.4173188572	0.1108664837	-0.3117723771
O2	-1.2242918994	0.2367078527	-2.2763615742
O3	1.4102350692	0.0668579878	-1.2494941981
C4	2.4995370441	-0.0071773719	-0.5997095777
C5	2.6978344098	-0.0795209619	0.7855896980
C6	1.6815261639	-0.0898244476	1.7574037072
O7	0.4298565614	-0.0210242991	1.5872306334
H8	2.0116447097	-0.1697072966	2.8080783728
H9	3.7241945273	-0.1425258612	1.1379292787
H10	3.4077830659	-0.0181816194	-1.2252527777
O11	-0.4302510981	-2.1703757049	-0.4417343272
C12	-0.8176102829	-2.7294294228	-1.4948165856
C13	-1.4555202712	-0.7886716582	-2.9860735744
C14	-1.3134340142	-2.1517752719	-2.6878189987
H15	-0.7741310658	-3.8403033332	-1.5107281171
H16	-1.8347055020	-0.5711449634	-4.0026036616
H17	-1.5878092526	-2.8450252003	-3.4801337024
C18	-0.4552994050	2.2095375201	-0.2048822882
H19	0.2032048357	2.5758464409	0.5974638669
H20	-0.1665790628	2.6918480766	-1.1482647766
C21	-1.9298298164	2.4541226197	0.1461483325
H22	-2.1330611632	3.3556729860	0.7514101321
H23	-2.5290942558	2.5396009905	-0.7691226214
C24	-3.2160674161	-1.0947004898	2.3221935737
C25	-3.3039642238	-1.0614541628	0.9419296322
C26	-2.8940187536	0.0810770517	0.2178601516
C27	-2.3708778985	1.2040603462	0.8999356995
C28	-2.3078763882	1.1490489875	2.3132541368
C29	-2.7195640160	0.0288533199	3.0117463590
H30	-3.5274412959	-1.9792764786	2.8724423386
H31	-3.6984088324	-1.9146077043	0.3964815265
H32	-3.1021092612	0.1470006862	-0.8436351661
H33	-1.9179696371	2.0111735219	2.8497382436
H34	-2.6556703194	0.0130246368	4.0977423089

D
Gas phase Energy: -1169.63219121691 hartrees
Solvation Energy:-1169.67249469628 hartrees
Zero Point Energy: 227.481 kcal/mol
Coordinates:

Ru1	-0.0587963590	0.0894154632	-0.1251543140
O2	-0.1214090669	-0.2876478700	2.1134565766
C3	0.9466302718	-0.4361406385	2.7543309902
C4	2.2800846106	-0.4338608358	2.2862579663
C5	2.7182010239	-0.2701773978	0.9661554481
O6	2.0559325170	-0.1002956097	-0.1018850845
H7	3.8146796719	-0.3033919310	0.8282645959

H8	3.0555537620	-0.5765589820	3.0350123406
H9	0.1538078288	1.7214432870	-2.2057765082
O10	-2.1412463474	0.2428979268	-0.1312402961
O11	0.2238535900	2.0716414176	0.3633948498
C12	-0.7635523475	2.8552535419	0.5111787819
C13	-2.7194004025	1.3440238101	0.1103230931
C14	-2.1365033323	2.5883854111	0.4021628158
H15	-0.4929001623	3.8927027868	0.7679487968
H16	-3.8219841804	1.3132895084	0.0916596464
H17	-2.8133475844	3.4205457132	0.5763064152
C18	-0.2531876689	-2.3195588335	-0.3040628027
H19	-0.9985864297	0.4568192688	-2.6401055079
C20	1.0758831588	-0.0492595192	-3.0271560953
H21	0.9139030887	-1.1365487294	-3.0384709090
H22	2.0474896983	0.1139953479	-2.5490429984
C23	-1.4088287833	-2.8469067192	0.2899124359
C24	-1.3828171497	-4.1210822662	0.8548244044
C25	-0.2117023945	-4.8854038720	0.8140881399
C26	0.9337302431	-4.3711004344	0.1989189654
C27	0.9116186659	-3.0961308979	-0.3669064181
H28	-2.3034126158	-2.2340437802	0.3199412858
H29	-2.2746225128	-4.5193811801	1.3337195392
H30	-0.1942536784	-5.8793573872	1.2540437500
H31	1.8458333950	-4.9633291816	0.1657786598
H32	1.7952502652	-2.6790373846	-0.8386667434
H33	0.8454785861	-0.5928723926	3.8486358248
H34	-0.3583865912	-1.4602232964	-1.0386126088
C35	-0.0161108025	0.6343796308	-2.1710385666
C36	1.1400924145	1.4103095202	-7.1186505779
C37	0.4082072867	0.2677730734	-6.7878287089
C38	0.4012262107	-0.2065905089	-5.4749868280
C39	1.1196243508	0.4412778721	-4.4575396471
C40	1.8486756982	1.5889994638	-4.8091559572
C41	1.8607234260	2.0694796043	-6.1189985189
H42	1.1501893308	1.7811924800	-8.1409586259
H43	-0.1562632354	-0.2577809219	-7.5553785815
H44	-0.1707233038	-1.0979524790	-5.2256452939
H45	2.4108524883	2.1073205434	-4.0355899775
H46	2.4374933123	2.9592827646	-6.3623948622

E
Gas phase Energy: -1169.64608757731 hartrees
Solvation Energy:-1169.68623298403 hartrees
Zero Point Energy: 227.481 kcal/mol
Coordinates:

Ru1	-.0988631021	-.0743439642	.0840747042
O2	.2009548904	.1395728626	2.0827690365
C3	1.3716107901	.1108967337	2.5777418534
C4	2.6061824226	-.0434145161	1.9304992537
C5	2.8048777080	-.1858365808	.5485950306
O6	1.9281075046	-.2225855617	-.3682418938
H7	3.8495787514	-.2695686637	.2074545686
H8	3.4929268167	-.0368101958	2.5582738774
H9	-.3300865718	.9176945130	-2.3242687348
O10	-2.1748150172	.1298407283	.4572551800
O11	.0583102242	2.1705734870	-.1950009956

C12	-.9486491902	2.9071352257	-.0228228795
C13	-2.7672827319	1.2466421645	.5107579234
C14	-2.2708239038	2.5444501332	.3033903120
H15	-.7859951719	3.9974768193	-.1508274926
H16	-3.8452320775	1.1874809526	.7486438492
H17	-2.9878367728	3.3558811506	.4017070084
C18	-.2403775365	-2.1086307385	.2954809122
H19	-1.3677082555	-.1896455082	-3.2307460125
C20	.7836527272	-.6150138166	-3.4117637363
H21	.6301422498	-1.6535237663	-3.7271024993
H22	1.6324301051	-.6080632063	-2.7207919383
C23	-1.2020182565	-2.6963099890	1.1508602036
C24	-1.3355478064	-4.0803797784	1.2881634901
C25	-.5070202183	-4.9507111759	.5720133633
C26	.4594601914	-4.4054303654	-.2765986575
C27	.5876709250	-3.0181082110	-.4044198302
H28	-1.8683100862	-2.0423353984	1.7079035174
H29	-2.0951336001	-4.4861182853	1.9568921671
H30	-.6118173624	-6.0293404551	.6749412333
H31	1.1202069149	-5.0637369684	-.8412813154
H32	1.3615953493	-2.6256580819	-1.0618601666
H33	1.4038795243	.2350110029	3.6711777641
H34	-.6319326473	-.7933946081	-1.7654690736
C35	-.4494151721	-.1214808948	-2.6364602332
C36	1.6541181126	1.8896450435	-6.8394969870
C37	1.0920640076	.6258409638	-7.0231983709
C38	.8174043661	-.1860000495	-5.9198624866
C39	1.0970643957	.2440002989	-4.6163437123
C40	1.6630476511	1.5176959632	-4.4466101009
C41	1.9385704418	2.3321384711	-5.5443007358
H42	1.8698645045	2.5239082326	-7.6956579440
H43	.8671184726	.2693060775	-8.0257973110
H44	.3804143261	-1.1710480224	-6.0692172672
H45	1.8839980203	1.8644544001	-3.4397275556
H46	2.3781265453	3.3142871293	-5.3889448233

G
Gas phase Energy: -1016.00841414685 hartrees
Solvation Energy:-1016.04902203370 hartrees
Zero Point Energy: 198.064 kcal/mol
Coordinates:

Ru1	-0.3094359941	0.0060583935	-0.3787873398
O2	-0.6529080522	-0.0237872640	-2.4680502431
O3	1.8058988203	-0.0210078007	-0.7853553227
C4	2.6366322829	-0.0583577239	0.1670016338
C5	2.4081660853	-0.0563497039	1.5526988722
C6	1.1582207761	-0.0298620827	2.1970524848
O7	0.0000777746	0.0037737212	1.6913402894
H8	1.1866470327	-0.0432675245	3.3008641940
H9	3.2858800077	-0.0876654358	2.1928287507
H10	3.7002375990	-0.0939456802	-0.1339748557
O11	0.0472130799	-2.2422007017	-0.4045567173
C12	-0.0065471103	-2.8708034518	-1.4902930851
C13	-0.5917629665	-1.0782022444	-3.1644213215
C14	-0.3116521125	-2.4004861644	-2.7849186045
H15	0.2110499634	-3.9578182079	-1.4356062821

H16	-0.7885864536	-0.9317607998	-4.2425318870
H17	-0.3090571001	-3.1396061500	-3.5823387300
C18	-0.0529957128	2.1185938561	-0.3672631960
H19	-0.6084899845	2.5991002037	0.4503028876
H20	1.0144513453	2.2543554031	-0.1413760808
C21	-0.3613333889	2.8516107065	-1.6882154296
H22	0.2104158067	2.3834528300	-2.4963990448
H23	-1.4193677116	2.7249720447	-1.9481701070
C24	0.5798093870	7.0851959221	-1.4326739976
C25	-0.7194514066	6.6350790431	-1.1882389924
C26	-1.0220469714	5.2759659491	-1.2861279425
C27	-0.0432847252	4.3294783822	-1.6278834421
C28	1.2575801334	4.8012621444	-1.8690775354
C29	1.5684751983	6.1578255737	-1.7738143077
H30	0.8190062820	8.1434251242	-1.3594032321
H31	-1.5006418077	7.3451978258	-0.9232502786
H32	-2.0366397394	4.9331454487	-1.0942420709
H33	2.0315516622	4.0846421282	-2.1321148027
H34	2.5851084063	6.4937299595	-1.9683722782
C35	-2.3446194349	0.6880401241	-0.0207786627
C36	-2.3211642634	-0.7123460623	-0.0616510174
H37	-2.3840710226	1.2069397095	0.9334093752
H38	-2.3206989277	-1.2903418176	0.8591728764
H39	-2.6524318294	-1.2499992526	-0.9475896578
H40	-2.7117320198	1.2551822253	-0.8723355479

TS1
Gas phase Energy: -937.33639447809 hartrees
Solvation Energy:-937.37910981114 hartrees
Zero Point Energy: 162.097 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-315.50 cm^{-1})
Coordinates:

Ru1	-0.0440491973	0.1639260172	0.0251532982
O2	-0.1198347570	0.1518995585	2.1245741474
O3	2.1899467081	-0.1847556371	0.0918676892
C4	2.8495901975	-0.1913646337	-0.9748518943
C5	2.4079182169	0.0028963723	-2.3041369823
C6	1.0937375114	0.2066837721	-2.7429394669
O7	0.0070865546	0.2480795473	-2.0887945581
H8	0.9784399622	0.3349734610	-3.8354008609
H9	3.1740514965	-0.0200285772	-3.0758026289
H10	3.9414053754	-0.3697357582	-0.8766542967
C11	-0.4127673402	-2.0629603462	-0.0408368905
C12	0.0251478489	-2.7397936333	1.1211829989
C13	0.6954708807	-3.9584807387	1.0458471455
C14	0.9285065502	-4.5676341862	-0.1918697149
C15	0.4740608985	-3.9323208855	-1.3539752261
C16	-0.1957951291	-2.7151727304	-1.2775434016
H17	-0.5480630224	-2.2326702525	-2.1844440705
H18	0.6445775466	-4.3914102704	-2.3263194696
H19	1.4473278491	-5.5218052582	-0.2503010282
H20	1.0445094592	-4.4354731941	1.9602177101
H21	-0.1374888092	-2.2657583590	2.0840247845
O22	0.5531868207	2.1693555289	-0.0408498702
C23	0.7082917087	2.8495522690	1.0147834805
C24	0.1603108694	1.1847663778	2.8043251290

C25	0.5449849109	2.4569756156	2.3550035868
H26	1.0133480787	3.8990775757	0.8549760215
H27	0.0883373620	1.0597081864	3.8990296331
H28	0.7377216770	3.2096506606	3.1152795308
C29	-1.9555397856	-1.1913238869	0.1028573734
C30	-2.0967904081	0.2879752906	-0.0197515014
H31	-2.4576756325	-1.7472130325	-0.6897144473
H32	-2.5090037859	0.6386855297	-0.9700150865
H33	-2.5626147620	0.7754821512	0.8423550656
H34	-2.2593799020	-1.5678910728	1.0796275411

TS2
Gas phase Energy: -1169.61866504600 hartrees
Solvation Energy:-1169.65812264499 hartrees
Zero Point Energy: 225.022 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -497.05 24.88 26.27 30.39 43.99 52.63
Coordinates:

Ru1	-0.0741997677	-0.0880180718	-0.1101423778
O2	-0.0169330345	0.0036643561	2.0704707159
C3	1.0806380898	-0.0511613400	2.6870776639
C4	2.3878632670	-0.1524624438	2.1754969112
C5	2.7563019195	-0.2135075633	0.8243014413
O6	2.0275578129	-0.2222708773	-0.2122829262
H7	3.8411322800	-0.2618335679	0.6267318955
H8	3.1962870487	-0.1721604076	2.9013238218
H9	0.1044812943	1.4515324863	-2.1560638574
O10	-2.1736465696	0.1353039066	0.0201083682
O11	0.1868811718	2.1261302802	0.1293577599
C12	-0.8139898308	2.8693495998	0.3031134535
C13	-2.7369525785	1.2501546771	0.2182693022
C14	-2.1797697952	2.5316059494	0.3531742873
H15	-0.5984939248	3.9489401910	0.4328969802
H16	-3.8381516282	1.2034954923	0.2908727565
H17	-2.8783410631	3.3482278959	0.5151827291
C18	-0.2000015262	-2.1591909201	0.1276998024
H19	-1.0748786349	0.2639682719	-2.7203581935
C20	0.9971579675	-0.2644887886	-3.1327741851
H21	0.7863478886	-1.3333179449	-3.2673136645
H22	1.9513364435	-0.1987157110	-2.6008803659
C23	-1.3220842018	-2.7295709921	0.7624061415
C24	-1.4001957661	-4.1004322837	1.0255233542
C25	-0.3591919863	-4.9563516907	0.6549487361
C26	0.7585537138	-4.4163617136	0.0138573588
C27	0.8308968565	-3.0447748041	-0.2463039349
H28	-2.1454034865	-2.0814896663	1.0478070206
H29	-2.2819126594	-4.5035577668	1.5230620595
H30	-0.4206758852	-6.0240737943	0.8559128407
H31	1.5793560403	-5.0665117387	-0.2879603704
H32	1.7094424191	-2.6451114107	-0.7456213116
H33	1.0112738645	-0.0064544585	3.7904369408
H34	-0.3881864138	-0.9969399751	-1.3295557520
C35	-0.0903378072	0.3779926966	-2.2480807695
C36	1.3011529227	1.6563898244	-7.0130918882
C37	0.5879211634	0.4647025987	-6.8721847116
C38	0.4997013573	-0.1573954207	-5.6251182129

C39	1.1175078380	0.3904778350	-4.4914558162
C40	1.8302487560	1.5897330254	-4.6511857372
C41	1.9224099198	2.2166555248	-5.8934956275
H42	1.3738119320	2.1424824830	-7.9829112826
H43	0.1009499070	0.0162110327	-7.7353319114
H44	-0.0561248545	-1.0870500163	-5.5231569712
H45	2.3154656385	2.0299471736	-3.7830993701
H46	2.4831054502	3.1437039766	-5.9897863771

TS3
Gas phase Energy: -1015.95393300453 hartrees
Solvation Energy:-1015.99634868038 hartrees
Zero Point Energy: 197.923 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -497.62 32.36 35.80 43.41 64.43 77.75
Coordinates:

Ru1	.0731904381	.1761348200	.0577121610
O2	-.2115668663	.2973330083	2.1261632285
O3	2.3026094570	.1378099149	.3861096050
C4	3.0834340411	.1130487250	-.5994334970
C5	2.7794635662	.0967194490	-1.9792928557
C6	1.5054427864	.0995027542	-2.5724684190
O7	.3576895824	.0747181260	-2.0363195839
H8	1.5022566630	.1055971195	-3.6780550782
H9	3.6266896518	.1051851456	-2.6613958208
H10	4.1685911552	.1013282614	-.3670860423
O11	.2851835192	2.2412911112	-.1523437335
C12	.1860451591	3.0183074096	.8423852215
C13	-.2065521613	1.4142802301	2.7277454916
C14	-.0363121743	2.7012544543	2.1944168265
H15	.2902275647	4.0930840632	.6102804470
H16	-.3602562410	1.3591414516	3.8197688849
H17	-.0767689009	3.5324824272	2.8940335741
C18	.0218239263	-2.2184855784	.1694907451
H19	1.0269383793	-1.8855121327	.4412062271
H20	-.3061713209	-2.8469067108	1.0017839858
C21	.0794819570	-3.0269402837	-1.1323303181
H22	-.9004865864	-3.4815849690	-1.3373102781
H23	.2925638400	-2.3469127682	-1.9613500669
C24	-1.7514692217	-1.3072014286	.1998133815
C25	-1.9928339053	.0589465897	-.2275034628
H26	-2.1145922396	-2.1098829155	-.4457228636
H27	-2.2848371156	.2108203918	-1.2693352586
H28	-2.5366708777	.6980417831	.4732636489
H29	-1.9717456920	-1.4989481963	1.2486377937
C31	3.0836418091	-6.1527710929	-.9446082345
C32	3.4299317587	-4.8589448610	-1.3445593931
C33	2.4610040082	-3.8582527152	-1.4151832644
C34	1.1216955758	-4.1248499710	-1.0863443114
C35	.7894985287	-5.4281105047	-.6878554055
C36	1.7563900882	-6.4330286336	-.6153677234
H37	3.8394131849	-6.9326130363	-.8911239653
H38	4.4605251308	-4.6279238920	-1.6040777598
H40	-.2438564325	-5.6543283760	-.4322387869
H41	1.4720409934	-7.4360324877	-.3043368201

Ir.acac

A
Gasphase Energy: -948.1427 hartrees
Solvation Energy: -948.1501 hartrees
Zero Point Energy: 165.12 kcal/mol
Coordinates:

Ir	-0.3047	0.0644	-0.1711
O	-1.9760	-0.1055	-1.3686
O	0.8108	0.2582	-1.9139
C	2.0791	0.3629	-1.8666
C	2.9197	0.3693	-0.7478
C	2.5138	0.2637	0.5854
O	1.3333	0.1622	1.0590
H	3.2980	0.2713	1.3513
H	3.9843	0.4601	-0.9315
H	2.5575	0.4549	-2.8494
C	-0.4410	2.1316	-0.2479
C	-1.1203	2.7369	-1.3158
C	-1.1444	4.1286	-1.4563
C	-0.4920	4.9463	-0.5317
C	0.1866	4.3564	0.5364
C	0.2089	2.9651	0.6764
H	0.7424	2.5297	1.5165
H	0.7012	4.9770	1.2664
H	-0.5119	6.0272	-0.6415
H	-1.6778	4.5717	-2.2941
H	-1.6343	2.1186	-2.0437
O	0.2174	-2.0612	-0.4638
C	-0.4674	-2.7763	-1.2484
C	-2.2715	-1.1930	-1.9734
C	-1.6331	-2.4336	-1.9600
H	-0.1039	-3.8067	-1.3829
H	-3.1746	-1.1120	-2.5908
H	-2.0779	-3.2113	-2.5716
C	-1.6217	0.5147	1.5474
C	-1.3989	-0.8606	1.4839
H	-1.0667	1.1293	2.2466
H	-0.6534	-1.3276	2.1196
H	-2.1426	-1.5235	1.0517
H	-2.5349	0.9487	1.1551

B
Gasphase Energy: -948.1389 hartrees
Solvation Energy: -948.1460 hartrees
Zero Point Energy: 165.73 kcal/mol
Coordinates:

Ir	-0.4681	0.0799	-0.3432
O	-1.2233	0.2652	-2.2540
O	1.3370	0.0482	-1.2606
C	2.4178	-0.0889	-0.5917
C	2.5865	-0.2162	0.7876
C	1.5543	-0.2206	1.7360

O	0.3032	-0.1017	1.5423
H	1.8382	-0.3380	2.7888
H	3.6006	-0.3268	1.1551
H	3.3173	-0.1042	-1.2176
O	-0.4067	-2.1427	-0.4870
C	-0.7128	-2.6998	-1.5750
C	-1.3747	-0.7502	-3.0205
C	-1.1711	-2.1069	-2.7725
H	-0.6155	-3.7980	-1.5950
H	-1.7300	-0.4851	-4.0247
H	-1.3755	-2.7803	-3.5987
C	-0.5143	2.1591	-0.2261
H	0.1628	2.5001	0.5661
H	-0.2078	2.5996	-1.1799
C	-1.9774	2.4801	0.1315
H	-2.1060	3.4110	0.6980
H	-2.5847	2.5527	-0.7775
C	-3.0319	-1.0548	2.4264
C	-3.1109	-1.0802	1.0472
C	-2.8040	0.0785	0.2841
C	-2.4195	1.2767	0.9441
C	-2.3608	1.2805	2.3537
C	-2.6705	0.1412	3.0788
H	-3.2613	-1.9428	3.0072
H	-3.4203	-1.9827	0.5297
H	-3.0964	0.1168	-0.7602
H	-2.0671	2.1925	2.8657
H	-2.6281	0.1673	4.1646

D
Gasphase Energy: -1180.3963 hartrees
Solvation Energy: -1180.4044 hartrees
Zero Point Energy: 230.15 kcal/mol
Coordinates:

Ir	0.4290	-0.9554	-0.0919
O	2.0753	-1.1388	1.4326
C	1.8901	-1.8411	2.4649
C	0.7097	-2.4795	2.8943
C	-0.5307	-2.4656	2.2550
O	-0.8925	-1.9151	1.1610
H	-1.3460	-3.0009	2.7590
H	0.7653	-3.0341	3.8254
H	2.7664	-1.9632	3.1228
O	1.7545	0.0102	-1.3241
C	-1.9698	1.2242	0.2898
C	-0.5675	1.2249	0.0167
H	-2.6667	1.3344	-0.5352
H	-0.2159	1.5464	-0.9564
C	-2.4279	1.1105	1.5812
C	0.3452	1.1286	1.0936
C	-1.5101	1.0148	2.6613
C	-0.1542	1.0295	2.4275
H	-1.8864	0.9468	3.6783
H	0.5498	0.9843	3.2520
H	-3.4951	1.1130	1.7837
H	1.3937	1.3534	0.9374

O	1.0290	-2.8239	-0.6229
C	1.9883	-2.9908	-1.4507
C	2.5859	-0.6427	-2.0332
C	2.7397	-2.0320	-2.1335
H	2.2300	-4.0441	-1.6325
H	3.2565	-0.0163	-2.6328
H	3.5141	-2.3961	-2.7993
C	-0.9020	-1.1198	-1.7136
H	-0.3189	-1.6034	-2.5090
H	-1.1947	-0.1395	-2.1036
C	-2.1600	-1.9600	-1.4352
H	-2.7344	-1.5096	-0.6196
H	-1.8578	-2.9529	-1.0851
C	-4.6238	-2.2936	-4.9908
C	-4.9135	-1.3299	-4.0219
C	-4.1257	-1.2332	-2.8727
C	-3.0359	-2.0917	-2.6652
C	-2.7591	-3.0556	-3.6472
C	-3.5423	-3.1581	-4.7980
H	-5.2368	-2.3738	-5.8843
H	-5.7563	-0.6564	-4.1580
H	-4.3629	-0.4858	-2.1178
H	-1.9221	-3.7355	-3.5005
H	-3.3117	-3.9159	-5.5429

E
Gasphase Energy: -1180.3945 hartrees
Solvation Energy: -1180.4037 hartrees
Zero Point Energy: 229.31 kcal/mol
Coordinates:

Ir	-1.2494	0.4656	0.0150
H	0.4426	1.2874	0.0786
O	-1.6510	0.3465	-2.1622
O	-0.5290	-1.4438	-0.0961
C	-0.4715	0.5760	4.8211
C	-1.5605	1.2481	4.2597
C	-1.7774	1.2154	2.8791
C	-0.9129	0.5099	2.0243
C	0.1752	-0.1653	2.6058
C	0.3963	-0.1314	3.9868
H	-0.3028	0.6020	5.8945
H	-2.2451	1.8025	4.8977
H	-2.6240	1.7494	2.4583
H	0.8563	-0.7337	1.9766
H	1.2470	-0.6625	4.4082
C	1.1888	1.0741	-0.7586
H	0.9529	0.2128	-1.3806
H	2.0728	0.8253	-0.1622
C	1.3680	2.3540	-1.5889
H	1.6089	3.1919	-0.9260
H	0.4196	2.5958	-2.0791
C	-3.4838	-1.2960	0.4067
O	-3.1513	-0.0611	0.3245
H	-4.5552	-1.4370	0.5805
C	-2.4936	2.9770	-0.9152
O	-1.9361	2.4089	0.0861

H -2.8618 3.9855 -0.6893
C -2.2640 1.2830 -2.7491
C -2.6838 2.5196 -2.2204
H -2.4863 1.1130 -3.8147
H -3.1931 3.1953 -2.8995
C -1.3055 -2.4415 0.0499
C -2.6852 -2.4326 0.2963
H -0.8110 -3.4153 -0.0377
H -3.1780 -3.3930 0.3953
C 4.4793 1.8006 -4.5491
C 4.7489 2.5091 -3.3765
C 3.7439 2.6964 -2.4241
C 2.4571 2.1827 -2.6295
C 2.1980 1.4716 -3.8112
C 3.1992 1.2816 -4.7640
H 5.2591 1.6555 -5.2913
H 5.7404 2.9184 -3.2023
H 3.9586 3.2516 -1.5136
H 1.2025 1.0670 -3.9818
H 2.9800 0.7317 -5.6753

G
Gasphase Energy: -1026.7664 hartrees
Solvation Energy: -1026.7741 hartrees
Zero Point Energy: 200.48 kcal/mol
Coordinates:
Ir -0.3207 0.0426 -0.3487
O -0.7691 0.0813 -2.3695
O 1.5942 -0.0786 -1.1230
C 2.6463 -0.2183 -0.4218
C 2.7559 -0.2528 0.9705
C 1.6759 -0.1366 1.8480
O 0.4364 0.0017 1.5850
H 1.8947 -0.1633 2.9223
H 3.7441 -0.3708 1.3996
H 3.5678 -0.3125 -1.0090
O -0.3127 -2.1951 -0.3153
C -0.4841 -2.8346 -1.3869
C -0.8234 -0.9936 -3.0656
C -0.7227 -2.3290 -2.6849
H -0.4430 -3.9329 -1.3029
H -0.9898 -0.7999 -4.1325
H -0.8260 -3.0613 -3.4788
C -0.2845 2.1318 -0.3341
H -1.3159 2.5098 -0.2960
H 0.1977 2.4448 0.6018
C 0.4272 2.7856 -1.5336
H 1.4771 2.4754 -1.5528
H -0.0228 2.4206 -2.4617
C 0.1454 7.1093 -1.3353
C -0.8035 6.3733 -2.0491
C -0.7023 4.9824 -2.1209
C 0.3441 4.2983 -1.4847
C 1.2891 5.0514 -0.7720
C 1.1939 6.4421 -0.6965
H 0.0712 8.1920 -1.2809

H	-1.6201	6.8826	-2.5546
H	-1.4411	4.4151	-2.6835
H	2.1107	4.5385	-0.2759
H	1.9404	7.0059	-0.1428
C	-2.0981	0.1444	0.9595
C	-2.5313	-0.0028	-0.3511
H	-2.0260	-0.7151	1.6171
H	-2.8185	-0.9779	-0.7323
H	-2.8627	0.8532	-0.9298
H	-2.0892	1.1166	1.4408

TS1
Gasphase Energy: -948.1027 hartrees
Solvation Energy: -948.1100 hartrees
Zero Point Energy: 164.56 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-349.24 cm^{-1})
Coordinates:

Ir	-0.0178	0.0607	0.0113
O	-0.0769	0.0341	2.0695
O	2.1444	-0.2063	0.1273
C	2.8384	-0.1812	-0.9262
C	2.4117	0.0002	-2.2584
C	1.1005	0.1530	-2.7022
O	0.0016	0.1494	-2.0436
H	0.9573	0.2804	-3.7826
H	3.1844	0.0149	-3.0198
H	3.9216	-0.3166	-0.7816
C	-0.3418	-2.1171	-0.0238
C	0.0654	-2.8130	1.1355
C	0.6210	-4.0880	1.0507
C	0.7694	-4.7107	-0.1923
C	0.3531	-4.0472	-1.3525
C	-0.2028	-2.7743	-1.2678
H	-0.5419	-2.2713	-2.1678
H	0.4571	-4.5268	-2.3221
H	1.1970	-5.7073	-0.2569
H	0.9410	-4.5960	1.9565
H	-0.0400	-2.3303	2.1011
O	0.4839	2.0707	-0.0869
C	0.6287	2.7643	0.9682
C	0.1753	1.0825	2.7529
C	0.5003	2.3652	2.3064
H	0.8869	3.8151	0.7841
H	0.1180	0.9300	3.8374
H	0.6716	3.1210	3.0650
C	-2.0210	-1.2514	0.1535
C	-2.0827	0.2008	-0.0340
H	-2.4824	-1.8653	-0.6136
H	-2.4469	0.5466	-1.0011
H	-2.4771	0.7723	0.8068
H	-2.2358	-1.6024	1.1585

TS2
TS3
Gasphase Energy: -1180.3436 hartrees
Solvation Energy: -1180.3817 hartrees

Zero Point Energy: 227.99 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-391.28 cm^{-1})
Coordinates:

Ir	0.0022	0.0555	0.0811
O	-0.1419	0.5413	2.1398
C	0.8930	0.5681	2.8748
C	2.2283	0.3272	2.5208
C	2.6951	-0.0050	1.2478
O	2.0433	-0.1826	0.1637
H	3.7764	-0.1420	1.1311
H	2.9705	0.4147	3.3070
H	0.4918	1.3119	-2.1024
O	-2.0364	0.3483	-0.0123
O	0.3958	2.2046	0.0017
C	-0.5647	3.0304	-0.0011
C	-2.5554	1.5154	-0.0191
C	-1.9455	2.7716	-0.0124
H	-0.2665	4.0893	-0.0042
H	-3.6517	1.4976	-0.0383
H	-2.6063	3.6320	-0.0210
C	-0.2743	-1.9146	0.7051
H	-0.7945	0.1796	-2.5747
C	1.2467	-0.5793	-2.8464
H	0.9188	-1.6249	-2.9146
H	2.1720	-0.5715	-2.2623
C	-1.4312	-2.2463	1.4237
C	-1.5936	-3.5308	1.9528
C	-0.6114	-4.5057	1.7620
C	0.5364	-4.1866	1.0330
C	0.7014	-2.9019	0.5050
H	-2.2040	-1.5005	1.5756
H	-2.4941	-3.7671	2.5155
H	-0.7412	-5.5039	2.1725
H	1.3073	-4.9365	0.8703
H	1.5988	-2.6683	-0.0608
H	0.6974	0.8222	3.9250
H	-0.2038	-1.0071	-1.0690
C	0.1930	0.2621	-2.1111
C	1.9316	1.0397	-6.8080
C	0.9801	0.0349	-6.6151
C	0.7682	-0.4938	-5.3399
C	1.5018	-0.0317	-4.2379
C	2.4544	0.9771	-4.4450
C	2.6690	1.5095	-5.7177
H	2.0999	1.4506	-7.8002
H	0.4048	-0.3405	-7.4579
H	0.0288	-1.2796	-5.1967
H	3.0346	1.3428	-3.5999
H	3.4153	2.2875	-5.8589

TS3
Gasphase Energy: -1026.7167 hartrees
Solvation Energy: -1026.7227 hartrees
Zero Point Energy: 200.37 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-447.79 cm^{-1})
Coordinates:

Ir	0.0601	0.0834	0.0255
O	-0.1953	0.1427	2.0566
O	2.2339	0.0325	0.3782
C	3.0283	0.0632	-0.6040
C	2.7243	0.1087	-1.9804
C	1.4552	0.0994	-2.5631
O	0.2999	0.0315	-2.0183
H	1.4182	0.1337	-3.6592
H	3.5664	0.1533	-2.6632
H	4.0996	0.0479	-0.3490
O	0.3434	2.0980	-0.1710
C	0.3155	2.8633	0.8477
C	-0.1136	1.2445	2.6947
C	0.1134	2.5296	2.1924
H	0.4736	3.9221	0.6106
H	-0.2476	1.1432	3.7781
H	0.1373	3.3420	2.9103
C	0.0142	-2.3075	0.1415
H	1.0142	-2.0010	0.4610
H	-0.3498	-2.9128	0.9719
C	0.1098	-3.1199	-1.1557
H	-0.8671	-3.5562	-1.4002
H	0.3734	-2.4577	-1.9839
C	-1.7720	-1.4319	0.1468
C	-1.9740	-0.0443	-0.2652
H	-2.1070	-2.2129	-0.5306
H	-2.2441	0.1205	-1.3086
H	-2.5412	0.5775	0.4295
H	-2.0095	-1.6339	1.1870
C	3.0324	-6.2985	-0.7686
C	3.4191	-5.0399	-1.2364
C	2.4755	-4.0197	-1.3693
C	1.1300	-4.2378	-1.0374
C	0.7545	-5.5057	-0.5701
C	1.6953	-6.5289	-0.4360
H	3.7657	-7.0939	-0.6681
H	4.4562	-4.8536	-1.5028
H	2.7796	-3.0422	-1.7373
H	-0.2867	-5.6942	-0.3160
H	1.3836	-7.5061	-0.0765

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A
Gas phase Energy: -952.93236665024 hartrees
Solvation Energy:-952.94785853476 hartrees
Zero Point Energy: 164.629 kcal/mol
Coordinates:

Rh1	-.2786677989	.0652540937	-.2002418372
O2	-1.9499999172	-.1073051037	-1.3971740905
O3	.8504689616	.2656390287	-1.9102504190
C4	2.1148975143	.3487981847	-1.8508492737
C5	2.9487687486	.3336037732	-.7242206474

C6	2.5207362019	.2362959317	.6018850330
O7	1.3344836480	.1593105236	1.0597693483
H8	3.2997382534	.2320541166	1.3756247403
H9	4.0166526727	.4056016802	-.8963772433
H10	2.6068574800	.4416487996	-2.8284235336
C11	-.4380559842	2.1165028951	-.2478734281
C12	-1.1716086321	2.7103728318	-1.2806215948
C13	-1.2240838703	4.1042650420	-1.3988415452
C14	-.5468242251	4.9200791321	-.4902721120
C15	.1867467502	4.3298970207	.5404165977
C16	.2400657067	2.9361544909	.6627384166
H17	.8132107349	2.4971629284	1.4733211817
H18	.7203445724	4.9499962909	1.2569769508
H19	-.5903611454	6.0017978485	-.5840406840
H20	-1.7991039398	4.5488562442	-2.2077322620
H21	-1.7037630400	2.0896526599	-1.9921164803
O22	.1751059453	-2.1065088197	-.4299458451
C23	-.5104940168	-2.8170658343	-1.2082230677
C24	-2.2632203605	-1.1996378549	-1.9831498189
C25	-1.6615436373	-2.4558202531	-1.9430774318
H26	-.1772149445	-3.8621416396	-1.3267928587
H27	-3.1599315357	-1.1120340582	-2.6122773140
H28	-2.1208054601	-3.2308987171	-2.5473687419
C29	-1.6755861407	.5134398670	1.5534579120
C30	-1.4333424276	-.8377063046	1.5122130470
H31	-1.1099712311	1.1606157460	2.2122710021
H32	-.6540247665	-1.2857035018	2.1189311632
H33	-2.1226588238	-1.5175142043	1.0228192999
H34	-2.5584445455	.9411948292	1.0922180929

B
Gas phase Energy: -952.94661274204 hartrees
Solvation Energy:-952.96159912555 hartrees
Zero Point Energy: 165.518 kcal/mol
Coordinates:

Rh1	-.4101124059	.0092321677	-.3799369596
O2	-1.2267176929	.2558727548	-2.2553952448
O3	1.3905545194	.1206504924	-1.2717291972
C4	2.4656651824	.0171024105	-.5947275133
C5	2.6340470288	-.1617874025	.7793702188
C6	1.5911313943	-.2675002320	1.7123285749
O7	.3425777223	-.2113302454	1.5056613438
H8	1.8752914136	-.4152345068	2.7629359411
H9	3.6494656351	-.2306275818	1.1525669493
H10	3.3736036210	.0814013869	-1.2074581288
O11	-.3679014870	-2.2258350441	-.6263800239
C12	-.6914629829	-2.7346396110	-1.7270268265
C13	-1.3896140899	-.7234249208	-3.0643033826
C14	-1.1727342394	-2.0876208636	-2.8916737935
H15	-.5990052763	-3.8330891391	-1.8044786927
H16	-1.7747061009	-.4158178941	-4.0469198179
H17	-1.3950649282	-2.7217448721	-3.7439391636
C18	-.4852111999	2.0582689247	-.1819179290
H19	.1690042126	2.3326822636	.6512176486
H20	-.1229485461	2.4910477529	-1.1172608985
C21	-1.9520793568	2.3942637557	.1146845738

H22	-2.0664226582	3.3647764928	.6153754353
H23	-2.5227994695	2.4309045317	-.8192336372
C24	-3.1446402582	-.9641688117	2.5828502430
C25	-3.1647180729	-1.0727328857	1.1989708402
C26	-2.8376339517	.0385341807	.3954063259
C27	-2.4720029857	1.2690126937	.9888646196
C28	-2.4668205063	1.3610647763	2.3896561902
C29	-2.8084002756	.2634969700	3.1740751070
H30	-3.3969418920	-1.8175825997	3.2049579067
H31	-3.4426067721	-2.0084453479	.7236425091
H32	-3.0003474245	-.0088881488	-.6772544321
H33	-2.1860460718	2.3000084553	2.8597425315
H34	-2.8079441002	.3568528170	4.2570379805

D
Gas phase Energy: -1185.20142950506 hartrees
Solvation Energy:-1185.21814627527 hartrees
Zero Point Energy: 229.617 kcal/mol
Coordinates:

Rh1	.4681487304	-1.0665515310	-.1164846325
O2	2.1082168100	-1.1763882648	1.4489559339
C3	1.9310039333	-1.8690033641	2.4822571728
C4	.7514066342	-2.5194220036	2.9109065917
C5	-.4837493739	-2.5175668239	2.2646873844
O6	-.8455652428	-1.9924029804	1.1581696166
H7	-1.2986874720	-3.0458724042	2.7803289818
H8	.8035430992	-3.0602759382	3.8504352923
H9	2.8008165425	-1.9766075644	3.1553866966
O10	1.7598320061	-.0651998024	-1.3561258014
C11	-1.9141902567	1.3475492261	.3345508059
C12	-.5153141574	1.3568153608	.1394546475
H13	-2.5744161855	1.4656860973	-.5193719895
H14	-.1009467667	1.5768876748	-.8376681673
C15	-2.4375734215	1.1991610437	1.6098362941
C16	.3425788731	1.2222697669	1.2444575795
C17	-1.5762555633	1.0665553879	2.7155501746
C18	-.2001605658	1.0768839454	2.5375674211
H19	-1.9939884418	.9573150286	3.7125635065
H20	.4650398428	.9765833692	3.3890322872
H21	-3.5134507109	1.1913629470	1.7595848972
H22	1.4153919251	1.3004156612	1.1128017778
O23	1.0687215469	-2.9000380423	-.6798346337
C24	2.0149391221	-3.0488225313	-1.5210816874
C25	2.5872431380	-.6945048411	-2.0824565711
C26	2.7543902564	-2.0819408888	-2.2059990917
H27	2.2601213751	-4.0997796299	-1.7188266949
H28	3.2474694496	-.0571157502	-2.6854685192
H29	3.5222384282	-2.4337738606	-2.8855622367
C30	-.8769313651	-1.1705428485	-1.6992826736
H31	-.2866627221	-1.5918038002	-2.5207254394
H32	-1.1658750531	-.1548554686	-1.9833922865
C33	-2.1084213629	-2.0370950994	-1.4252679827
H34	-2.6761835369	-1.6231153675	-.5868468964
H35	-1.7855841130	-3.0371733189	-1.1175996534
C36	-4.6222677465	-2.2938623137	-4.9533443896
C37	-4.9139855428	-1.3692497894	-3.9478113086

C38	-4.1077206080	-1.2940562613	-2.8097131661
C39	-2.9984754053	-2.1373180255	-2.6507924822
C40	-2.7179154728	-3.0608965517	-3.6698690703
C41	-3.5197884602	-3.1411145582	-4.8095411731
H42	-5.2500698122	-2.3575964113	-5.8379153223
H43	-5.7727518306	-.7101021121	-4.0464039956
H44	-4.3460740445	-.5783778944	-2.0254420235
H45	-1.8656633529	-3.7284019356	-3.5602573966
H46	-3.2878697426	-3.8685632876	-5.5833074616

E
Gas phase Energy: -1185.20029235114 hartrees
Solvation Energy: -1185.20887524631 hartrees
Zero Point Energy: 229.352 kcal/mol
Coordinates:

Rh1	-1.2273763551	0.4618077629	0.0414617639
H2	0.5638657802	1.3724061119	0.2136089341
O3	-1.4540471850	0.4245627629	-2.1788017542
O4	-0.4865013671	-1.4395666924	-0.0630757639
C5	-0.6390374409	0.5328251906	4.8295017437
C6	-1.7182863334	1.1956413979	4.2417719619
C7	-1.8974457415	1.1664246287	2.8557614872
C8	-0.9932518775	0.4704679513	2.0463676050
C9	0.0843565426	-0.2015505180	2.6367230817
C10	0.2612578095	-0.1647706347	4.0241523634
H11	-0.5020319080	0.5586409672	5.9073312115
H12	-2.4246306867	1.7417018031	4.8628184879
H13	-2.7318153298	1.6939892328	2.4053149261
H14	0.7854453795	-0.7602221105	2.0229541760
H15	1.1037816625	-0.6868511822	4.4719576605
C16	1.3261415341	1.1854436201	-0.5842261788
H17	1.0924807480	0.3029848538	-1.1804476084
H18	2.2313067453	0.9633954858	-0.0087784985
C19	1.4730222817	2.4383238475	-1.4617148572
H20	1.8015501441	3.2832305848	-0.8466727890
H21	0.4916746038	2.7050779678	-1.8680678811
C22	-3.4514192425	-1.3178900349	0.3078220536
O23	-3.1273225781	-0.0826754640	0.2601836713
H24	-4.5295609501	-1.4711556045	0.4337919826
C25	-2.3816458802	3.0009909988	-0.8932219344
O26	-1.8775371017	2.4064567933	0.1208541528
H27	-2.7613049075	4.0054923293	-0.6610552797
C28	-2.0454886754	1.3686584929	-2.7657350074
C29	-2.5078269214	2.5845777362	-2.2170526095
H30	-2.2117254103	1.2412107875	-3.8494575341
H31	-2.9863185229	3.2797742834	-2.8988056761
C32	-1.2562776383	-2.4423679321	0.0320183666
C33	-2.6466407609	-2.4512174871	0.2152952949
H34	-0.7542455940	-3.4153222955	-0.0453248322
H35	-3.1373402847	-3.4155651517	0.2782707785
C36	4.2475616428	1.7261259454	-4.7063806516
C37	4.6104663670	2.5633106158	-3.6518074723
C38	3.7158944477	2.8016107709	-2.6061212353
C39	2.4479094041	2.2103455420	-2.5991237847
C40	2.0941329365	1.3693091829	-3.6651108659
C41	2.9847230029	1.1289241568	-4.7096799203

H42	4.9421122542	1.5398779661	-5.5209668912
H43	5.5904923067	3.0329773280	-3.6413722395
H44	4.0050507090	3.4565879167	-1.7870556229
H45	1.1122504523	0.9004399556	-3.6701437415
H46	2.6929842774	0.4766253287	-5.5286973814

G
Gas phase Energy: -1031.56339202470 hartrees
Solvation Energy:-1031.57109839059 hartrees
Zero Point Energy: 200.381 kcal/mol
Coordinates:

Rh1	-0.2758222456	0.0209788146	-0.3884326531
O2	-0.6638902750	0.0016870109	-2.4107712114
O3	1.7388616456	-0.0032840162	-0.8428427400
C4	2.6087350681	-0.0496939950	0.0813555634
C5	2.4239045522	-0.0415058634	1.4699485311
C6	1.1918887620	0.0078072684	2.1316824083
O7	0.0206798940	0.0529103876	1.6393813895
H8	1.2186197254	0.0097893098	3.2293064323
H9	3.3141149653	-0.0792633139	2.0873227821
H10	3.6464975414	-0.0943226393	-0.2759953608
O11	-0.0247230633	-2.2178123779	-0.3627839805
C12	-0.0705722764	-2.8612170141	-1.4414247355
C13	-0.6118292213	-1.0660277325	-3.1112307373
C14	-0.3534248245	-2.3840114563	-2.7410123993
H15	0.1255909090	-3.9448921930	-1.3670965743
H16	-0.8121605225	-0.8940803780	-4.1781304976
H17	-0.3600255517	-3.1182571365	-3.5394799616
C18	-0.0596444996	2.1124666266	-0.3786351914
H19	-0.7018665078	2.5460628676	0.3907615980
H20	0.9772598625	2.2245893813	-0.0505207569
C21	-0.2669299685	2.7968780458	-1.7300024605
H22	0.3953179056	2.3448922557	-2.4738617056
H23	-1.2892271556	2.6389838292	-2.0893098793
C24	0.5323538587	7.0402696945	-1.3466352412
C25	-0.7729563362	6.5584954552	-1.2323745883
C26	-1.0296371826	5.1934491091	-1.3679168532
C27	0.0071694299	4.2852893058	-1.6217413705
C28	1.3129392725	4.7834739079	-1.7351489623
C29	1.5756053582	6.1467668897	-1.5994312558
H30	0.7345141070	8.1025680450	-1.2436941297
H31	-1.5926056303	7.2460213099	-1.0415772486
H32	-2.0497002201	4.8254998189	-1.2827524618
H33	2.1283479514	4.0928277334	-1.9379274458
H34	2.5943906789	6.5125668791	-1.6955201558
C35	-2.4127899399	0.6752147584	-0.0078552890
C36	-2.3601289381	-0.6978807590	0.0084147067
H37	-2.3801804924	1.2353868307	0.9193081942
H38	-2.2562945135	-1.2414360836	0.9409079952
H39	-2.6105533278	-1.2813236913	-0.8709920866
H40	-2.7125967856	1.2128320945	-0.9001357763

TS1
Gas phase Energy: -952.90836509180 hartrees iterations: 12
Solvation Energy:-952.92392418039 hartrees
Zero Point Energy: 164.197 kcal/mol

Number and Magnitude of negative Eigen values: 1 (-343.59 cm^{-1})
Coordinates:

Rh1	0.0180001475	0.0840926737	0.0102881860
O2	-0.0233801274	0.0506392538	2.0715650134
O3	2.1766037876	-0.1732012406	0.0638623250
C4	2.8417534437	-0.1248985278	-1.0020365027
C5	2.3800709207	0.0708296818	-2.3235415747
C6	1.0548987101	0.2052498964	-2.7256548077
O7	-0.0238705476	0.1770602168	-2.0380776632
H8	0.8818312429	0.3389645088	-3.8024309496
H9	3.1314815968	0.1048565919	-3.1052467633
H10	3.9314751943	-0.2523555174	-0.8918642686
C11	-0.2682422379	-2.0721662488	-0.0250224069
C12	0.0821236307	-2.7557277330	1.1536008254
C13	0.5870721148	-4.0552210474	1.0984682916
C14	0.7385121320	-4.7022298862	-0.1313877349
C15	0.3791417226	-4.0391418895	-1.3089829166
C16	-0.1262696520	-2.7405319849	-1.2558333034
H17	-0.4191961454	-2.2376541685	-2.1714037731
H18	0.4866120280	-4.5353997290	-2.2699350515
H19	1.1268443309	-5.7161791614	-0.1718075750
H20	0.8631874374	-4.5623867313	2.0191992078
H21	-0.0247821492	-2.2550380704	2.1092637901
O22	0.4193024849	2.1466636792	-0.0544365152
C23	0.5307195975	2.8302738878	1.0019909267
C24	0.1761822564	1.1026511528	2.7629976585
C25	0.4293823728	2.4077175078	2.3396081249
H26	0.7317664833	3.9002660811	0.8418809605
H27	0.1313561479	0.9371497282	3.8481732701
H28	0.5625667317	3.1596684907	3.1094833678
C29	-2.0248206420	-1.1393069582	0.0862891177
C30	-2.0504961064	0.2950364785	0.0048949216
H31	-2.3964566216	-1.6957823619	-0.7661293696
H32	-2.3379063519	0.7480255990	-0.9403535296
H33	-2.3363785073	0.8504794055	0.8948363214
H34	-2.2669194860	-1.5861797657	1.0443710530

TS2
Gas phase Energy: -1185.16579760783 hartrees
Solvation Energy:-1185.18144257048 hartrees
Zero Point Energy: 226.564 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1233.63 cm^{-1})
Coordinates:

Rh1	0.0047530146	0.0165633548	0.0217502562
O2	0.0060309915	0.0115297462	2.1414656552
C3	1.0877215558	0.0118085761	2.7907652351
C4	2.4081336212	0.0002183257	2.3003842125
C5	2.7801712674	-0.0538469421	0.9592119793
O6	2.0524416661	-0.1092534429	-0.0895322965
H7	3.8576889383	-0.0653280152	0.7470175425
H8	3.2082774481	0.0225284880	3.0320591268
H9	-0.1165210766	1.1950905441	-2.1500960372
O10	-2.0445354260	0.1964549374	0.0951589158
O11	0.2843157275	2.1295498440	0.2147909746
C12	-0.6964060698	2.9097018559	0.3663305104
C13	-2.6184295797	1.3211344402	0.2792095643

C14	-2.0675983878	2.5950892056	0.4145559023
H15	-0.4394519742	3.9760999560	0.4654182177
H16	-3.7136741594	1.2528766655	0.3255274114
H17	-2.7605532285	3.4173075379	0.5554523890
C18	-0.1940245152	-2.0967870817	-0.2386550011
H19	-1.0858722339	-0.2060407243	-2.6171271425
C20	1.0663904032	-0.3950964123	-3.0548843445
H21	1.0400323327	-1.4890049960	-3.1245240296
H22	1.9964951087	-0.1303348232	-2.5441925268
C23	-1.4324205337	-2.6985261299	0.0365393678
C24	-1.5286421093	-4.0870525046	0.1497899057
C25	-0.3970153985	-4.8894752831	-0.0244049081
C26	0.8345193875	-4.2986260250	-0.3175300774
C27	0.9362236742	-2.9094521761	-0.4268404919
H28	-2.3100161753	-2.0760477781	0.1687481896
H29	-2.4898399553	-4.5423222469	0.3734940212
H30	-0.4768489296	-5.9697989598	0.0600456500
H31	1.7167604376	-4.9162903218	-0.4629776012
H32	1.8908963958	-2.4516735563	-0.6620484650
H33	0.9759675098	0.0228351617	3.8857198943
H34	-0.2030285287	-1.0449405168	-1.2386245545
C35	-0.1164765562	0.1067989374	-2.2149462844
C36	0.9842798536	1.3350041277	-7.0283649485
C37	0.3224498461	0.1314426495	-6.7724754095
C38	0.3559830766	-0.4283788248	-5.4937205996
C39	1.0497602815	0.2010670763	-4.4502006320
C40	1.7098742366	1.4090642364	-4.7199602095
C41	1.6790188228	1.9723699985	-5.9970664363
H42	0.9625487413	1.7701641259	-8.0236188822
H43	-0.2160960863	-0.3743368807	-7.5695129929
H44	-0.1559338261	-1.3691782807	-5.3025252628
H45	2.2574086150	1.9057588072	-3.9218868437
H46	2.2019376493	2.9057482986	-6.1881126849

TS3
Gas phase Energy: -1031.52765552698 hartrees
Solvation Energy:-1031.53594935788 hartrees
Zero Point Energy: 200.154 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-404.90 cm^{-1})
Coordinates:

Rh1	.0622705529	.1597597124	.0203716156
O2	-.2000857925	.1696453394	2.0493218612
O3	2.2490000883	.0727124382	.3339220768
C4	3.0262818320	.1504741077	-.6528557168
C5	2.7019006671	.2389141888	-2.0248984869
C6	1.4238793259	.2204347661	-2.5827529285
O7	.2791366139	.1265571931	-2.0236055610
H8	1.3720869600	.2733014232	-3.6789910255
H9	3.5315839593	.3145083085	-2.7197471979
H10	4.1043771686	.1386043741	-.4198919554
O11	.3103206364	2.2133260591	-.1115896878
C12	.2761706171	2.9372112700	.9270545567
C13	-.1304685107	1.2516732012	2.7170079978
C14	.0819385400	2.5557276628	2.2639212193
H15	.4178102624	4.0107445095	.7387204796
H16	-.2664159459	1.1188703908	3.7984040660

H17	.0962877102	3.3419062487	3.0101794522
C18	.0152859655	-2.1912919064	.1203341458
H19	1.0196128219	-1.8849420622	.4191504269
H20	-.3859023340	-2.7414790079	.9697100993
C21	.0827631407	-3.0328546433	-1.1556732568
H22	-.8858911336	-3.5083130926	-1.3521782600
H23	.2984760066	-2.3842792696	-2.0088044818
C24	-1.8319135193	-1.2553430856	.0066082415
C25	-1.9764216087	.1504087780	-.2617781027
H26	-2.0805318922	-1.9490607124	-.7888649874
H27	-2.1798780251	.4601040265	-1.2841801149
H28	-2.4424272641	.7648944587	.5060335678
H29	-2.1267749636	-1.5830149537	.9977507742
C31	3.1273509516	-6.0898208738	-.7659839427
C32	3.4507795315	-4.8385464758	-1.2949151627
C33	2.4673381652	-3.8582801118	-1.4302197533
C34	1.1447207462	-4.1106420492	-1.0397051043
C35	.8324493861	-5.3703715470	-.5111408883
C36	1.8135068954	-6.3535002390	-.3746025800
H37	3.8921716358	-6.8542450284	-.6629475309
H38	4.4697516675	-4.6266806233	-1.6069117520
H39	2.7230997758	-2.8860310811	-1.8447698065
H40	-.1907360690	-5.5843173587	-.2097860810
H41	1.5511486615	-7.3256952088	.0335200296

Pt.acac.+

A
Gas phase Energy: -962.30771073878 hartrees
Solvation Energy:-962.39183988631 hartrees
Zero Point Energy: 165.252 kcal/mol
Coordinates:

Pt1	-.2869602560	.0729130729	-.1954427771
O2	-1.9430623705	-.0918573905	-1.3765886346
O3	.8153514316	.2641703728	-1.9162026499
C4	2.0915003475	.3367422271	-1.8631069651
C5	2.9306902576	.3111678514	-.7467105004
C6	2.5142010866	.2260749741	.5788673499
O7	1.3217748904	.1662848743	1.0534790856
H8	3.2804687430	.2166373087	1.3595985731
H9	3.9970327305	.3697554385	-.9272855476
H10	2.5540871431	.4272929046	-2.8509469841
C11	-.4499170241	2.1638211544	-.2474510752
C12	-1.1774116516	2.7276446934	-1.2910667164
C13	-1.2186757923	4.1238983990	-1.4005640239
C14	-.5472612829	4.9292304581	-.4794965234
C15	.1739916598	4.3409920906	.5605252669
C16	.2268622996	2.9470957519	.6862420186
H17	.7876167732	2.5039765136	1.5012959972
H18	.6993612246	4.9573912870	1.2840292122
H19	-.5867482241	6.0100999124	-.5707597672
H20	-1.7811243705	4.5719874097	-2.2142707348
H21	-1.7005286601	2.1110067364	-2.0109091636

O22	.1788657142	-2.0889563194	-.3951496070
C23	-.4877576640	-2.8055194340	-1.1948970365
C24	-2.2316410941	-1.1976436483	-1.9868613624
C25	-1.6219701681	-2.4399584665	-1.9530410363
H26	-.1403390453	-3.8423583060	-1.2952858593
H27	-3.1192154346	-1.0869278681	-2.6171172065
H28	-2.0663447466	-3.2104837187	-2.5722013533
C29	-1.6974952828	.5307631001	1.5911477735
C30	-1.4509060805	-.8275988122	1.5553994595
H31	-1.1246324350	1.1800432226	2.2424932299
H32	-.6673222852	-1.2683216907	2.1634923673
H33	-2.1468532672	-1.5074190501	1.0744868150
H34	-2.5802474086	.9532061039	1.1230949607

B
Gas phase Energy: -962.33650559780 hartrees
Solvation Energy:-962.41773222938 hartrees
Zero Point Energy: 166.440 kcal/mol
Coordinates:

Pt1	-.4880897435	.0343774842	-.3709053781
O2	-1.2516961457	.2866616513	-2.2405198722
O3	1.3684060512	.1072590015	-1.2701923503
C4	2.4280577127	-.0504677904	-.5728707485
C5	2.5578604915	-.2522377279	.8029754091
C6	1.5080184472	-.2997889321	1.7199876581
O7	.2484710626	-.1778634806	1.5197595554
H8	1.7604305042	-.4526125200	2.7739152121
H9	3.5611431577	-.3719498603	1.1932660558
H10	3.3434361156	-.0112712578	-1.1729856362
O11	-.4073509615	-2.1705062003	-.5799023044
C12	-.6586339313	-2.6946700947	-1.7010544247
C13	-1.3388140678	-.7080734326	-3.0664977239
C14	-1.0830572499	-2.0567094970	-2.8898545092
H15	-.5411281051	-3.7860134943	-1.7488017497
H16	-1.6890525040	-.3846465239	-4.0514235535
H17	-1.2429626158	-2.6920565092	-3.7533009934
C18	-.5392033524	2.1262510801	-.2015495558
H19	.1752870606	2.3711695196	.5860367117
H20	-.2122687141	2.4981938423	-1.1728475604
C21	-1.9728289484	2.5264626812	.1732453937
H22	-1.9995635216	3.4913554769	.6889601075
H23	-2.5945167555	2.6015832666	-.7249641328
C24	-2.9188836775	-.9424822858	2.5886924309
C25	-2.8746336748	-1.0443686680	1.2137950639
C26	-2.6135292194	.1147554479	.4095749655
C27	-2.4516694852	1.4000750378	1.0515849255
C28	-2.5128582820	1.4765147365	2.4386665931
C29	-2.7580538904	.3222220381	3.1910937695
H30	-3.1023791157	-1.8162726828	3.2044337245
H31	-3.0362838392	-1.9981300829	.7225538074
H32	-3.0124462419	.1150824622	-.6049539443
H33	-2.3645977145	2.4289541897	2.9380649657
H34	-2.8161340179	.4018378121	4.2735095115

D
Gas phase Energy: -1194.58998385532 hartrees

Solvation Energy:-1194.67073876680 hartrees
Zero Point Energy: 230.201 kcal/mol
Coordinates:

Pt1	.3357548072	-1.0310662708	-.1344317036
O2	1.9372125483	-1.0804583759	1.4553470755
C3	1.7643908124	-1.7783180698	2.4906828945
C4	.5975913603	-2.4739554500	2.8850316362
C5	-.6110158278	-2.5157426322	2.2117864040
O6	-.9804699936	-1.9919761534	1.0879176721
H7	-1.4288115325	-3.0704111105	2.6830242969
H8	.6441430923	-3.0175134830	3.8218368138
H9	2.6224997496	-1.8401677059	3.1757257787
O10	1.6483747466	-.0510891408	-1.3559996215
C11	-1.7410257369	.8966053539	.8107229203
C12	-.4127522744	1.1055713504	.3167612961
H13	-2.5290912913	.6307938544	.1139572808
H14	-.2887363794	1.3932001460	-.7251401886
C15	-2.0165885512	1.0259562722	2.1614154117
C16	.5996948653	1.5318686241	1.2363828641
C17	-.9920392370	1.4154742940	3.0414487233
C18	.3127981172	1.6614768185	2.5865269666
H19	-1.2168736128	1.5331175526	4.0980735886
H20	1.0841464144	1.9687237763	3.2845574856
H21	-3.0189188372	.8508490564	2.5375818517
H22	1.5950696776	1.7371291658	.8573978118
O23	.9902550382	-2.9126345993	-.6390613823
C24	1.9795710611	-3.0531473769	-1.4381749634
C25	2.5268832579	-.7006387610	-2.0236966590
C26	2.7282857713	-2.0798965115	-2.1021109847
H27	2.2440057289	-4.1029311492	-1.6038770608
H28	3.1893744928	-.0539673819	-2.6072480353
H29	3.5336947114	-2.4259349942	-2.7384290537
C30	-1.0030001134	-1.1506655559	-1.7731719806
H31	-.3437795990	-1.4215448221	-2.6017775188
H32	-1.3862178951	-.1429882698	-1.9493115011
C33	-2.1205819400	-2.1695752080	-1.5830357978
H34	-2.7465300610	-1.8998791872	-.7283466470
H35	-1.6952775286	-3.1543380923	-1.3689654470
C36	-4.4649641011	-2.2534659495	-5.2222424878
C37	-4.8244953343	-1.3992858009	-4.1763274602
C38	-4.0703906756	-1.3775017286	-3.0024063774
C39	-2.9529898905	-2.2121122945	-2.8538524430
C40	-2.5985072992	-3.0621669960	-3.9118815871
C41	-3.3506764338	-3.0861811257	-5.0870517084
H42	-5.0533116517	-2.2745813080	-6.1346183080
H43	-5.6948043725	-.7566637342	-4.2720760832
H44	-4.3638040053	-.7204739705	-2.1860189224
H45	-1.7395572367	-3.7215385527	-3.8063927888
H46	-3.0722937590	-3.7583868927	-5.8933729123

E
Gas phase Energy: -1194.56804198211 hartrees
Solvation Energy: -1194.60716131044 hartrees
Zero Point Energy: 229.180 kcal/mol
Coordinates:

Pt1	-1.2913585839	0.4419432309	0.0097632501

H2	0.3727518780	1.1657507835	-0.1545745487
O3	-1.7760031163	0.2230036233	-2.1394181579
O4	-0.5540941045	-1.4568771400	-0.0660061592
C5	-0.3134459729	0.7341554258	4.7281072428
C6	-1.4286738861	1.3851429034	4.1991786063
C7	-1.7132255447	1.3068551321	2.8320357599
C8	-0.8615908172	0.5688438401	2.0141987844
C9	0.2545869818	-0.0945017392	2.5217637520
C10	0.5256415576	-0.0017586194	3.8916805306
H11	-0.1009864628	0.7975193096	5.7907250610
H12	-2.0858079789	1.9595939166	4.8455836323
H13	-2.5770484456	1.8195567604	2.4246449199
H14	0.9037831450	-0.6842099845	1.8828713417
H15	1.3937625849	-0.5135166223	4.2968887523
C16	1.1483989166	1.0206109587	-1.0189195074
H17	0.8198505781	0.2831405652	-1.7480680022
H18	1.9907949305	0.6239571211	-0.4440402331
C19	1.3882963765	2.4058539469	-1.6266852515
H20	1.6399179399	3.1258701112	-0.8429834301
H21	0.4802971156	2.7554978519	-2.1271099335
C22	-3.4974860088	-1.3344803817	0.5286870607
O23	-3.1883131016	-0.0890139077	0.4333467353
H24	-4.5599372207	-1.4718987058	0.7526232510
C25	-2.5523741031	2.8923402159	-0.9663121976
O26	-1.9397521887	2.3669257791	0.0469671729
H27	-2.8992605931	3.9054008385	-0.7414136182
C28	-2.4165786685	1.1331126214	-2.7378702936
C29	-2.8091402535	2.3918608180	-2.2310965295
H30	-2.6862453225	0.9167717503	-3.7808261011
H31	-3.3532898453	3.0436611624	-2.9048957290
C32	-1.3292720237	-2.4576025829	0.1027120907
C33	-2.6994779791	-2.4616184098	0.3847756094
H34	-0.8216325192	-3.4222641490	0.0075703762
H35	-3.1801163116	-3.4254677591	0.5000555973
C36	4.6354430501	1.8774311064	-4.4208723469
C37	4.9005385455	2.2899773359	-3.1132641367
C38	3.8526971757	2.4712274978	-2.2125958006
C39	2.5260782834	2.2540732235	-2.6138446408
C40	2.2706393477	1.8316942919	-3.9279638629
C41	3.3178924594	1.6504612419	-4.8278207986
H42	5.4522916574	1.7353670842	-5.1220296987
H43	5.9229520842	2.4727187403	-2.7967065388
H44	4.0623322620	2.7981000838	-1.1968179617
H45	1.2457815859	1.6594229776	-4.2499250889
H46	3.1089880397	1.3364638622	-5.8461969556

G
Gas phase Energy: -1040.94267344265 hartrees
Solvation Energy:-1040.98463899261 hartrees
Zero Point Energy: 201.258 kcal/mol
Coordinates:

Pt1	-0.3444729186	0.0375020479	-0.3622940728
O2	-1.2222395857	0.0818759638	-2.1913504065
O3	1.4677199625	-0.0328830533	-1.3257529586
C4	2.5508567033	-0.1604714149	-0.6548919933
C5	2.7345934170	-0.1819876584	0.7285474627

C6	1.7256053311	-0.0703381389	1.6842242890
O7	0.4609793431	0.0540460567	1.5113589334
H8	2.0130114540	-0.0829074958	2.7396508100
H9	3.7494328603	-0.2888960547	1.0912983695
H10	3.4378531420	-0.2477561763	-1.2901820083
O11	-0.0838395963	-2.2168757736	-0.4256678561
C12	-0.3768886481	-2.8233281683	-1.4919870707
C13	-1.3106053837	-0.9839556049	-2.9250380140
C14	-0.9521115233	-2.2957692025	-2.6732436518
H15	-0.1679016061	-3.9022633581	-1.4950127065
H16	-1.7601235120	-0.7619955945	-3.8973732820
H17	-1.1373292896	-3.0003565714	-3.4755480053
C18	-0.3134518672	2.2034194286	-0.4708296763
H19	-1.2604223339	2.4361851243	-0.9556065756
H20	-0.3143598684	2.5257510854	0.5711177761
C21	0.8556980072	2.7774398096	-1.2579634888
H22	1.8069996195	2.5756705116	-0.7593888083
H23	0.8962296561	2.3480478602	-2.2616354737
C24	0.1089264682	7.0344748121	-1.4181417869
C25	-0.3842232540	6.1987752743	-2.4234052160
C26	-0.1388966894	4.8273296481	-2.3741934160
C27	0.6124554893	4.2769854155	-1.3256145881
C28	1.0962575759	5.1224996155	-0.3167730044
C29	0.8505123362	6.4942520240	-0.3650291820
H30	-0.0799903974	8.1026029119	-1.4579314151
H31	-0.9542667604	6.6160246864	-3.2479684581
H32	-0.5153080828	4.1809806971	-3.1638844378
H33	1.6804564028	4.7068549808	0.5015184025
H34	1.2412479592	7.1410686995	0.4146868939
C35	-2.2546237853	-0.7530789567	0.6125278432
C36	-2.3425620052	0.6233938393	0.6357497112
H37	-2.7354175474	-1.3279775846	-0.1721567424
H38	-2.9051288129	1.1501555349	-0.1270450588
H39	-2.0465849903	1.1794416954	1.5186915947
H40	-1.8640260845	-1.3042197620	1.4615852288

TS1
Gas phase Energy: -962.29614733085 hartrees
Solvation Energy:-962.33735029457 hartrees
Zero Point Energy: 164.924 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-226.57 cm^{-1})

Pt1	-.0000012873	.0125071215	-.0069931899
O2	-.0848936878	-.0058030698	2.0353330542
O3	2.1149898078	-.1136083939	.1533817784
C4	2.8402051404	-.0201241821	-.8837484289
C5	2.4418044831	.1456179475	-2.2215021024
C6	1.1360337887	.1933758593	-2.6851208611
O7	.0224101851	.0962478075	-2.0416518016
H8	.9822915476	.3141555191	-3.7615373194
H9	3.2273988560	.2295984734	-2.9623786918
H10	3.9169064929	-.0800364713	-.6854008507
C11	-.1968117685	-2.0778703461	-.0179747438
C12	.1418831033	-2.7872429661	1.1508227026
C13	.3893477508	-4.1560157804	1.0773083733
C14	.2933718759	-4.8256477145	-.1470777629
C15	-.0558134580	-4.1260684853	-1.3075241485

C16	-.3067107784	-2.7582566036	-1.2487418742
H17	-.5874383873	-2.2186364654	-2.1458140272
H18	-.1352261159	-4.6467683172	-2.2564007243
H19	.4861274849	-5.8928303228	-.1967086829
H20	.6637950425	-4.6995340807	1.9756522314
H21	.2284876159	-2.2657507917	2.0961972935
O22	.2505938046	2.1422639307	-.0900161743
C23	.3953220066	2.8185924828	.9705631497
C24	.1374853932	1.0664168577	2.7225442972
C25	.3650766685	2.3666290261	2.3046197394
H26	.5554277185	3.8919544375	.8113953643
H27	.1210328915	.8743680268	3.7993131928
H28	.5186613827	3.1076240668	3.0797675375
C29	-2.2781389786	-1.2432583120	.2558523034
C30	-2.1412077839	.1296119391	-.0794980537
H31	-2.6345722588	-1.9689392878	-.4633679964
H32	-2.3961530103	.4350210426	-1.0910258703
H33	-2.3654322766	.8520799396	.7029088827
H34	-2.3124944276	-1.5385582255	1.2985854370

TS2
Gas phase Energy: -1194.54285426943 hartrees
Solvation Energy:-1194.61993044776 hartrees
Zero Point Energy: 226.559 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1255.35 cm^{-1})
Coordinates:

Pt1	0.0511599230	0.2112760458	0.2661030579
O2	-0.1504797415	0.5741262888	2.3422488606
C3	0.8768323397	0.6386647438	3.0855632233
C4	2.2289608087	0.4965928485	2.7288657459
C5	2.7119024992	0.2080119579	1.4612821750
O6	2.0760558009	-0.0023937697	0.3587548457
H7	3.7954598691	0.1220300990	1.3362344709
H8	2.9623317059	0.6132113899	3.5178029694
H9	0.3699519563	1.0132374683	-2.0749865815
O10	-1.9678287541	0.4804044994	0.1217979397
O11	0.4444684557	2.3200174993	0.1616052772
C12	-0.5053784071	3.1605888089	0.1617513081
C13	-2.4909883502	1.6607721747	0.1446866900
C14	-1.8895190008	2.9094503325	0.1758087927
H15	-0.1877505567	4.2102555760	0.1351914258
H16	-3.5841613518	1.6236523327	0.1203396691
H17	-2.5489779538	3.7691196783	0.1807869204
C18	-0.2442555812	-1.9025690206	0.2643670072
H19	-0.8394045305	-0.2487951128	-2.4249266641
C20	1.2901122647	-0.8671031938	-2.6823124286
H21	1.0760896188	-1.9391877386	-2.6351129298
H22	2.2223841326	-0.6855660546	-2.1407421834
C23	-1.5445248588	-2.3950717284	0.4538655135
C24	-1.7239895440	-3.7572383372	0.6976918767
C25	-0.6222348126	-4.6174127136	0.7476396382
C26	0.6687919200	-4.1215720022	0.5451352869
C27	0.8666873011	-2.7609081242	0.3041535707
H28	-2.3964167220	-1.7273960885	0.4191305538
H29	-2.7266914510	-4.1435780055	0.8516707666
H30	-0.7709034089	-5.6755752914	0.9398556694

H31	1.5240472185	-4.7894894212	0.5744775251
H32	1.8657087320	-2.3771665802	0.1366048598
H33	0.6535091431	0.8342066240	4.1411293128
H34	-0.0845706943	-1.0250728912	-0.9445390688
C35	0.1632264546	-0.0557372730	-2.0345549452
C36	1.6016425187	0.4576768181	-6.7850738059
C37	0.7350171232	-0.5865053518	-6.4513602172
C38	0.6378535021	-1.0174948765	-5.1275604110
C39	1.4116647282	-0.4133609688	-4.1261046102
C40	2.2752978790	0.6379002525	-4.4682859856
C41	2.3729280061	1.0682384472	-5.7917087630
H42	1.6798242990	0.7909691736	-7.8154825849
H43	0.1397309714	-1.0682269873	-7.2211888317
H44	-0.0303199219	-1.8373056894	-4.8731717676
H45	2.8843451041	1.1081238774	-3.6992607802
H46	3.0546319558	1.8734018276	-6.0488757253

TS3
Gas phase Energy: -1040.90490683252 hartrees
Solvation Energy:-1040.94672158429 hartrees
Zero Point Energy: 200.834 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-352.81 cm^{-1})
Coordinates:

Pt1	.0584509981	.1491053302	.0093835093
O2	-.2155101147	.1451284928	2.0254974270
O3	2.2238334918	.0466631536	.3711037218
C4	3.0259844605	.1525591791	-.6010722958
C5	2.7208510255	.2850822229	-1.9735089631
C6	1.4607659826	.2546757551	-2.5476367911
O7	.2918797835	.1240959807	-2.0081666255
H8	1.3979939302	.3250758429	-3.6374072239
H9	3.5582717606	.3884989099	-2.6533991661
H10	4.0905641928	.1248754734	-.3343301984
O11	.3411056652	2.1915018058	-.1300753658
C12	.3554472324	2.9063646513	.9288026395
C13	-.0826178998	1.2262704786	2.7052654679
C14	.1800457816	2.5195755215	2.2606969825
H15	.5284720920	3.9681832946	.7243840813
H16	-.2117156062	1.0696156914	3.7801976383
H17	.2420646116	3.2966086981	3.0125899642
C18	-.0424838929	-2.2813127601	.0753505840
H19	.9514401051	-1.9442626640	.3846079766
H20	-.4303284073	-2.8252873777	.9344646160
C21	.0344697029	-3.0839343761	-1.2195285563
H22	-.9269123844	-3.5666390686	-1.4261090417
H23	.2549570036	-2.4246199614	-2.0622656297
C24	-1.8723896534	-1.3653170700	.0366416133
C25	-1.9873259002	.0417967525	-.3018209664
H26	-2.1623618019	-2.0857144205	-.7199247514
H27	-2.1782122584	.2972769769	-1.3416526919
H28	-2.4831328076	.6830773705	.4244280455
H29	-2.1417942490	-1.6234449673	1.0549154283
C31	3.1169516331	-6.0725001752	-.7157698663
C32	3.4240724843	-4.8458304138	-1.3088545184
C33	2.4292489836	-3.8836960367	-1.4793681440
C34	1.1148656298	-4.1385958994	-1.0639452215

C35	.8164352879	-5.3723576594	-.4686805330
C36	1.8111134748	-6.3350249095	-.2976367889
H37	3.8905767305	-6.8229070250	-.5866564113
H38	4.4358538403	-4.6431438864	-1.6462306583
H39	2.6694768209	-2.9349764361	-1.9535438946
H40	-.2018394218	-5.5875923884	-.1531409104
H41	1.5656637903	-7.2903988450	.1553621855

Pd.acac+

A
Gas phase Energy: -969.85101092989 hartrees
Solvation Energy:-969.89244982499 hartrees
Zero Point Energy: 164.249 kcal/mol
Coordinates:

Pd1	-0.2642090078	0.0769972187	-0.2227750626
O2	-1.9204178548	-0.0947475112	-1.3890294371
O3	0.8395194709	0.3021775513	-1.9245425580
C4	2.1116723276	0.3415150409	-1.8679680160
C5	2.9534377978	0.2792906226	-0.7539375775
C6	2.5221599696	0.1997755270	0.5677279790
O7	1.3301541692	0.1684395133	1.0323634371
H8	3.2879995854	0.1719874464	1.3509707222
H9	4.0208379034	0.3129574929	-0.9311942351
H10	2.5809929025	0.4402678435	-2.8540368065
C11	-0.4511826430	2.1700061905	-0.2464354669
C12	-1.2014420595	2.7064910571	-1.2785990996
C13	-1.2546631306	4.1048344801	-1.3758883119
C14	-0.5747147123	4.9086218734	-0.4606560896
C15	0.1692398700	4.3243223016	0.5644102998
C16	0.2409732053	2.9291976126	0.6858108271
H17	0.8178917760	2.4829088957	1.4858139301
H18	0.7008758021	4.9409311004	1.2829231529
H19	-0.6240926725	5.9893009033	-0.5464289632
H20	-1.8325833183	4.5508791239	-2.1796707704
H21	-1.7276263797	2.0840821726	-1.9899362922
O22	0.1658761058	-2.0924165677	-0.3827947022
C23	-0.4941422928	-2.8156100293	-1.1730433926
C24	-2.2156020441	-1.2024023782	-1.9889317205
C25	-1.6242897957	-2.4506930690	-1.9443779460
H26	-0.1577744693	-3.8586926534	-1.2621606834
H27	-3.0998518938	-1.0887382550	-2.6263012672
H28	-2.0737028994	-3.2221150551	-2.5580166876
C29	-1.7454874457	0.5412173908	1.6093400926
C30	-1.4870181695	-0.8037850383	1.5710534424
H31	-1.1714532646	1.2002870572	2.2496315464
H32	-0.6871510409	-1.2404025697	2.1603072075
H33	-2.1524958036	-1.4871349477	1.0539643586
H34	-2.6121396093	0.9624682074	1.1112944314

B
Gas phase Energy: -969.88853692673 hartrees
Solvation Energy:-969.92924760320 hartrees
Zero Point Energy: 165.848 kcal/mol
Coordinates:

Pd1	-0.4939493366	0.0175342126	-0.3724341066
O2	-1.2672664436	0.2829843364	-2.2275756542
O3	1.3595657712	0.1485559369	-1.2477365380
C4	2.4134091315	-0.0260653117	-0.5532221768
C5	2.5446347012	-0.2664416357	0.8163476162
C6	1.4849208352	-0.3231022822	1.7232893014
O7	0.2328756875	-0.1885479588	1.5164552447
H8	1.7345183759	-0.4936629963	2.7768898155
H9	3.5456640728	-0.3964858063	1.2076825083
H10	3.3341374064	0.0357319013	-1.1464649658
O11	-0.4459484762	-2.1861287746	-0.5935771848
C12	-0.6696771248	-2.6990406031	-1.7193399622
C13	-1.3230152764	-0.6980451485	-3.0710294365
C14	-1.0629698202	-2.0455274323	-2.9156129648
H15	-0.5594406036	-3.7919244683	-1.7819066272
H16	-1.6506574451	-0.3599325976	-4.0605035625
H17	-1.1987546936	-2.6676640898	-3.7922704622
C18	-0.5512348105	2.1245537985	-0.2266552435
H19	0.1625127416	2.3177730059	0.5726147677
H20	-0.1970778060	2.4054251688	-1.2164672333
C21	-1.9866148896	2.4837314769	0.1156289337
H22	-2.0321831765	3.4553800568	0.6205440547
H23	-2.5988864421	2.5392893691	-0.7886486098
C24	-2.9031896302	-0.9501478335	2.5877274687
C25	-2.9264050370	-1.0615654179	1.2114953392
C26	-2.6870954428	0.0847642119	0.4009750837
C27	-2.4484227217	1.3594256022	1.0147797250
C28	-2.4407586635	1.4484780500	2.4045119994
C29	-2.6782667281	0.3094373757	3.1776784095
H30	-3.0788987386	-1.8170499863	3.2150992878
H31	-3.1310652443	-2.0135543915	0.7343384979
H32	-3.0023955353	0.0629641667	-0.6391682288
H33	-2.2445152217	2.4011916250	2.8865471115
H34	-2.6825908788	0.3961437188	4.2604424748

D
Gas phase Energy: -1202.14467306384 hartrees
Solvation Energy:-1202.18355606793 hartrees
Zero Point Energy: 229.668 kcal/mol
Coordinates:

Pd1	0.4305695123	-1.0317706747	-0.1475253741
O2	2.1328830681	-1.0732080508	1.3638553092
C3	2.0128584661	-1.7734677189	2.3973321861
C4	0.8558098849	-2.4591863558	2.8526170923
C5	-0.3920068565	-2.4500177404	2.2612611958
O6	-0.8241836580	-1.8941294813	1.1759940728
H7	-1.1926135068	-2.9899645258	2.7802120984
H8	0.9462889979	-3.0165985135	3.7776544254
H9	2.9019015000	-1.8535635854	3.0426958729
O10	1.6607557412	-0.0815859860	-1.4636958484
C11	-1.8079764549	1.1123448042	0.3832227403
C12	-0.3963799303	1.2207480111	0.2547982879
H13	-2.4279395840	1.1044996279	-0.5072189057
H14	0.0360555929	1.5053801953	-0.6995867633
C15	-2.3906148353	1.0463550133	1.6367504649
C16	0.4002317889	1.3253924096	1.4269522056

C17	-1.5823082480	1.1174813669	2.7859251517
C18	-0.1956580178	1.2540621348	2.6848006827
H19	-2.0465185856	1.0767045482	3.7670001012
H20	0.4123229062	1.3254401532	3.5801618572
H21	-3.4675267480	0.9622733708	1.7382375057
H22	1.4709266583	1.4648286699	1.3308503151
O23	1.0550691926	-2.9171350984	-0.6628489032
C24	2.0331757567	-3.0656672829	-1.4685514139
C25	2.5367857176	-0.7283491024	-2.1263006905
C26	2.7658797247	-2.1064825209	-2.1693439062
H27	2.3051800406	-4.1175560779	-1.6200114854
H28	3.1767704424	-0.0903995061	-2.7465931891
H29	3.5667005944	-2.4591552662	-2.8069908308
C30	-0.9838830539	-1.2381308352	-1.7543652725
H31	-0.3308872669	-1.6894522258	-2.5005102808
H32	-1.2113525983	-0.2046096299	-2.0089788490
C33	-2.1715184238	-2.0866554249	-1.3770761701
H34	-2.7301157217	-1.6482176731	-0.5483021019
H35	-1.8536289960	-3.0876489344	-1.0780459929
C36	-4.5363200418	-2.1757607052	-4.9986863785
C37	-4.7912828815	-1.2106598299	-4.0205124633
C38	-4.0300339022	-1.1835981199	-2.8537299728
C39	-3.0158541174	-2.1307416243	-2.6427976533
C40	-2.7608967879	-3.0897793405	-3.6356906138
C41	-3.5212185482	-3.1161085927	-4.8033437050
H42	-5.1293538069	-2.1973263808	-5.9076062786
H43	-5.5857262777	-0.4850615141	-4.1651170978
H44	-4.2406543798	-0.4403106755	-2.0882476865
H45	-1.9790217693	-3.8293041422	-3.4806599073
H46	-3.3264132897	-3.8715544118	-5.5581519058

E
Gas phase Energy: -1202.12185764263 hartrees
Solvation Energy: -1202.16028385060 hartrees
Zero Point Energy: 228.105 kcal/mol
Coordinates:

Pd1	-1.3562617678	0.4415783313	0.0236916871
H2	0.3494904046	1.3176430351	-0.2274674718
O3	-1.7944308670	0.2988913194	-2.1387268312
O4	-0.5738772062	-1.4335991438	-0.1005155358
C5	-0.2550205985	0.7383690694	4.6813798085
C6	-1.4078786393	1.3573187292	4.1958149543
C7	-1.7494269000	1.2629791875	2.8397658768
C8	-0.8961522559	0.5428893049	2.0219357916
C9	0.2517246541	-0.1009025246	2.4590604434
C10	0.5705956225	0.0158184248	3.8202379292
H11	-0.0022916641	0.8156647922	5.7341791749
H12	-2.0531529293	1.9217052950	4.8627330103
H13	-2.6369151163	1.7504756959	2.4550270319
H14	0.8837293048	-0.6785176842	1.7947266202
H15	1.4668473291	-0.4713807373	4.1934262664
C16	1.1588955122	1.1364842236	-1.0074049455
H17	0.8497482861	0.3622367318	-1.7087119137
H18	2.0051907545	0.7732338758	-0.4165432449
C19	1.4319548103	2.4810006975	-1.7059641577
H20	1.6751223966	3.2465645296	-0.9635323460

H21	0.5352356019	2.8070357873	-2.2419596593
C22	-3.4967990755	-1.4141503812	0.5495991517
O23	-3.2227405690	-0.1642372661	0.5033489099
H24	-4.5503070433	-1.5947323693	0.7969543269
C25	-2.6418555982	2.8944538955	-0.8918428053
O26	-2.0140441538	2.3534673087	0.1004962900
H27	-3.0342657176	3.8834768966	-0.6280255148
C28	-2.4402581494	1.2072416567	-2.7213801211
C29	-2.8754939054	2.4417125235	-2.1776340466
H30	-2.6849000654	1.0281647547	-3.7793522936
H31	-3.4340455374	3.1017521874	-2.8310901111
C32	-1.3142918795	-2.4583435708	0.0367908786
C33	-2.6804491932	-2.5192844947	0.3384650651
H34	-0.7847685732	-3.4084639979	-0.1024750932
H35	-3.1337087709	-3.4992644660	0.4204817036
C36	4.7275400205	1.7704567867	-4.3983458626
C37	4.9701683555	2.2597275334	-3.1115342142
C38	3.9067733744	2.4981925181	-2.2450539215
C39	2.5837820547	2.2649138120	-2.6578640128
C40	2.3529335656	1.7632990422	-3.9510253564
C41	3.4153213544	1.5248450947	-4.8173435009
H42	5.5569614275	1.5817553991	-5.0733880894
H43	5.9876175657	2.4564157608	-2.7875327811
H44	4.0975645282	2.8824226643	-1.2459326016
H45	1.3334528463	1.5745023219	-4.2800755841
H46	3.2254686735	1.1516059433	-5.8193116094

G
Gas phase Energy: -1048.48894797611 hartrees iterations: 14
Solvation Energy:-1048.53028330986 hartrees
Zero Point Energy: 199.566 kcal/mol
Coordinates:

Pd1	-0.2365360077	0.0663016178	-0.3622691878
O2	-0.9004711685	0.1540757770	-2.2795289877
O3	1.6177916980	-0.0754056026	-1.1950116880
C4	2.6476678434	-0.3244385624	-0.4837460830
C5	2.7629663878	-0.4277480231	0.9015609381
C6	1.7124210176	-0.2191522257	1.7959989347
O7	0.4888751327	0.0518137095	1.5559333664
H8	1.9404107833	-0.2739323024	2.8668712340
H9	3.7397961765	-0.6488816144	1.3121392559
H10	3.5572553643	-0.4519879796	-1.0827979612
O11	-0.3607902535	-2.1978821779	-0.3330205198
C12	-0.5801265176	-2.8093221627	-1.4055258152
C13	-0.9940879067	-0.9177833209	-3.0033788942
C14	-0.8704266530	-2.2541767844	-2.6835467742
H15	-0.5567844363	-3.9091356545	-1.3578519569
H16	-1.2290125191	-0.6723385177	-4.0453920158
H17	-1.0175780816	-2.9555063325	-3.4965965371
C18	-0.1647633876	2.2185475834	-0.4094242687
H19	-1.2210016948	2.4302534312	-0.5726700923
H20	0.1489458822	2.4333108845	0.6123961784
C21	0.7266190319	2.7644559029	-1.4951502786
H22	1.7789687131	2.5568914780	-1.2953624756
H23	0.4641361693	2.3398411373	-2.4659274566
C24	-0.0893429562	7.0101965217	-1.3643656112

C25	-0.8214131324	6.1833033195	-2.2215204494
C26	-0.5589307012	4.8156885302	-2.2638024328
C27	0.4516243360	4.2623813755	-1.4614440357
C28	1.1719923298	5.0975443408	-0.5933250996
C29	0.9082086198	6.4656276422	-0.5516553584
H30	-0.2938168287	8.0757937217	-1.3327780169
H31	-1.5910018316	6.6058967249	-2.8599442885
H32	-1.1214357167	4.1753002291	-2.9388925891
H33	1.9556582975	4.6774419298	0.0325096145
H34	1.4820838825	7.1068694525	0.1099515888
C35	-2.1975779976	0.1914618949	1.0851415430
C36	-2.6913810470	0.0193163421	-0.1702935148
H37	-1.9669715933	-0.6584651313	1.7183790498
H38	-2.8743380715	-0.9732968375	-0.5680032715
H39	-3.0024233113	0.8579942911	-0.7839847205
H40	-2.1079841179	1.1764776803	1.5322966376

TS1
Gas phase Energy: -969.84532125825 hartrees
Solvation Energy:-969.88674477418 hartrees
Zero Point Energy: 164.031 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-214.22 cm^{-1})
Coordinates:

Pd1	-.0105104804	.0094497070	-.0041023207
O2	-.1020099719	-.0015283219	2.0327585170
O3	2.0934621970	-.1758256354	.1332425004
C4	2.8102776023	-.0632722655	-.9014557203
C5	2.4076051970	.1444789283	-2.2349003567
C6	1.0962242478	.2023096783	-2.6801275324
O7	-.0087051652	.0918273146	-2.0303562323
H8	.9343898234	.3441113448	-3.7547383532
H9	3.1875894730	.2412949065	-2.9797889410
H10	3.8900238511	-.1464221037	-.7184904666
C11	-.2242250396	-2.0963829255	-.0200245676
C12	.1133737863	-2.7631527035	1.1625183819
C13	.4210967143	-4.1233062500	1.0941807069
C14	.3786106697	-4.7980750117	-.1296058273
C15	.0251286948	-4.1171661900	-1.2991775630
C16	-.2868025465	-2.7581651025	-1.2539410133
H17	-.5730274005	-2.2315819940	-2.1560685701
H18	-.0150126490	-4.6416178699	-2.2488707767
H19	.6178753823	-5.8559059253	-.1722018763
H20	.6988115547	-4.6506196603	2.0013716507
H21	.1569777632	-2.2335201476	2.1057622070
O22	.2329837080	2.1401857146	-.0781388494
C23	.4017668131	2.8134078637	.9751124723
C24	.1448577165	1.0613775260	2.7203768808
C25	.3880426179	2.3611643408	2.3122558895
H26	.5672210920	3.8883500435	.8200715458
H27	.1371922981	.8657034775	3.7985632451
H28	.5600725215	3.0966332825	3.0884550977
C29	-2.3016450756	-1.1677177295	.2080147790
C30	-2.1713533444	.2056689509	-.0537603112
H31	-2.6249881093	-1.8514620975	-.5659114573
H32	-2.3540875347	.5787980885	-1.0570438670
H33	-2.2992867334	.9084498011	.7640423161

H34	-2.3722105785	-1.5196059319	1.2308202007

TS2
Gas phase Energy: -1202.09790211630 hartrees
Solvation Energy:-1202.13543983512 hartrees
Zero Point Energy: 225.962 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -1212.06 27.26 30.87 33.10 45.80 52.69
Coordinates:

Pd1	0.0622705847	0.2373040508	0.2802126878
O2	-0.1714964726	0.4785388569	2.3805374617
C3	0.8446583299	0.5353734301	3.1278660124
C4	2.2060381036	0.4351196443	2.7776311800
C5	2.6959296619	0.1912767668	1.5044438205
O6	2.0727074986	0.0048961988	0.3944764979
H7	3.7836567051	0.1227430097	1.3890232367
H8	2.9320926666	0.5376302007	3.5746289352
H9	0.3722174482	0.9120112933	-2.0376806953
O10	-1.9391165074	0.5194646169	0.0638119461
O11	0.4570964575	2.3512717415	0.1845938297
C12	-0.4856792854	3.1901151611	0.2127649291
C13	-2.4655997518	1.6931669535	0.1354912395
C14	-1.8738193216	2.9418076296	0.2259333651
H15	-0.1742100110	4.2439619703	0.2095945785
H16	-3.5602208812	1.6568209495	0.0985305735
H17	-2.5346512653	3.7991819429	0.2621630498
C18	-0.2350186250	-1.8899505496	0.1563532325
H19	-0.7989571463	-0.3606848333	-2.4932474383
C20	1.3575374582	-0.9234827093	-2.7079381156
H21	1.1887436842	-2.0026942006	-2.6614669368
H22	2.2803847965	-0.6945754433	-2.1696464793
C23	-1.5435478681	-2.3470637772	0.3413597895
C24	-1.7359062153	-3.6913108291	0.6643324450
C25	-0.6406005346	-4.5493310100	0.7994413171
C26	0.6590219241	-4.0746614040	0.6034751671
C27	0.8751367232	-2.7335973630	0.2812577538
H28	-2.3854920028	-1.6737040756	0.2450636815
H29	-2.7446049241	-4.0626496777	0.8152959265
H30	-0.8008921549	-5.5918694701	1.0557748790
H31	1.5084840521	-4.7431668288	0.7013511120
H32	1.8787702452	-2.3605207744	0.1219992054
H33	0.6196850871	0.6807088373	4.1934421186
H34	-0.0523826881	-1.0280802005	-0.9991103938
C35	0.1938367896	-0.1616406164	-2.0816856970
C36	1.5255123210	0.4481142277	-6.7985156410
C37	0.7490062751	-0.6650064830	-6.4663245841
C38	0.6948035421	-1.1080691342	-5.1460548947
C39	1.4298907989	-0.4505205253	-4.1473977533
C40	2.1978689363	0.6740918402	-4.4871178098
C41	2.2508739597	1.1160507892	-5.8071882518
H42	1.5682360561	0.7926122575	-7.8270097665
H43	0.1903499090	-1.1891289937	-7.2354226595
H44	0.0967548007	-1.9793914982	-4.8905782985
H45	2.7701731208	1.1885298268	-3.7187630713
H46	2.8614651568	1.9757213610	-6.0648546728

TS3
Gas phase Energy: -1048.46581809139 hartrees
Solvation Energy:-1048.50728181853 hartrees
Zero Point Energy: 199.663 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -321.62 23.70 28.94 38.86 53.75 65.65
Coordinates:

Pd1	.0761064016	.1826153054	-.0041067191
O2	-.1464701868	.1140917801	2.0032112787
O3	2.2526949177	.0604420125	.2763377087
C4	3.0221866900	.2098851042	-.7092143672
C5	2.6728579764	.3826969792	-2.0699762250
C6	1.3917844786	.3434241859	-2.5931268737
O7	.2490158950	.1746988568	-2.0163478515
H8	1.2895415623	.4440367179	-3.6793360940
H9	3.4835335490	.5211839023	-2.7754427372
H10	4.0981280577	.1855139031	-.4833479710
O11	.2413074189	2.2650676098	-.0791825611
C12	.2790791476	2.9345706636	.9980853357
C13	-.0163679363	1.1694441961	2.7184284575
C14	.1850648746	2.4883931973	2.3257790924
H15	.3948663450	4.0153469060	.8424323043
H16	-.0940508509	.9666988137	3.7927680393
H17	.2539263646	3.2340896364	3.1077956024
C18	-.0137886031	-2.3380878552	.0278624654
H19	.9409110392	-1.9111441418	.3376202581
H20	-.4278506891	-2.8803161268	.8738078818
C21	.0779026709	-3.1030898657	-1.2760284100
H22	-.8789303991	-3.5709713569	-1.5268298370
H23	.3557500749	-2.4398324570	-2.0977691125
C24	-1.8756862208	-1.3490512859	-.0431168303
C25	-1.9931126386	.0621261204	-.2623891951
H26	-2.1247444823	-1.9956510703	-.8776573642
H27	-2.1467127716	.4276463812	-1.2739811194
H28	-2.3977534416	.6777475836	.5368367851
H29	-2.1672516886	-1.7013512803	.9406073658
C31	3.0909816730	-6.1208173599	-.5818224832
C32	3.4476731770	-4.8992273213	-1.1611100957
C33	2.4779632324	-3.9248980925	-1.3878856916
C34	1.1378503797	-4.1667809577	-1.0486179247
C35	.7902535354	-5.3927927702	-.4592438670
C36	1.7610250461	-6.3666884050	-.2327926133
H37	3.8467500308	-6.8802001821	-.4084279242
H38	4.4791834979	-4.7116833840	-1.4428136505
H39	2.7542800987	-2.9803155979	-1.8508439653
H40	-.2461810350	-5.5926915093	-.1981855820
H41	1.4801497757	-7.3173324884	.2096228380

Os.Tp.CO

A
Gas phase Energy: -1217.14541356499 hartrees

Solvation Energy:-1217.15309575323 hartrees
Zero Point Energy: 224.573 kcal/mol
Coordinates:

Os1	-2.4053607497	1.4936607391	-0.1527747401
N2	-2.4582690895	3.6948223021	-0.3362723208
N3	-4.5577730952	1.6343021804	-0.1688734331
N4	-2.7248421051	1.5488455142	-2.3678030091
N5	-5.1903097511	2.5311882570	-0.9769356151
N6	-3.3723955174	4.2665668454	-1.1724937579
N7	-3.5960218284	2.4463948796	-2.9005427584
B8	-4.3804521445	3.4006076844	-1.9697013156
C9	-1.7515197573	4.6940405799	0.2096003739
C10	-5.4991423203	0.9949938208	0.5368132589
C11	-2.2491384274	0.8135865228	-3.3801361258
C12	-3.6634306772	2.2733778852	-4.2400115464
C13	-3.2299579528	5.6099916381	-1.1470432399
C14	-6.5241864803	2.4435945902	-0.7783892871
H15	-5.1132427194	4.1024716958	-2.6065472143
C16	-6.7672654748	1.4737705884	0.1842996107
C17	-2.8125997465	1.2360893055	-4.5926915182
C18	-2.1999172876	5.9299233550	-0.2744082442
H19	-0.9798349439	4.4835798512	0.9339526043
H20	-5.2114710713	0.2522206334	1.2652253291
H21	-1.5344503250	0.0269496272	-3.1891148298
H22	-4.3098761106	2.8976358567	-4.8383007015
H23	-3.8717060825	6.2364154629	-1.7480810102
H24	-7.1985738220	3.0741738917	-1.3379948325
H25	-7.7216693355	1.1595452338	0.5769849296
H26	-2.6266879909	0.8414758703	-5.5795134626
H27	-1.8312882057	6.9111782064	-0.0190035415
O28	-2.3623821951	-1.5235511809	-0.0629634998
C29	-2.3884069512	-0.3574107686	-0.0873347864
C30	-0.3042863496	1.5672071836	-0.8285570543
C31	-0.3206083592	1.6200506713	0.5783181480
H32	-0.0080688218	0.6532129425	-1.3349932620
H33	-0.0576994511	0.7463407548	1.1642545889
H34	-0.1552265387	2.5563602824	1.0996147280
H35	-0.1582011788	2.4759256946	-1.4053190710
C37	-3.0917791407	1.7882875485	4.7882315641
C38	-3.5187084171	2.8031310763	3.9321997011
C39	-3.3048930632	2.7070577707	2.5532044161
C40	-2.6508527923	1.6034448425	1.9701417069
C41	-2.2391382461	0.5918339173	2.8618501365
C42	-2.4527490982	0.6752935599	4.2399689022
H43	-3.2561734996	1.8606252004	5.8599292518
H44	-4.0252252093	3.6776163939	4.3346720317
H45	-3.6676269418	3.5132320488	1.9230534855
H46	-1.7347555195	-0.2924637759	2.4794159932
H47	-2.1166989883	-0.1339812886	4.8843238515

B
Gas phase Energy: -1217.13060950233 hartrees
Solvation Energy:-1217.13806479621 hartrees
Zero Point Energy: 224.905 kcal/mol
Coordinates:

Os1	-2.4956196557	1.3303780063	-0.2483385867

N2	-2.4057836503	3.5499538670	-0.2742397943
N3	-4.5333841126	1.6465166364	-0.1819990742
N4	-2.7041269824	1.5427704543	-2.4624463408
N5	-5.1287351787	2.5647408417	-0.9982099177
N6	-3.2533690634	4.2177491283	-1.1060364323
N7	-3.5319313536	2.5100420541	-2.9454788647
B8	-4.2825779980	3.4348754014	-1.9648593106
C9	-1.7141083102	4.4794852646	0.4008422579
C10	-5.4969452144	1.0800746448	0.5582906462
C11	-2.2303361818	0.8734290610	-3.5197361279
C12	-3.5691685229	2.4479976673	-4.2976904959
C13	-3.0879897939	5.5498684397	-0.9517115188
C14	-6.4608753100	2.5717252240	-0.7578660170
H15	-4.9893859802	4.1982259182	-2.5608401864
C16	-6.7407139719	1.6349947225	0.2253021509
C17	-2.7464815163	1.4110468113	-4.7103064391
C18	-2.1044592983	5.7656592067	0.0030481186
H19	-0.9868298709	4.1833091482	1.1418258896
H20	-5.2410907630	0.3154822712	1.2757652670
H21	-1.5510295877	0.0473176674	-3.3694223794
H22	-4.1764237752	3.1413812867	-4.8602767784
H23	-3.6835558734	6.2427769712	-1.5270526073
H24	-7.1056740027	3.2440130863	-1.3033846152
H25	-7.7035025649	1.3871179201	0.6445078292
H26	-2.5510020133	1.0877005779	-5.7212664558
H27	-1.7299018907	6.7111296972	0.3636768354
O28	-2.8753679451	-1.6633426840	-0.1817816334
C29	-2.7030043811	-0.5057094727	-0.2196602045
C30	-2.2213780047	1.4098952039	1.8903709928
H31	-2.7055408444	0.5754193104	2.4104858633
H32	-2.6424892423	2.3307145825	2.3124336016
C33	-0.6921603315	1.3467239444	2.1322455444
H34	-0.4133973385	0.7893458503	3.0359068563
H35	-0.2667591079	2.3522583081	2.2477897262
C36	0.9932021381	-0.5301728432	-1.4096680381
C37	0.6151544310	0.8024200772	-1.4430725401
C38	0.0828787881	1.4269396719	-0.2918645803
C39	-0.0730532532	0.6950681642	0.9093285063
C40	0.3315778004	-0.6567135773	0.9214761072
C41	0.8574000091	-1.2561141559	-0.2133713080
H42	1.4068467843	-1.0076525323	-2.2929292784
H43	0.7443194406	1.3887532449	-2.3478309010
H44	-0.0196248838	2.5067679119	-0.2867503348
H45	0.2232293046	-1.2290531614	1.8385256746
H46	1.1667180640	-2.2971079668	-0.1771521418

D
Gas phase Energy: -1449.38799350416 hartrees
Solvation Energy:-1449.39685396639 hartrees
Zero Point Energy: 288.563 kcal/mol
Coordinates:

Os1	-2.7300330758	1.7183350520	-0.1698737111
N2	-2.8563255309	3.8771313976	-0.5810667524
N3	-4.8029717623	1.8169818141	-0.0171917994
N4	-3.0998329079	1.5216875648	-2.3606550207
N5	-5.5264702698	2.5571011062	-0.9076711809

N6	-3.8236347782	4.3250734359	-1.4297730202
N7	-4.0518259911	2.3082779111	-2.9305593049
B8	-4.8277630906	3.3237123409	-2.0628616349
C9	-2.1795669854	4.9530154212	-0.1535480662
C10	-5.6693440412	1.2627137464	0.8428158113
C11	-2.6081362797	0.7371519498	-3.3260260266
C12	-4.1553960022	2.0162237623	-4.2486834530
C13	-3.7491748118	5.6704718246	-1.5299116749
C14	-6.8392679380	2.4633660236	-0.5959980476
H15	-5.6397597742	3.9110342363	-2.7200315115
C16	-6.9769555078	1.6446489740	0.5149117261
C17	-3.2460395666	1.0124614410	-4.5464173384
C18	-2.7047487418	6.1170642227	-0.7317411498
H19	-1.3645734840	4.8370196033	0.5458600463
H20	-5.3078918721	0.6267843027	1.6361173522
H21	-1.8252619325	0.0291912325	-3.0964970035
H22	-4.8649160335	2.5411898667	-4.8708503158
H23	-4.4444288229	6.2092891064	-2.1561012493
H24	-7.5747910021	2.9857673279	-1.1888336826
H25	-7.8891945461	1.3633705499	1.0175157470
H26	-3.0705175449	0.5461337422	-5.5036588353
H27	-2.3764410657	7.1340898623	-0.5834399489
O28	-2.7355388103	-1.2425414159	0.4395539566
C29	-2.7194313077	-0.0983288069	0.1956741793
C30	-2.5366560134	2.1819354237	1.9388520295
H31	-3.5182136584	2.0680732585	2.4202507946
H32	-2.2939233922	3.2492222802	2.0481073229
C33	-1.5067446893	1.3696356018	2.7592375222
H34	-0.5099632066	1.4599552516	2.3054704252
H35	-1.7651078428	0.3046889953	2.7137941259
C36	-1.2620074334	2.6031224839	6.9085694023
C37	-2.1719399895	1.6183277937	6.5187177389
C38	-2.2421630756	1.2177187719	5.1840066570
C39	-1.4102064425	1.7893811568	4.2112603482
C40	-0.5017852368	2.7762815268	4.6186852457
C41	-0.4256839536	3.1815806351	5.9517693957
H42	-1.2011002005	2.9122754191	7.9482993387
H43	-2.8227713811	1.1561113329	7.2563331434
H44	-2.9466683656	0.4428903278	4.8892920873
H45	0.1601017228	3.2244699503	3.8802372100
H46	0.2917793620	3.9436668758	6.2449193439
C47	0.2935480843	0.4023176811	-0.6746217328
C48	-0.3823483516	1.6277623176	-0.7930018004
H49	0.0094005738	-0.2956101902	0.1052115406
H50	-0.9297477366	2.0044106211	0.1518708631
C52	1.6968245721	0.9919085702	-2.5541675665
C53	1.3186783086	0.0816145821	-1.5631657154
H54	2.4969986793	0.7416145875	-3.2447290467
H55	1.8253393265	-0.8752584060	-1.4784797746
C56	1.0556164186	2.2305662516	-2.6461768607
C57	0.0264461261	2.5551477570	-1.7639510220
H58	1.3560724554	2.9435411137	-3.4083951209
H59	-0.4741176570	3.5135809763	-1.8372767736

E
Gas phase Energy: -1449.39249551472 hartrees

Solvation Energy:-1449.40185550063 hartrees
Zero Point Energy: 288.564 kcal/mol
Coordinates:

Os1	-1.7088927563	-1.2323083956	-0.9573165087
N2	-0.9399526372	-0.6403535418	1.0059945162
N3	-0.3035479930	-2.9551455955	-0.7397948870
N4	-3.0417183750	-2.3650792012	0.1143616669
N5	-0.2488086947	-3.5915252090	0.4626326605
N6	-0.7457564717	-1.6100535670	1.9432620572
N7	-2.6130753237	-3.1038923280	1.1819285822
B8	-1.1245874620	-3.0826998589	1.6289366452
C9	-0.6218800276	0.5301365618	1.5774823128
C10	0.5183911412	-3.6140346222	-1.5665801547
C11	-4.3630269616	-2.5559493395	-0.0101540514
C12	-3.6736774662	-3.7509112279	1.7183491524
C13	-0.3031182095	-1.0483002877	3.0894178778
C14	0.6040137691	-4.6396801458	0.3869586187
H15	-0.9762101593	-3.7680943308	2.6004317094
C16	1.1215109636	-4.6912942270	-0.8989481544
C17	-4.8085859161	-3.4341103440	0.9867423651
C18	-0.2012452369	0.3235643027	2.8988139623
H19	-0.7366613110	1.4510159530	1.0262676852
H20	0.6266742503	-3.2895984210	-2.5917009896
H21	-4.9065120117	-2.0467615369	-0.7909620962
H22	-3.5399436801	-4.3853798777	2.5814689641
H23	-0.1001044580	-1.6621320157	3.9543450276
H24	0.7762033792	-5.2681859381	1.2479480634
H25	1.8266315258	-5.4044424374	-1.2973109765
H26	-5.8166236313	-3.7818882817	1.1509486272
H27	0.1144843269	1.0665173028	3.6147684407
O28	-2.9163430870	-2.1301152692	-3.5845483741
C29	-2.4344927167	-1.7814776052	-2.5803828509
C30	0.2462482237	0.4474486428	-1.9422697294
H31	-0.2452856834	1.0924510701	-1.2184106416
H32	0.1785683647	0.9439388561	-2.9151577136
C33	1.6911614527	0.1115940421	-1.5436905778
H34	2.1499180091	-0.5039542097	-2.3263512248
H35	1.6742604180	-0.4943889470	-0.6332176985
C36	3.9828128101	3.7243424284	-0.8929198737
C37	3.3921143045	3.0618814792	0.1844295949
C38	2.6650553862	1.8897817225	-0.0271276235
C39	2.5161049823	1.3604783008	-1.3157878489
C40	3.1160101717	2.0326851174	-2.3888728040
C41	3.8431476822	3.2052996654	-2.1817361052
H42	4.5501370914	4.6360615167	-0.7295585660
H43	3.4996687298	3.4553213290	1.1914901531
H44	2.2076847472	1.3764155916	0.8152785626
H45	3.0157361424	1.6305744555	-3.3947207492
H46	4.3030252105	3.7117955738	-3.0257140613
H47	-0.3071792464	-0.5246414865	-2.1304172606
C48	-4.5566163456	2.8281844914	-0.8277041065
C49	-4.4503548090	1.9921359776	0.2843588384
C50	-3.6670250306	0.8355755401	0.2277912710
C51	-2.9532347506	0.4599995233	-0.9319023463
C52	-3.0993008658	1.3216234802	-2.0425553839
C53	-3.8754391376	2.4820779817	-1.9965332268

H54	-5.1630316399	3.7290822599	-0.7871655733
H55	-4.9782328496	2.2391862942	1.2030999103
H56	-3.6080992521	0.2113023664	1.1157988920
H57	-2.5952260895	1.0802016936	-2.9770558427
H58	-3.9510987170	3.1146084463	-2.8783004962

G
Gas phase Energy: -1295.77256830645 hartrees
Solvation Energy:-1295.78066750769 hartrees
Zero Point Energy: 260.189 kcal/mol
Coordinates:

Os1	-2.4842508710	1.6915084410	-0.2595295754
N2	-2.7611887858	3.8451110861	-0.6593547681
N3	-4.6236814828	1.6828437373	0.0786511077
N4	-3.1920675166	1.4304450635	-2.3702765876
N5	-5.4530457876	2.4357635483	-0.6959284000
N6	-3.8474160719	4.2516204316	-1.3778458897
N7	-4.1923503860	2.2197067123	-2.8408007832
B8	-4.8881512387	3.2317400394	-1.9005438590
C9	-2.0907762324	4.9506219932	-0.3087765603
C10	-5.3863078776	1.0466576094	0.9776191465
C11	-2.8447483021	0.6016412116	-3.3619808496
C12	-4.4703962743	1.8862852496	-4.1222230973
C13	-3.8490254056	5.6000090079	-1.4713657444
C14	-6.7280788146	2.2656866244	-0.2819215714
H15	-5.7714374278	3.8016910548	-2.4755765817
C16	-6.7325559189	1.3864331236	0.7920093115
C17	-3.6262259340	0.8526945881	-4.4994822116
C18	-2.7378092264	6.0915607310	-0.8024992266
H19	-1.1913526701	4.8784048204	0.2835393906
H20	-4.9298426057	0.3908334071	1.7037690753
H21	-2.0609091736	-0.1254320346	-3.2106429942
H22	-5.2457457407	2.4060272586	-4.6648031275
H23	-4.6391676825	6.1073998307	-2.0041242246
H24	-7.5348827413	2.7792735342	-0.7828869589
H25	-7.5838428084	1.0397877380	1.3569084752
H26	-3.5821710000	0.3517717181	-5.4541290683
H27	-2.4405528901	7.1219394776	-0.6841564836
O28	-2.2586303309	-1.2879323435	0.1639506699
C29	-2.3341069335	-0.1303610189	0.0295368078
C30	-2.3886723077	2.2173279658	1.8565244385
H31	-3.4108715473	2.4851232331	2.1496772422
H32	-1.8070813229	3.1410529307	1.9624877019
C33	-1.8524856871	1.1912488596	2.8747684643
H34	-0.8510621472	0.8555851225	2.5821901768
H35	-2.4879232664	0.2962209160	2.8673199386
C36	-1.6829627909	2.8443119729	6.8809962239
C37	-2.8512674250	2.2334563566	6.4209332603
C38	-2.8992400422	1.6902009552	5.1365899909
C39	-1.7872720194	1.7439970075	4.2847846424
C40	-0.6213300479	2.3592911867	4.7621293341
C41	-0.5661003928	2.9049122249	6.0453839952
H42	-1.6420047439	3.2647083340	7.8819707934
H43	-3.7247823534	2.1757473783	7.0650266809
H44	-3.8120160977	1.2119977962	4.7877274524
H45	0.2552413784	2.4047359172	4.1191669775

H46	0.3508340811	3.3722791732	6.3950207097
C47	-0.3264370431	2.0035966703	0.0476107104
H48	0.1187781080	1.2250491009	0.6579730928
H49	-0.1236190055	3.0088500549	0.4037039038
C50	-0.5652530873	1.7752135830	-1.3237651989
H51	-0.2961537180	0.8235441229	-1.7729193954
H52	-0.5879129780	2.6129300492	-2.0152941299

TS1
Gas phase Energy: -1217.09396598218 hartrees
Solvation Energy:-1217.10119444688 hartrees
Zero Point Energy: 223.959 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-336.88 cm^{-1})
Coordinates:

Os1	-0.0768981542	-0.1524512868	0.0097394363
N2	-0.0589333537	-0.1179106463	2.2321502743
N3	2.1163517376	0.0768686917	0.1900308644
N4	0.3445541846	-2.1987410545	0.2925350259
N5	2.7870964855	-0.6078286419	1.1544293964
N6	0.9463702851	-0.7689235618	2.8776893666
N7	1.2663838405	-2.6062260253	1.2112679967
B8	2.0169448791	-1.5674825942	2.0813688932
C9	-0.8737656508	0.3718757667	3.1788111725
C10	3.0143464017	0.8269185296	-0.4580695379
C11	-0.1503186010	-3.3002899217	-0.2903806097
C12	1.3382117022	-3.9568575649	1.2044110892
C13	0.7617382043	-0.6838080462	4.2133396733
C14	4.1018238161	-0.2874846084	1.1103413790
H15	2.7639281407	-2.1186784010	2.8400757196
C16	4.2928877435	0.6304133844	0.0886739062
C17	0.4513023387	-4.4428904610	0.2553889810
C18	-0.3935742170	0.0457963855	4.4543792540
H19	-1.7589332888	0.9258539639	2.9043156231
H20	2.6945922550	1.4693999508	-1.2650640637
H21	-0.9031700442	-3.2080562882	-1.0583123611
H22	2.0128797458	-4.4677080216	1.8747999188
H23	1.4619177007	-1.1500985483	4.8900712963
H24	4.7976463729	-0.7361829665	1.8036297395
H25	5.2199854990	1.0893695990	-0.2186273922
H26	0.2634461383	-5.4732929202	-0.0036378009
H27	-0.8265267082	0.3015001527	5.4090124471
O28	-0.1201366403	-0.4756395115	-2.9905997032
C29	-0.0952237345	-0.3415138706	-1.8280030100
C30	-2.1854068926	-0.0284398099	0.1195947298
C31	-1.9106145797	1.4322108561	0.0270912734
H32	-2.7666216113	-0.4308373617	-0.7097249858
H33	-2.3198498485	1.9069303971	-0.8604981794
H34	-2.1552237779	2.0101210424	0.9159093020
H35	-2.5928120232	-0.3605337640	1.0758116500
C36	1.2933750872	4.5123260988	-0.5483975445
C37	1.0539659512	4.0123296631	0.7340568004
C38	0.2986468213	2.8559170231	0.9128979796
C39	-0.2203852662	2.1322280482	-0.1857679574
C40	-0.0005397941	2.6873145496	-1.4704509236
C41	0.7534985871	3.8425791564	-1.6513313552
H42	1.8768328762	5.4177996329	-0.6864161256

H43	1.4562024296	4.5265619969	1.6027695537
H44	0.1250192118	2.4932375468	1.9199903506
H45	-0.4310724617	2.1992960362	-2.3397982906
H46	0.9116907614	4.2265013159	-2.6556335143

TS2 – Ph-H

TS2 – intermediate

TS2 – CH2-H
Gas phase Energy: -1449.37786663405 hartrees
Solvation Energy:-1449.38663925067 hartrees
Zero Point Energy: 287.025 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -456.94 24.56 26.25 30.22 45.66 53.75
Coordinates:

Os1	-0.2449393610	0.0026759272	0.0604060016
N2	-0.0048680247	-0.1589170941	2.2257340065
N3	1.9795016813	0.1576974894	0.0388157720
N4	0.2319017171	-2.1097853068	0.0519607637
N5	2.7063514583	-0.6197759875	0.8847650148
N6	1.0197357191	-0.8936374511	2.7435755970
N7	1.1796250924	-2.6029414157	0.8994928920
B8	1.9971178590	-1.6447305896	1.8046722076
C9	-0.6876628440	0.3519884590	3.2588024697
C10	2.8513362888	0.8596570379	-0.6972360035
C11	-0.2761277778	-3.1449615989	-0.6282116701
C12	1.2631514410	-3.9425915633	0.7407996767
C13	0.9745826522	-0.8376719786	4.0934212179
C14	4.0254366764	-0.4027654036	0.6799405967
H15	2.8006056598	-2.2589379260	2.4469051500
C16	4.1656518744	0.5439296572	-0.3242080347
C17	0.3475582578	-4.3334349790	-0.2266081060
C18	-0.1036593767	-0.0479870441	4.4684943336
H19	-1.5640529118	0.9568297531	3.0785266271
H20	2.4960750826	1.5431045498	-1.4547474319
H21	-1.0653296185	-2.9798934928	-1.3460025090
H22	1.9680688611	-4.5158928599	1.3240940325
H23	1.7086529736	-1.3638481814	4.6850361724
H24	4.7621088173	-0.9386835952	1.2595264073
H25	5.0815883813	0.9435638876	-0.7309787093
H26	0.1573332330	-5.3318120542	-0.5886069954
H27	-0.4241725635	0.1973302874	5.4690537952
O28	-0.4693039497	0.2104946885	-2.9483847723
C29	-0.3952582212	0.1337978695	-1.7875320541
C30	-0.1445206607	2.2745386623	0.2709310621
H31	0.8773821909	2.4304561697	-0.0793454948
H32	-0.1541053036	2.5086662258	1.3400504326
C33	-1.0874151344	3.2297454650	-0.4920952739
H34	-2.1204123184	3.0992030285	-0.1447155435
H35	-1.0846196504	2.9667229804	-1.5556390595
C36	0.1345909288	7.3505069258	0.0394909151
C37	0.5415081564	6.6383525520	-1.0897739797
C38	0.1373898483	5.3139534041	-1.2665446780
C39	-0.6781692846	4.6777893704	-0.3218312136
C40	-1.0819231507	5.4060490857	0.8064836655
C41	-0.6801403156	6.7294520606	0.9882687022

H42	0.4449806684	8.3824378033	0.1771044159
H43	1.1684561034	7.1153665568	-1.8371293121
H44	0.4506487818	4.7670354475	-2.1531171874
H45	-1.7253322129	4.9308522484	1.5454671554
H46	-1.0076772512	7.2775045802	1.8675819172
H47	-1.2771984478	1.1907121165	0.3461638870
C48	-4.9934091245	-1.4989640623	0.4310313817
C49	-4.0079301258	-1.9987555216	1.2823583943
C50	-2.6837477665	-1.5629951407	1.1703743196
C51	-2.2915609728	-0.6147775340	0.2058301004
C52	-3.3101006685	-0.1242800135	-0.6368494827
C53	-4.6339234202	-0.5565586700	-0.5337983058
H54	-6.0228195124	-1.8357455586	0.5179486132
H55	-4.2662874822	-2.7340872650	2.0409485980
H56	-1.9449234355	-1.9785451354	1.8489020878
H57	-3.0672585296	0.6141650907	-1.3974152256
H58	-5.3844721767	-0.1515284761	-1.2086085344

TS3
Gas phase Energy: -1295.70757067820 hartrees
Solvation Energy:-1295.71558931332 hartrees
Zero Point Energy: 259.629 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -470.53 25.64 27.88 33.66 60.24 63.69
Coordinates:

Os1	0.0117346299	-0.3290843244	-0.0924449459
N2	-0.0695371497	0.2314522181	2.0350324666
N3	2.1962087839	-0.0493977165	0.1366377303
N4	0.3872003698	-2.2497186827	0.6281221407
N5	2.7991664893	-0.5103497833	1.2651149150
N6	0.8735783216	-0.2724429465	2.8752822099
N7	1.2433461827	-2.4431616812	1.6739643312
B8	1.9608268129	-1.2414270346	2.3384596494
C9	-0.8812558698	0.9999799268	2.7751961961
C10	3.1552679790	0.4957556509	-0.6235577422
C11	-0.0869762517	-3.4521167179	0.2728483697
C12	1.2940071063	-3.7629546414	1.9700261697
C13	0.6533232799	0.1779708286	4.1299088997
C14	4.1271228376	-0.2509713727	1.2127924230
H15	2.6600884450	-1.6173295725	3.2366799898
C16	4.4004073635	0.3960056308	0.0175414835
C17	0.4623997578	-4.4458258850	1.0958332969
C18	-0.4632803905	1.0018240470	4.1132017659
H19	-1.7199204230	1.5038407071	2.3182293107
H20	2.9072035754	0.9198837792	-1.5858102877
H21	-0.7873835082	-3.5312055685	-0.5444223959
H22	1.9173486658	-4.1138891286	2.7785714946
H23	1.3038647341	-0.1212565130	4.9380196710
H24	4.7742533305	-0.5476918239	2.0246484102
H25	5.3578719723	0.7407262040	-0.3414585296
H26	0.2768709349	-5.5080455408	1.0576494699
H27	-0.9104724977	1.5234505745	4.9450869241
O28	0.1768839899	-1.2424167153	-2.9696206298
C29	0.1153110108	-0.8744424891	-1.8596720228
C30	-2.1086869293	-0.3118319688	-0.1017597484
C31	-1.9110691605	1.0517925712	-0.6058291555

H32	-2.5895784973	-0.9958999997	-0.8011223299
H33	-2.0827292974	1.1751137430	-1.6710317507
H34	-2.3635535222	1.8632175015	-0.0350216799
H35	-2.5459077815	-0.3903092135	0.8951371336
C36	-0.2218908642	2.1113418776	-0.5313790753
H37	0.8257356242	1.8678937212	-0.7027843903
H38	-0.2939734857	2.5531217914	0.4625064200
C39	-0.6119364936	3.1216159357	-1.6200913012
H40	-0.5123066470	2.6523768828	-2.6058923676
H41	-1.6626757541	3.4195051980	-1.5127660843
C42	0.2663278780	4.3547906024	-1.5491327520
C43	1.9408351401	6.6087270772	-1.3397455493
C44	1.4246473852	4.4628755575	-2.3294501131
C45	-0.0413448662	5.3981376441	-0.6654108597
C46	0.7869250217	6.5153688713	-0.5588538532
C47	2.2563881442	5.5788891577	-2.2274518397
H48	1.6726532690	3.6661783892	-3.0273530596
H49	-0.9411102034	5.3334973387	-0.0573227076
H50	0.5299876450	7.3142695492	0.1311329676
H51	3.1485992638	5.6453613569	-2.8439252085
H52	2.5862869986	7.4786139002	-1.2596108140

Ru.Tp.CO

A
Gasphase Energy: -1219.951597 Hartrees
Solvation Energy: -1219.958609 Hartrees
Zero Point Energy: 223.95 kcal/mol
Coordinates:

Ru1	-2.4184739896	1.5125597271	-0.1206001402
N2	-2.4662740509	3.7259748643	-0.3286717763
N3	-4.5654914562	1.6410517322	-0.1437774340
N4	-2.6808420265	1.5492672292	-2.3825033476
N5	-5.1825238800	2.5152663748	-0.9852105533
N6	-3.3760322446	4.2677526753	-1.1864493890
N7	-3.5706456401	2.4305685065	-2.9090502555
B8	-4.3669507457	3.3780334608	-1.9813904878
C9	-1.7743068629	4.7454813418	0.1962571170
C10	-5.5184926856	1.0280554977	0.5677011499
C11	-2.1939700745	0.8329723667	-3.4018087776
C12	-3.6382300834	2.2673735183	-4.2508530767
C13	-3.2474569021	5.6137111370	-1.1952061316
C14	-6.5205006496	2.4422167948	-0.8004355447
H15	-5.1049800348	4.0681661683	-2.6269890541
C16	-6.7815856522	1.5013894247	0.1856885875
C17	-2.7674752196	1.2503963635	-4.6131798910
C18	-2.2286964072	5.9665359470	-0.3220925914
H19	-1.0056476752	4.5616865301	0.9321391330
H20	-5.2455881841	0.3057724900	1.3224469953
H21	-1.4626850348	0.0580882494	-3.2214401865
H22	-4.2975483706	2.8837468195	-4.8436103153
H23	-3.8899203341	6.2182292772	-1.8177829131
H24	-7.1840657759	3.0627685864	-1.3838778626

H25	-7.7426647624	1.2034673765	0.5753021848
H26	-2.5757669203	0.8666004980	-5.6033892904
H27	-1.8719097789	6.9578994441	-0.0891174597
O28	-2.4380186714	-1.5041172118	-0.0518745544
C29	-2.4309406777	-0.3449832758	-0.0606660095
C30	-0.2621382611	1.5747654639	-0.7691360202
C31	-0.2799691581	1.6316347220	0.6147334773
H32	-0.0231108684	0.6482400403	-1.2809375417
H33	-0.0670108420	0.7540543091	1.2132787967
H34	-0.1804691433	2.5724126464	1.1422460360
H35	-0.1783873222	2.4776782981	-1.3637247121
X36	-0.4742280869	1.5709608672	-0.0247244879
C37	-3.0482870333	1.7634191736	4.8054727071
C38	-3.4590650253	2.7934310100	3.9587663883
C39	-3.2540154805	2.7045361950	2.5777325197
C40	-2.6240669467	1.5915772934	1.9907872205
C41	-2.2263188947	0.5640774283	2.8675053874
C42	-2.4332365158	0.6421186150	4.2482979854
H43	-3.2070257953	1.8315687632	5.8782640069
H44	-3.9470333773	3.6742102630	4.3702351293
H45	-3.6036939634	3.5195327145	1.9528637398
H46	-1.7382215466	-0.3269505141	2.4792041965
H47	-2.1097399892	-0.1776705093	4.8857475177

B
Gasphase Energy: -1219.957559 Hartrees
Solvation Energy: -1219.964251 Hartrees
Zero Point Energy: 224.64 kcal/mol
Coordinates:

Ru1	-2.4933520457	1.3351131945	-0.2350469563
N2	-2.4040799771	3.5684394949	-0.2529186102
N3	-4.5390361339	1.6319598914	-0.1418951493
N4	-2.6909216110	1.5619402616	-2.4912859839
N5	-5.1322947574	2.5403920906	-0.9647573515
N6	-3.2695276556	4.2145207943	-1.0819778336
N7	-3.5487366127	2.5171768656	-2.9392244585
B8	-4.2950159007	3.4211553828	-1.9343707963
C9	-1.7103918053	4.5160461115	0.3918298899
C10	-5.4994074980	1.0756361123	0.6064153910
C11	-2.2111551157	0.9366577386	-3.5708125908
C12	-3.6006802668	2.4918726309	-4.2926799039
C13	-3.1148462691	5.5518093168	-0.9543438268
C14	-6.4639904640	2.5513947482	-0.7239533686
H15	-5.0179786728	4.1810288369	-2.5168126095
C16	-6.7446971593	1.6269065584	0.2711136172
C17	-2.7544123066	1.4902886251	-4.7431940314
C18	-2.1186583492	5.7936050637	-0.0199569172
H19	-0.9652703231	4.2406163739	1.1237781949
H20	-5.2450563405	0.3195464495	1.3338793170
H21	-1.5061795347	0.1260295347	-3.4524414044
H22	-4.2331606458	3.1830970955	-4.8297420769
H23	-3.7253068811	6.2289164284	-1.5329476996
H24	-7.1088541477	3.2173114305	-1.2772652968
H25	-7.7072662255	1.3852838319	0.6945380873
H26	-2.5616383771	1.2006210386	-5.7649094116
H27	-1.7473304450	6.7487277966	0.3180286386

O28	-2.9061468077	-1.6513806667	-0.1779488041
C29	-2.7143599295	-0.5052939541	-0.2125802538
C30	-2.2587736003	1.3595438314	1.8880415749
H31	-2.7202630819	0.4900377783	2.3683716025
H32	-2.7377679415	2.2571529402	2.2931527891
C33	-0.7376051138	1.3619588561	2.1590627961
H34	-0.4697658340	0.8633116513	3.1000957505
H35	-0.3606197068	2.3894259025	2.2358831004
C36	1.0738883631	-0.6298886971	-1.2489725001
C37	0.6837381530	0.7003532946	-1.3426405070
C38	0.1328637426	1.3596440636	-0.2275783282
C39	-0.0471787019	0.6765601338	0.9946713481
C40	0.3654941786	-0.6664782968	1.0707386310
C41	0.9218611949	-1.3074510585	-0.0306121578
H42	1.5063693030	-1.1380367073	-2.1056408412
H43	0.8174382197	1.2495366449	-2.2698562473
H44	-0.0412070380	2.4298584475	-0.2833058197
H45	0.2410316682	-1.2045442749	2.0065934323
H46	1.2389155255	-2.3432883831	0.0537940086

D
Gasphase Energy: -1452.210791 Hartrees
Solvation Energy: -1452.218899 Hartrees
Zero Point Energy: 288.34 kcal/mol
Coordinates:

Ru1	-2.6944703642	1.7332028029	-0.1537139843
N2	-2.8505214683	3.8996759204	-0.5468863599
N3	-4.7561706487	1.7677069692	-0.0306731369
N4	-2.9914815988	1.5523440853	-2.4063029318
N5	-5.4708145412	2.4849658306	-0.9426696068
N6	-3.8122604662	4.3165978396	-1.4147841108
N7	-3.9641510480	2.3233828321	-2.9631157262
B8	-4.7747868104	3.2928201212	-2.0757256477
C9	-2.2017381934	4.9944790305	-0.1279547484
C10	-5.6294295958	1.1897892960	0.8041578553
C11	-2.4609567009	0.8241025976	-3.3930493550
C12	-4.0401882768	2.0776671574	-4.2931787779
C13	-3.7625809012	5.6623941789	-1.5369075173
C14	-6.7897081127	2.3544033946	-0.6699496079
H15	-5.6004690987	3.8678275962	-2.7281111068
C16	-6.9381841032	1.5326226117	0.4372723715
C17	-3.0907374021	1.1195688150	-4.6146185890
C18	-2.7393471222	6.1416993411	-0.7311457358
H19	-1.3953879277	4.9070263210	0.5862649375
H20	-5.2746195255	0.5659349203	1.6102563558
H21	-1.6561968661	0.1345647810	-3.1807438367
H22	-4.7606172408	2.5984062669	-4.9065289370
H23	-4.4582747169	6.1774254218	-2.1824385878
H24	-7.5213492592	2.8553025510	-1.2856422229
H25	-7.8565589626	1.2250013323	0.9125703954
H26	-2.8856616473	0.6954921690	-5.5857153541
H27	-2.4331230148	7.1672002476	-0.5936634224
O28	-2.6974429416	-1.2429588395	0.3689479442
C29	-2.6696544527	-0.0984981440	0.1680113577
C30	-2.5166666372	2.1434338887	1.9453986112
H31	-3.5082716914	2.0435919066	2.4038338272

H32	-2.2540038599	3.2064051293	2.0368763120
C33	-1.5058001531	1.3094829668	2.7622953784
H34	-0.5119257265	1.3528891869	2.2973254803
H35	-1.8040186252	0.2538432597	2.7475775163
C36	-1.1509521253	2.6452592242	6.8719879390
C37	-2.1163676497	1.6995041342	6.5201186936
C38	-2.2233049943	1.2652359241	5.1984338307
C39	-1.3721648993	1.7635682105	4.2023287466
C40	-0.4078682290	2.7117406086	4.5710258623
C41	-0.2957743407	3.1507135120	5.8908730215
H42	-1.0623935151	2.9807583094	7.9014507292
H43	-2.7824682048	1.2943600824	7.2772834077
H44	-2.9717727069	0.5216111363	4.9332577269
H45	0.2685833402	3.1025586772	3.8135014566
H46	0.4640407653	3.8818061782	6.1544732052
C47	0.5279761793	0.5347148399	-0.4447105453
C48	-0.0994770587	1.7772144798	-0.5963462170
H49	0.2695614555	-0.1023925507	0.3945865492
H50	-0.7421046182	2.1570672165	0.2248276346
X51	-0.3191567369	1.5578181861	-0.1054602026
C52	1.8187291636	0.9586350089	-2.4442503869
C53	1.4845238886	0.1241771523	-1.3740485012
H54	2.5647385461	0.6391979072	-3.1664326922
H55	1.9693276746	-0.8410707267	-1.2625899639
C56	1.2030113768	2.2057701361	-2.5846691303
C57	0.2423967321	2.6182396221	-1.6612560525
H58	1.4681314051	2.8527519644	-3.4154772216
H59	-0.2494475818	3.5787353670	-1.7681641478

E
Gasphase Energy: -1452.216535 Hartrees
Solvation Energy: -1452.224588 Hartrees
Zero Point Energy: 288.27 kcal/mol
Coordinates:

Ru1	-1.6390503335	-1.2718473439	-0.8537321237
N2	-0.9367194547	-0.9337349391	1.1895531587
N3	-0.3961905554	-3.1731410538	-0.7199032420
N4	-3.1574575756	-2.3452508139	0.0117906005
N5	-0.5146368364	-3.8968599184	0.4253890160
N6	-0.9117137979	-1.9957207670	2.0410489828
N7	-2.8700685388	-3.2072886120	1.0281670026
B8	-1.4193480685	-3.3832864758	1.5684681945
C9	-0.4974873570	0.1301541163	1.8732036728
C10	0.4271340383	-3.8541657716	-1.5243252603
C11	-4.4779418931	-2.3909412319	-0.2051717903
C12	-4.0188643451	-3.7892426589	1.4438681611
C13	-0.4533771284	-1.5961287858	3.2490952370
C14	0.2325626520	-5.0224202434	0.3374226337
H15	-1.4198220738	-4.1587485517	2.4826008763
C16	0.8584543866	-5.0364201451	-0.9000647178
C17	-5.0703051413	-3.2999759663	0.6822798274
C18	-0.1692804014	-0.2388472282	3.1865595486
H19	-0.4691775905	1.0997045367	1.3981872461
H20	0.6643580571	-3.4697578944	-2.5067580358
H21	-4.9203695011	-1.7648219548	-0.9647091411
H22	-4.0008776961	-4.5049953541	2.2517765482

H23	-0.3678552102	-2.3023422596	4.0614511529
H24	0.2627028831	-5.7252677121	1.1566711782
H25	1.5234494766	-5.7894259457	-1.2941239898
H26	-6.1154186936	-3.5567790409	0.7586501646
H27	0.2091945674	0.3921634360	3.9758335431
O28	-2.7358717518	-1.8369524597	-3.6204412309
C29	-2.2988309135	-1.6149877857	-2.5701622683
C30	0.5296825970	0.3471395773	-1.8079177063
H31	-0.1646014574	1.0852228486	-1.4072950642
H32	0.5766561766	0.4852437253	-2.8920870455
C33	1.9176265125	0.4618532535	-1.1530515844
H34	2.5848768768	-0.3007890247	-1.5698364365
H35	1.8230332911	0.2502176900	-0.0825881361
C36	3.5493216530	4.4217278639	-1.7858674518
C37	2.6952421541	4.1761526236	-0.7084463980
C38	2.1853731062	2.8949739132	-0.4982723891
C39	2.5160250395	1.8380782945	-1.3575435304
C40	3.3743594134	2.0972786353	-2.4334065797
C41	3.8885803850	3.3773352926	-2.6475973084
H42	3.9485714971	5.4184007071	-1.9507003606
H43	2.4277169249	4.9816149669	-0.0301599456
H44	1.5245386346	2.7104027396	0.3456946363
H45	3.6445116711	1.2874363626	-3.1073642964
H46	4.5553377073	3.5579201557	-3.4862502874
H47	0.1533815911	-0.6949642973	-1.6548769112
C48	-4.1116705023	2.9912725165	-0.5815762602
C49	-4.1170282273	2.0910206757	0.4852161186
C50	-3.4453682392	0.8684131205	0.3844103765
C51	-2.7396980568	0.4984442965	-0.7778831270
C52	-2.7713840657	1.4189717902	-1.8459788142
C53	-3.4356813555	2.6458751281	-1.7524475107
H54	-4.6307010476	3.9428424650	-0.5043581116
H55	-4.6439904112	2.3397044371	1.4038665666
H56	-3.4686109379	0.1942729404	1.2359101586
H57	-2.2640755171	1.1837006222	-2.7799051805
H58	-3.4263970449	3.3284819334	-2.5991953755

G
Gas phase Energy: -1298.57938671424 hartrees
Solvation Energy: -1298.58679224331 hartrees
Zero Point Energy: 259.543 kcal/mol
Coordinates:

Ru1	-2.4732901523	1.7271963360	-0.2260991201
N2	-2.7491542117	3.8911131017	-0.6197116121
N3	-4.6138693539	1.7017212436	0.0943656323
N4	-3.1330718676	1.4713887539	-2.4025926446
N5	-5.4263484339	2.4430051294	-0.7060969262
N6	-3.8271902134	4.2827275474	-1.3539829206
N7	-4.1399485082	2.2639737313	-2.8515055552
B8	-4.8490488341	3.2526490865	-1.8962575436
C9	-2.0936974804	5.0052377016	-0.2706701172
C10	-5.3957716579	1.0761486150	0.9824370708
C11	-2.7738161218	0.6861925711	-3.4239543702
C12	-4.4092922596	1.9771035345	-4.1473216825
C13	-3.8395764385	5.6310583713	-1.4620247910
C14	-6.7111297415	2.2788860655	-0.3180681820

H15	-5.7331186653	3.8227420057	-2.4721226067
C16	-6.7397534696	1.4112249863	0.7642997297
C17	-3.5522593878	0.9677298105	-4.5588873204
C18	-2.7417945375	6.1387927516	-0.7832044683
H19	-1.2020394080	4.9473572290	0.3359367556
H20	-4.9566337686	0.4301143091	1.7284400113
H21	-1.9813668709	-0.0382518644	-3.3001660299
H22	-5.1876568667	2.5088345457	-4.6746535538
H23	-4.6267143376	6.1270518458	-2.0097842990
H24	-7.5061337832	2.7895166219	-0.8406744169
H25	-7.6033963175	1.0706228478	1.3138553272
H26	-3.4983939468	0.5030393614	-5.5316451460
H27	-2.4549261750	7.1729893498	-0.6699564884
O28	-2.2279341200	-1.2357999320	0.2963714286
C29	-2.3180995675	-0.0945443403	0.1044708326
C30	-2.3474070188	2.2219612082	1.8820955308
H31	-3.3699900314	2.5077758351	2.1474834624
H32	-1.7411542099	3.1289405544	1.9770897950
C33	-1.8443005637	1.1754992597	2.8915623041
H34	-0.8500726892	0.8128043566	2.6049481761
H35	-2.5049408357	0.2986818670	2.8790407314
C36	-1.6501854569	2.7980899266	6.9077263569
C37	-2.8223818922	2.1925925984	6.4502048832
C38	-2.8792138166	1.6605800007	5.1613086985
C39	-1.7709874824	1.7202408726	4.3048411700
C40	-0.6021289942	2.3313306054	4.7788642839
C41	-0.5389906813	2.8659423914	6.0657281196
H42	-1.6024919150	3.2090882214	7.9121307371
H43	-3.6912118123	2.1292477550	7.0992384196
H44	-3.7943124252	1.1859084470	4.8139372618
H45	0.2713250930	2.3804953345	4.1308814560
H46	0.3798378602	3.3297362453	6.4136454509
C47	-0.2632116580	2.0353211584	0.0679260801
H48	0.1322380335	1.2547491220	0.7074793465
H49	-0.1176697876	3.0456077226	0.4327502219
C50	-0.5020689903	1.7977027973	-1.2790345494
H51	-0.2955311418	0.8257520264	-1.7159946514
H52	-0.5853217248	2.6200420905	-1.9819136482

TS1
Gasphase Energy: -1219.917714 Hartrees
Solvation Energy: -1219.924248 Hartrees
Zero Point Energy: 223.49 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-352.85 cm^{-1})
Coordinates:

Ru1	-0.0623750086	-0.0825472582	0.0154909358
N2	-0.0347844199	-0.0724245467	2.2542742711
N3	2.1553780578	0.1074778810	0.2030385831
N4	0.2896315036	-2.1766502321	0.2846447472
N5	2.7971299381	-0.6307825054	1.1475182333
N6	0.9525600578	-0.7739241445	2.8744837017
N7	1.2193952603	-2.6028385738	1.1811814886
B8	1.9977113857	-1.5860986849	2.0571159637
C9	-0.8206797043	0.4226608206	3.2199791981
C10	3.0787481623	0.8588636833	-0.4032889135
C11	-0.2392927111	-3.2649955212	-0.2874951271

C12	1.2651784407	-3.9549276592	1.1727689723
C13	0.7843465797	-0.7124472033	4.2148015663
C14	4.1201283132	-0.3404586042	1.1314982010
H15	2.7340356817	-2.1666243603	2.8053715484
C16	4.3470666440	0.6114948049	0.1489708188
C17	0.3480431460	-4.4232159756	0.2431983811
C18	-0.3419524791	0.0510824026	4.4849242553
H19	-1.6872957076	1.0167198639	2.9674041906
H20	2.7851043033	1.5422697400	-1.1872491694
H21	-1.0049663320	-3.1590338583	-1.0418451698
H22	1.9440103013	-4.4800229865	1.8278505160
H23	1.4749526054	-1.2167144044	4.8739524025
H24	4.7962133009	-0.8312193002	1.8158252583
H25	5.2886234631	1.0601584807	-0.1286941679
H26	0.1335394221	-5.4491718145	-0.0131724759
H27	-0.7561547030	0.3005148461	5.4496370525
O28	-0.0839013216	-0.5350161223	-2.9633344762
C29	-0.0681707966	-0.3210693682	-1.8208381942
C30	-2.1830183219	-0.0530360125	0.0950029558
C31	-1.9430480634	1.3828301497	0.0152700155
H32	-2.6943769883	-0.5057422394	-0.7523881515
H33	-2.3167252086	1.8733301229	-0.8781070247
H34	-2.1584228786	1.9644702768	0.9075245813
H35	-2.5200769262	-0.4464054955	1.0519438818
C36	1.1635963904	4.6288978738	-0.5518325692
C37	0.9636013960	4.1052031546	0.7279299308
C38	0.2874656296	2.8978998108	0.9011765586
C39	-0.1903185257	2.1582701336	-0.1998890100
C40	-0.0062529009	2.7249086702	-1.4801445398
C41	0.6691681777	3.9315632951	-1.6573512291
H42	1.6825293158	5.5738190480	-0.6851471931
H43	1.3347813846	4.6390795922	1.5986553690
H44	0.1466635183	2.5149823507	1.9060547829
H45	-0.4083822486	2.2186178603	-2.3533338003
H46	0.7984834112	4.3319665339	-2.6596375097

TS2
Gasphase Energy: -1452.178668 Hartrees
Solvation Energy: -1452.186275 Hartrees
Zero Point Energy: 285.87 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1137.17 cm^{-1})
Coordinates:

Ru1	-.1319293883	-.0180283147	-.0303528805
N2	-.0129487910	.0256054963	2.1851214513
N3	2.0611932575	.1022929580	.0783443219
N4	.1891298499	-2.1680735255	.2157694018
N5	2.7200922465	-.6616855188	.9874079682
N6	.9578743675	-.7184254194	2.7858904511
N7	1.1119361657	-2.6026836536	1.1168417337
B8	1.9356110442	-1.5886720592	1.9492505436
C9	-.6845723420	.6489204241	3.1623512509
C10	2.9840504458	.8024491533	-.5916764574
C11	-.3800706435	-3.2511244297	-.3233954410
C12	1.1173704697	-3.9559414455	1.1385196389
C13	.8899681649	-.5566404317	4.1265550137
C14	4.0509761048	-.4388497608	.8887123558

H15	2.6927073006	-2.1675520527	2.6770253714
C16	4.2674446654	.4953736171	-.1139153732
C17	.1761764226	-4.4155805068	.2287159997
C18	-.1511587850	.3141377402	4.4153870460
H19	-1.5225543517	1.2858623217	2.9211232584
H20	2.6836926859	1.4855040647	-1.3733068688
H21	-1.1572596554	-3.1375264376	-1.0650514975
H22	1.7880421561	-4.4882797315	1.7964832531
H23	1.5838770309	-1.0726970317	4.7731184378
H24	4.7408710569	-.9593822127	1.5361024754
H25	5.2117975978	.8942987506	-.4507236883
H26	-.0718933761	-5.4401767604	-.0019615755
H27	-.4783060094	.6536145025	5.3860153195
O28	-.0286697275	-.1433798904	-3.0462473069
C29	-.0925870487	-.0951583719	-1.8901880337
C30	-.2585556534	2.2426504755	-.0815435898
H31	-.0175761092	2.5139600840	-1.1116212831
H32	.6193642471	2.4256214448	.5403862170
C33	-1.4134450524	3.1539071448	.4023366258
H34	-1.6555059154	2.9292865004	1.4475872818
H35	-2.3245970603	2.9643139303	-.1770557652
C36	-.2543773898	7.3085622731	.0115223686
C37	-1.0396957190	6.7031110006	-.9715171642
C38	-1.4255432868	5.3683073298	-.8358074766
C39	-1.0365132241	4.6163742954	.2804289499
C40	-.2502487855	5.2371799691	1.2614436672
C41	.1390789529	6.5702129767	1.1304683473
H42	.0463906698	8.3474165002	-.0913344316
H43	-1.3548585878	7.2702009587	-1.8435857849
H44	-2.0402724168	4.9026577399	-1.6033114921
H45	.0585455925	4.6676607868	2.1353779515
H46	.7474870948	7.0338320316	1.9029069141
H47	-1.3578069992	1.0196398794	.0440993488
C48	-5.0456196218	-.8923134528	-.1459693283
C49	-4.2707132654	-1.2138288214	.9707103368
C50	-2.9160472739	-.8781504943	1.0156284530
C51	-2.2879580970	-.2259880295	-.0632655419
C52	-3.0935409323	.1011448738	-1.1724703003
C53	-4.4500087679	-.2279120254	-1.2184069971
H54	-6.1002770724	-1.1509585030	-.1766705417
H55	-4.7212181461	-1.7328044656	1.8131336834
H56	-2.3374136959	-1.1495572449	1.8911271534
H57	-2.6579457257	.6284770646	-2.0174177217
H58	-5.0377274465	.0368528876	-2.0937946199

TS3
Gas phase Energy: -1298.53505262389 hartrees
Solvation Energy:-1298.54227357060 hartrees
Zero Point Energy: 259.120 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-439.64 cm^{-1})
Coordinates:

Ru1	-0.0286068800	-0.2880575951	-0.0758177680
N2	-0.0633583676	0.1643960102	2.0836240463
N3	2.2145678750	-0.0360331354	0.1326878210
N4	0.3429603054	-2.2804097443	0.5417334054
N5	2.8080450641	-0.5932091352	1.2219009335

N6	0.8961135290	-0.3963303444	2.8656273132
N7	1.2163258170	-2.5208471830	1.5579250657
B8	1.9582412779	-1.3559915136	2.2647224287
C9	-0.8298350024	0.9136873689	2.8865408854
C10	3.1887564423	0.5172315009	-0.5981522803
C11	-0.1391796209	-3.4636318614	0.1433217412
C12	1.2734803615	-3.8520445695	1.7946458855
C13	0.7309368258	0.0010321991	4.1477104666
C14	4.1453936540	-0.3857110258	1.1725082044
H15	2.6601373892	-1.7859954984	3.1373546462
C16	4.4361052450	0.3270108545	0.0193244743
C17	0.4221648077	-4.4963707776	0.9095199141
C18	-0.3668478442	0.8467430493	4.2092513986
H19	-1.6710962939	1.4585553543	2.4832667066
H20	2.9520526066	1.0184323290	-1.5262846416
H21	-0.8570524150	-3.5092969346	-0.6620629013
H22	1.9148408157	-4.2386059073	2.5723719908
H23	1.4034612155	-0.3473018136	4.9172147536
H24	4.7864349285	-0.7603790334	1.9566606396
H25	5.4039364484	0.6562517874	-0.3263085525
H26	0.2332979033	-5.5556718846	0.8289145817
H27	-0.7726808070	1.3392186630	5.0793659888
O28	0.1322094237	-1.0666214145	-2.9903709567
C29	0.0655152313	-0.7518073458	-1.8728329141
C30	-2.1428984711	-0.3813118930	-0.0596588021
C31	-2.0116642071	0.9929823670	-0.4908727493
H32	-2.5507733370	-1.0840092053	-0.7840738649
H33	-2.2012064148	1.1803755287	-1.5428229794
H34	-2.4324918909	1.7689828948	0.1456464936
H35	-2.5083657791	-0.5545744461	0.9512487813
C36	-0.2821159024	2.1073555611	-0.4205529338
H37	0.7725611643	1.8883061336	-0.5815725644
H38	-0.3807222110	2.5225930458	0.5823064187
C39	-0.7018351695	3.1156331965	-1.4960399346
H40	-0.5916415123	2.6586996916	-2.4868197261
H41	-1.7586550902	3.3869001601	-1.3868525573
C42	0.1414088736	4.3741612068	-1.4171823452
C43	1.7442812128	6.6789873335	-1.1863082213
C44	1.3937593879	4.4440339572	-2.0433824676
C45	-0.2954687497	5.4817782762	-0.6782158986
C46	0.4967888833	6.6255721284	-0.5625149248
C47	2.1899855646	5.5832621449	-1.9292946127
H48	1.7440092584	3.5973370072	-2.6301631602
H49	-1.2677297902	5.4475488203	-0.1925374089
H50	0.1379740932	7.4749770344	0.0124247153
H51	3.1566929544	5.6182103937	-2.4230499430
H52	2.3625123539	7.5677527030	-1.0978015879

Ir.Tp.CO^{+}

A
Gas phase Energy: -1230.56473888375 hartrees

Solvation Energy:-1230.60307505538 hartrees
Zero Point Energy: 225.450 kcal/mol
Coordinates:

Ir1	-2.4435141011	1.5426983075	-0.1318200231
N2	-2.4654506480	3.6589174793	-0.3064878603
N3	-4.5353835931	1.6490914240	-0.1415066553
N4	-2.6797829278	1.5459405698	-2.3565516074
N5	-5.1658360937	2.5085461990	-0.9912288734
N6	-3.3514501643	4.2351722590	-1.1721702008
N7	-3.5595661224	2.4245385009	-2.9066672390
B8	-4.3553430827	3.3786560890	-1.9900787737
C9	-1.7567923050	4.6512222627	0.2623334011
C10	-5.4724995927	1.0034851230	0.5729786170
C11	-2.1877598370	0.7941374726	-3.3542913712
C12	-3.6126347516	2.2266924060	-4.2422349223
C13	-3.1869752870	5.5732651744	-1.1430377275
C14	-6.4976400895	2.3922597717	-0.8079756696
H15	-5.0824972694	4.0791862281	-2.6246545623
C16	-6.7372243950	1.4438224172	0.1795369227
C17	-2.7478107511	1.1920204761	-4.5724638520
C18	-2.1761188443	5.8833312568	-0.2411818109
H19	-1.0121626548	4.4429058746	1.0148638067
H20	-5.1879163730	0.2908059245	1.3323238143
H21	-1.4672675039	0.0131513225	-3.1578612873
H22	-4.2591762399	2.8325344771	-4.8592717370
H23	-3.8009028902	6.2098102706	-1.7623926356
H24	-7.1792669533	2.9909543148	-1.3934298375
H25	-7.6918182444	1.1197306272	0.5632605712
H26	-2.5508384549	0.7835262954	-5.5513473278
H27	-1.8019244938	6.8607545798	0.0200684290
O28	-2.4976736266	-1.4830365911	-0.0461811419
C29	-2.4748066025	-0.3384755116	-0.0618683698
C30	-0.2637809717	1.6019810433	-0.7966694241
C31	-0.2643723760	1.6136798915	0.5878702990
H32	-0.0527038512	0.6858633514	-1.3372773675
H33	-0.0702092383	0.7094578737	1.1517763491
H34	-0.1551672192	2.5322871965	1.1488136100
H35	-0.1815983504	2.5218875156	-1.3643244743
C37	-3.0182555652	1.7712565828	4.7791666396
C38	-3.4684233963	2.7963844250	3.9476975829
C39	-3.2824389353	2.7251674151	2.5632595806
C40	-2.6299169806	1.6280444117	1.9844949012
C41	-2.1906522670	0.5973687464	2.8298203978
C42	-2.3833379617	0.6666972536	4.2128377319
H43	-3.1636770892	1.8298722254	5.8531607327
H44	-3.9735484064	3.6597896631	4.3708839579
H45	-3.6628862442	3.5305981645	1.9466133796
H46	-1.6839696184	-0.2787542536	2.4338503666
H47	-2.0318313962	-0.1464782127	4.8411923948

B
Gas phase Energy: -1230.58298076215 hartrees
Solvation Energy:-1230.61959926768 hartrees
Zero Point Energy: 226.329 kcal/mol
Coordinates:

Ir1	-2.4659102311	1.3981411693	-0.2761603246

N2	-2.3864231653	3.5295443759	-0.2641133062
N3	-4.5063933649	1.6578443087	-0.1612385904
N4	-2.7006801766	1.5907284138	-2.4859077389
N5	-5.1199545061	2.5609935008	-0.9752613371
N6	-3.2445713280	4.2081167591	-1.0766382961
N7	-3.5559912871	2.5437661301	-2.9453463491
B8	-4.2905775688	3.4560805352	-1.9428004920
C9	-1.6721269044	4.4463793869	0.4141444218
C10	-5.4468209560	1.0585687480	0.5874047492
C11	-2.2492714166	0.9150837865	-3.5528386254
C12	-3.6305711244	2.4694264995	-4.2933546471
C13	-3.0612175922	5.5339822557	-0.9093293943
C14	-6.4463625232	2.5279819044	-0.7278954822
H15	-5.0031955074	4.2288550910	-2.5072143633
C16	-6.6993937584	1.5820688892	0.2581042346
C17	-2.8071448304	1.4391352083	-4.7252854664
C18	-2.0600732387	5.7324569882	0.0327663691
H19	-0.9303749606	4.1453682360	1.1380254790
H20	-5.1774688495	0.3006453786	1.3076153345
H21	-1.5596259459	0.0929528952	-3.4275183732
H22	-4.2616583594	3.1496252549	-4.8455551524
H23	-3.6564004022	6.2401025645	-1.4686282545
H24	-7.1145835162	3.1800718346	-1.2700618565
H25	-7.6541451530	1.3095379563	0.6797132502
H26	-2.6376288579	1.1124661007	-5.7394626371
H27	-1.6714512511	6.6713515000	0.3946044678
O28	-2.7478263844	-1.6077572616	-0.3025884212
C29	-2.6226329143	-0.4660823809	-0.2933893024
C30	-2.2753597324	1.4167247423	1.8509800947
H31	-2.7973153436	0.5580353907	2.2797804188
H32	-2.7577979749	2.3241339755	2.2195812956
C33	-0.7759424005	1.3617254220	2.2246762531
H34	-0.6052332317	0.8227835978	3.1616899553
H35	-0.3673173389	2.3694267082	2.3624849463
C36	0.9309064646	-0.6049049174	-1.2403562313
C37	0.4520073361	0.6915478266	-1.3370233306
C38	-0.0769213798	1.3532125173	-0.1934928060
C39	-0.0740850238	0.6861465550	1.0747642229
C40	0.4223419893	-0.6173794091	1.1493061564
C41	0.9305920535	-1.2456355790	0.0104547863
H42	1.3339729491	-1.1126209701	-2.1101136711
H43	0.4973676477	1.2289482004	-2.2786664126
H44	-0.0955797508	2.4394724172	-0.2160576424
H45	0.4133871266	-1.1417530998	2.0999225535
H46	1.3287717471	-2.2529157752	0.0936992320

D
Gas phase Energy: -1462.83129402175 hartrees
Solvation Energy:-1462.86824716210 hartrees
Zero Point Energy: 290.184 kcal/mol
Coordinates:

Ir1	-2.4782691281	1.8612221707	-0.2966593643
N2	-2.9397036701	3.9286092224	-0.4954606674
N3	-4.4903764341	1.6125758287	-0.0074992751
N4	-2.9587720177	1.6650151119	-2.4949781430
N5	-5.3703549210	2.2707655288	-0.8160546938

N6	-3.9783366827	4.2852874554	-1.3063725321
N7	-4.0469816726	2.3488571469	-2.9427024315
B8	-4.8741390650	3.2041747583	-1.9639119703
C9	-2.4455401753	5.0581992453	0.0418097376
C10	-5.1953911045	0.8841352163	0.8754846090
C11	-2.5378218512	0.8905314335	-3.5052607418
C12	-4.2977247524	2.0096480222	-4.2280879949
C13	-4.1231613086	5.6264637080	-1.2752245533
C14	-6.6234960052	1.9527778352	-0.4301820517
H15	-5.8048090868	3.7090862367	-2.5143645133
C16	-6.5589663250	1.0709497292	0.6417084903
C17	-3.3505362038	1.0794529093	-4.6304976401
C18	-3.1583853228	6.1623342288	-0.4313140332
H19	-1.6289668138	5.0260497335	0.7476975091
H20	-4.6948070248	0.2806874095	1.6163421181
H21	-1.6798669375	0.2471313300	-3.3793216825
H22	-5.1273445582	2.4518403026	-4.7595306893
H23	-4.9034899311	6.1032397536	-1.8494504223
H24	-7.4715054769	2.3774678788	-0.9462682060
H25	-7.3814639297	0.6263302788	1.1797389354
H26	-3.2622479980	0.6056778067	-5.5958038838
H27	-2.9998991345	7.2008710361	-0.1864247174
O28	-1.9977579648	-1.1138097748	-0.0966413626
C29	-2.1517598670	0.0224121404	-0.1527229879
C30	-2.2167840653	2.2201447088	1.7891315452
H31	-3.1153395370	2.7577303708	2.1066903860
H32	-1.3813674906	2.9234192511	1.8901802256
C33	-1.9711476845	1.0254023340	2.7275199823
H34	-1.1118073725	0.4381164097	2.3843082213
H35	-2.8315397150	0.3451827566	2.7082795752
C36	-1.2427046761	2.3664932787	6.7782395346
C37	-2.5498484983	2.2695422265	6.2956630809
C38	-2.7843164681	1.8266089447	4.9941687120
C39	-1.7192934550	1.4734060012	4.1545713732
C40	-0.4133663921	1.5729231156	4.6510557942
C41	-0.1736394960	2.0155734244	5.9527419626
H42	-1.0596197019	2.7060299785	7.7930448074
H43	-3.3868163872	2.5324363835	6.9356767119
H44	-3.8060264929	1.7454505961	4.6292194482
H45	0.4254362773	1.2848275609	4.0200842019
H46	0.8452358352	2.0780787300	6.3234085968
C47	0.5670866711	1.4980906956	0.1655163700
C48	-0.0622197641	2.5177710186	-0.5953705535
H49	0.5278440241	1.5432553803	1.2477808063
H50	-0.3367993681	3.4445257509	-0.1057571076
C52	1.3513106859	0.4654177868	-1.8677308019
C53	1.2519882811	0.4672326629	-0.4717127189
H54	1.9051472985	-0.3268445982	-2.3630276607
H55	1.7252194047	-0.3165486371	0.1103303529
C56	0.7573958485	1.4769375442	-2.6350731329
C57	0.0616171320	2.5038750433	-2.0068801613
H58	0.8581542595	1.4691728318	-3.7153746305
H59	-0.3793144555	3.3073197685	-2.5867462458

E
Gas phase Energy: -1462.82727333094 hartrees

Solvation Energy:-1462.86353318977 hartrees
Zero Point Energy: 289.214 kcal/mol
Coordinates:

Ir1	-0.1512527304	-0.1613438627	0.0273321026
N2	-0.1082849669	-0.1517679273	2.1301061974
N3	2.0456871431	0.1490775904	0.1705955982
N4	0.2246186290	-2.1513038136	0.1515598230
N5	2.7258445722	-0.6206243969	1.0650125051
N6	0.8904480434	-0.8228339550	2.7740341910
N7	1.1692175598	-2.5978374246	1.0285394775
B8	1.9488793207	-1.6119341212	1.9568509638
C9	-0.8925156537	0.4136538631	3.0639528140
C10	2.9485672192	0.9021320436	-0.4757344026
C11	-0.3033498418	-3.2091724197	-0.4885763143
C12	1.2290896650	-3.9424801685	0.9302120494
C13	0.7301269433	-0.6695982429	4.1046039074
C14	4.0465977409	-0.3439071882	0.9805195913
H15	2.6819021228	-2.2165449165	2.6774440530
C16	4.2339695765	0.6277192581	0.0067889636
C17	0.3134277605	-4.3719291499	-0.0240728775
C18	-0.3934481041	0.1170644119	4.3345384000
H19	-1.7698977653	0.9723927019	2.7741690887
H20	2.6383282106	1.5951213472	-1.2451704973
H21	-1.0893888599	-3.0747831374	-1.2159264587
H22	1.9187917464	-4.4986711077	1.5473079864
H23	1.4218405117	-1.1315228887	4.7933600279
H24	4.7551614278	-0.8547055950	1.6155325200
H25	5.1650480411	1.0714536481	-0.3099884814
H26	0.1160974307	-5.3850170467	-0.3380082621
H27	-0.7970674601	0.4235370860	5.2867215060
O28	-0.1699107036	-0.2512051228	-3.0053098691
C29	-0.1636617532	-0.2090733924	-1.8611813977
C30	-0.3244706281	2.5786342645	-0.0219106655
H31	-0.0484527315	2.6913164349	-1.0700072305
H32	0.5557217248	2.6548039126	0.6137195300
C33	-1.4505984326	3.5539773030	0.3857725069
H34	-1.6913824556	3.4044432933	1.4428920423
H35	-2.3533674836	3.3270317716	-0.1889096062
C36	-0.1612202197	7.6131188532	-0.3342988305
C37	-0.8340283759	6.9043860776	-1.3321246318
C38	-1.2528109104	5.5950943252	-1.0968543444
C39	-1.0082499055	4.9805056014	0.1389493328
C40	-0.3287177705	5.6981132300	1.1325465028
C41	0.0899047393	7.0079786972	0.8990643600
H42	0.1595679999	8.6345138689	-0.5145666110
H43	-1.0403980613	7.3736964801	-2.2891948292
H44	-1.7895001449	5.0526317216	-1.8720922485
H45	-0.1416812525	5.2353744582	2.0989507307
H46	0.6040541732	7.5580954392	1.6812539877
H47	-0.8399725066	1.5609959857	0.1269406055
C48	-5.0214996668	-0.7920764316	0.1543414219
C49	-4.1919423319	-1.5248020962	1.0039060018
C50	-2.8037530755	-1.3631189268	0.9529061756
C51	-2.2185962354	-0.4613351612	0.0521398624
C52	-3.0652176255	0.2592239218	-0.8078406492
C53	-4.4528351573	0.1013761470	-0.7538847876

H54	-6.0987763608	-0.9190189742	0.1955458697
H55	-4.6218094975	-2.2269797987	1.7124479916
H56	-2.1841268497	-1.9432816446	1.6284682112
H57	-2.6555905108	0.9572022092	-1.5348854306
H58	-5.0841407204	0.6740430900	-1.4273770037

G
Gas phase Energy: -1309.19620732843 hartrees
Solvation Energy:-1309.23492488040 hartrees
Zero Point Energy: 261.210 kcal/mol
Coordinates:

Ir1	-2.5412816660	1.7632254098	-0.2181269461
N2	-2.8089911905	3.8370070371	-0.5776530478
N3	-4.6160643351	1.6980685511	0.1092562766
N4	-3.1496316906	1.4533305934	-2.3649890177
N5	-5.4491405216	2.4038227274	-0.7058926261
N6	-3.8643901390	4.2373632520	-1.3464644902
N7	-4.1631675395	2.2224788363	-2.8423698915
B8	-4.8867550897	3.2154305790	-1.9070556325
C9	-2.1585699494	4.9466181411	-0.1829193745
C10	-5.3729563757	1.0467064656	1.0100333832
C11	-2.7792065765	0.6230075538	-3.3527219232
C12	-4.4231222388	1.8775411613	-4.1235184789
C13	-3.8633891813	5.5834931077	-1.4298680607
C14	-6.7215513454	2.1915126474	-0.3122162711
H15	-5.7674204255	3.7794065759	-2.4806050947
C16	-6.7194816617	1.3329684512	0.7809447672
C17	-3.5571914630	0.8574164036	-4.4919280244
C18	-2.7871833481	6.0783989740	-0.7042382642
H19	-1.2928299190	4.8890169331	0.4584346895
H20	-4.9166574083	0.4259269534	1.7665293988
H21	-1.9857002391	-0.0954147302	-3.2056296699
H22	-5.2023723837	2.3792834615	-4.6774711619
H23	-4.6283809027	6.0935833200	-1.9957276661
H24	-7.5374805540	2.6650269589	-0.8372548936
H25	-7.5712007085	0.9672838408	1.3326256014
H26	-3.4977048831	0.3545752649	-5.4447402703
H27	-2.5023915836	7.1097051893	-0.5665468705
O28	-2.2954840139	-1.2201319036	0.2255739026
C29	-2.3777685013	-0.0861697958	0.0823878507
C30	-2.3944601105	2.2376807083	1.8967556702
H31	-3.4003328823	2.5762725513	2.1521905151
H32	-1.7350860808	3.1013885873	1.9968272530
C33	-1.9478472367	1.1302302012	2.8621972345
H34	-0.9824127808	0.7114838451	2.5547868816
H35	-2.6656767796	0.3006894728	2.8457871767
C36	-1.5921207371	2.6841640141	6.8852303518
C37	-2.8117693363	2.1719191389	6.4381206149
C38	-2.9242500723	1.6633352561	5.1439467451
C39	-1.8222053354	1.6573468970	4.2794897713
C40	-0.6027791505	2.1732970958	4.7394469920
C41	-0.4860501198	2.6828985133	6.0327262072
H42	-1.5017143699	3.0745431978	7.8941431644
H43	-3.6733383004	2.1614690045	7.0993334583
H44	-3.8748424508	1.2554568821	4.8067848505
H45	0.2675715888	2.1615070569	4.0861223584

H46	0.4686843204	3.0696117743	6.3773676821
C47	-0.3019739738	2.0798505477	0.0649213099
H48	0.0761048543	1.2956511788	0.7102162758
H49	-0.1624374116	3.0893491361	0.4287143869
C50	-0.5404828574	1.8432115882	-1.2801130104
H51	-0.3475206099	0.8680378461	-1.7121000583
H52	-0.6335706637	2.6651294564	-1.9805474842

TS1
Gas phase Energy: -1230.53765495878 hartrees
Solvation Energy:-1230.57495959577 hartrees
Zero Point Energy: 224.784 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-319.26 cm^{-1})
Coordinates:

Ir1	-.0222806431	-.0822770006	.0397155847
N2	-.0336359283	-.0529625002	2.1813498497
N3	2.1328174734	.0959315720	.1998748853
N4	.2440144222	-2.1689783591	.3117164396
N5	2.7854762264	-.6626341119	1.1192270920
N6	.9404529102	-.7515744206	2.8298498856
N7	1.1895359025	-2.6119064395	1.1849963247
B8	1.9870372326	-1.5998175288	2.0486508521
C9	-.8420724099	.4681218471	3.1229506747
C10	3.0487296606	.8327736510	-.4455146277
C11	-.3193345009	-3.2429140788	-.2642325874
C12	1.2085634875	-3.9617763716	1.1605238901
C13	.7433507816	-.6589344446	4.1606651834
C14	4.1095374021	-.3981712577	1.0532659270
H15	2.7109726940	-2.1692193306	2.8073483340
C16	4.3225359928	.5516598290	.0632616687
C17	.2630225842	-4.4070446691	.2455350243
C18	-.3847031332	.1175603925	4.3945938460
H19	-1.6998432668	1.0648214556	2.8525323064
H20	2.7488461534	1.5236691944	-1.2199082972
H21	-1.1009790685	-3.1253094915	-1.0003655687
H22	1.8893210391	-4.5079423357	1.7962381475
H23	1.4160997764	-1.1531701358	4.8454437499
H24	4.8012245040	-.9013864149	1.7124948939
H25	5.2642431945	.9782052272	-.2459022232
H26	.0263585725	-5.4271853772	-.0130573577
H27	-.8140766595	.3880853084	5.3464120403
O28	.0989402048	-.5127817013	-2.9437749845
C29	.0448843202	-.3117242751	-1.8148947404
C30	-2.1649693820	-.0656542408	.0767907932
C31	-2.0825080204	1.3736965152	-.0054704868
H32	-2.6042874213	-.5663934992	-.7828416587
H33	-2.3733072179	1.8571887689	-.9304008828
H34	-2.2767627242	1.9739553925	.8757647274
H35	-2.4863447797	-.4864786399	1.0260947388
C36	1.0449423455	4.6531906406	-.5068992011
C37	.8786419860	4.1173093767	.7731385028
C38	.2776384555	2.8721334363	.9429916462
C39	-.1582086003	2.1140235049	-.1669111591
C40	-.0124740626	2.6949219042	-1.4495688586
C41	.5900481745	3.9389899011	-1.6195785475
H42	1.5135609765	5.6241618542	-.6357480593

H43	1.2234191635	4.6680652039	1.6430282179
H44	.1779704187	2.4776003237	1.9461951969
H45	-.3847706176	2.1783592505	-2.3296682837
H46	.6970225810	4.3535655955	-2.6172340816

TS2
Gas phase Energy: -1462.79489112585 hartrees
Solvation Energy:-1462.83062450321 hartrees
Zero Point Energy: 287.201 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-1156.58 cm^{-1})
Coordinates:

Ir1	-0.0977983899	-0.0249762058	0.0248643332
N2	0.0365034521	-0.0141121830	2.1376958196
N3	2.0554791813	0.0723395806	0.0861683689
N4	0.1868663507	-2.1424095783	0.1724596112
N5	2.7330101603	-0.7265689301	0.9567458670
N6	0.9811135620	-0.7877054357	2.7475033702
N7	1.1035942183	-2.6368801671	1.0502157872
B8	1.9535222911	-1.6680362627	1.9091918533
C9	-0.6217260266	0.6576855546	3.0990391903
C10	2.9609309073	0.7843446821	-0.6034583345
C11	-0.4238798521	-3.1821331663	-0.4161296118
C12	1.0653383952	-3.9863260581	1.0059491190
C13	0.9077724912	-0.5963675859	4.0805041011
C14	4.0578261047	-0.5091390197	0.8120859862
H15	2.6972565471	-2.2683211512	2.6226742190
C16	4.2489739775	0.4489906580	-0.1755770362
C17	0.1048408683	-4.3771607351	0.0811342275
C18	-0.1041032334	0.3183179403	4.3503077663
H19	-1.4296093135	1.3278449969	2.8457379753
H20	2.6481258129	1.4923177279	-1.3575343655
H21	-1.2036053614	-3.0179822236	-1.1455125851
H22	1.7223274660	-4.5709777513	1.6324330239
H23	1.5785936103	-1.1231040734	4.7425877917
H24	4.7682743803	-1.0491514619	1.4199841404
H25	5.1851996127	0.8472214133	-0.5341807707
H26	-0.1726833509	-5.3826747464	-0.1940562346
H27	-0.4207860927	0.6845360790	5.3142750374
O28	-0.0770668269	-0.0817871755	-3.0030587385
C29	-0.1060415711	-0.0570481946	-1.8586196919
C30	-0.2190522437	2.2612665910	0.0592801850
H31	0.2754265685	2.5091046939	-0.8791806494
H32	0.4595243287	2.4340931509	0.8926649072
C33	-1.4904296806	3.1373253443	0.2018993239
H34	-1.9938203501	2.9328453192	1.1542129452
H35	-2.2108304320	2.9050086467	-0.5885042418
C36	-0.3884050386	7.3113718173	-0.0342733802
C37	-0.8594027073	6.6452005026	-1.1672295592
C38	-1.2179962322	5.2990668951	-1.0875408176
C39	-1.1135316829	4.6038366232	0.1241360096
C40	-0.6388323623	5.2811377861	1.2551111586
C41	-0.2789059966	6.6264323672	1.1778037100
H42	-0.1144287790	8.3602403048	-0.0936523843
H43	-0.9561566309	7.1746736994	-2.1102195223
H44	-1.5967480835	4.7889949265	-1.9707044591
H45	-0.5634329521	4.7570108844	2.2053851547

H46	0.0785025696	7.1419043234	2.0641525831
H47	-1.3216537968	1.0509437607	0.1893647781
C48	-5.0163928473	-0.7584386000	-0.0091036775
C49	-4.2343135957	-1.1609616589	1.0765906490
C50	-2.8673041284	-0.8827512570	1.1087748438
C51	-2.2583817409	-0.2042115158	0.0396761270
C52	-3.0549790247	0.1994104540	-1.0470543611
C53	-4.4235711317	-0.0759969993	-1.0711129103
H54	-6.0805178117	-0.9719218493	-0.0242031064
H55	-4.6886854965	-1.6961539550	1.9048219636
H56	-2.2799558720	-1.2120478979	1.9570729016
H57	-2.6210018763	0.7485421026	-1.8777453781
H58	-5.0203359695	0.2471836290	-1.9185159293

TS3
Gas phase Energy: -1309.15260500323 hartrees
Solvation Energy:-1309.18981195820 hartrees
Zero Point Energy: 260.769 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-395.36 cm^{-1})
Coordinates:

Ir1	-0.0193365148	-0.3098536332	-0.0793894101
N2	-0.0477558702	0.1507957239	1.9860055311
N3	2.1741150105	-0.0591706114	0.0624684890
N4	0.3244334101	-2.2707921950	0.5265053644
N5	2.8031560457	-0.6004596440	1.1392774542
N6	0.9117294219	-0.3898681313	2.7872792469
N7	1.2253030056	-2.5212960501	1.5170862735
B8	1.9841242869	-1.3554714557	2.2089760526
C9	-0.8428425957	0.9066600839	2.7648011236
C10	3.1158279916	0.5123494785	-0.7057110719
C11	-0.2011612012	-3.4437061334	0.1355320492
C12	1.2574434415	-3.8512397826	1.7454322457
C13	0.7163944834	0.0276600291	4.0547350633
C14	4.1310743564	-0.3646694202	1.0481240267
H15	2.6883636123	-1.7692843658	3.0783880217
C16	4.3754105235	0.3471619919	-0.1180510497
C17	0.3658347907	-4.4783070263	0.8838546912
C18	-0.3945976844	0.8616717409	4.0863289338
H19	-1.6882804557	1.4343120009	2.3498060843
H20	2.8500309900	1.0105864020	-1.6273107875
H21	-0.9455879489	-3.4801673187	-0.6458329436
H22	1.9108690605	-4.2560762684	2.5037519249
H23	1.3785412914	-0.2980066964	4.8430015941
H24	4.8035387933	-0.7183675989	1.8155290309
H25	5.3267183785	0.6936985916	-0.4905411594
H26	0.1545687178	-5.5335041449	0.8091418021
H27	-0.8196515200	1.3610712974	4.9427952475
O28	0.1046402600	-1.0610101760	-3.0075352402
C29	0.0598408034	-0.7712704220	-1.8983085080
C30	-2.1205805972	-0.3320058015	-0.0786232908
C31	-1.9782835197	1.0403874732	-0.5447005800
H32	-2.5457070805	-1.0359887072	-0.7912411490
H33	-2.1382960355	1.2030350724	-1.6046960804
H34	-2.3835362998	1.8357389863	0.0728108039
H35	-2.5055309110	-0.4767137953	0.9282678308
C36	-0.2126768596	2.0904276822	-0.4658952168

H37	0.8511548350	1.8675692095	-0.5242220514
H38	-0.3829609897	2.5488632809	0.5058771096
C39	-0.5332533008	3.0304549508	-1.6373218881
H40	-0.4266729806	2.4937549059	-2.5871575866
H41	-1.5673921706	3.3872222899	-1.5788688620
C42	0.4238763325	4.2069042291	-1.6001389763
C43	2.2432234766	6.3408041201	-1.4505463391
C44	1.6027225428	4.1930868368	-2.3575449124
C45	0.1664771370	5.3057506090	-0.7693579639
C46	1.0694509377	6.3663415815	-0.6944578066
C47	2.5067780162	5.2532702175	-2.2856876248
H48	1.8040675120	3.3574967362	-3.0251325171
H49	-0.7509564566	5.3373611717	-0.1857310250
H50	0.8541934170	7.2143977752	-0.0515194786
H51	3.4106632052	5.2348387509	-2.8871481409
H52	2.9443197657	7.1678236105	-1.3957352184

Rh.Tp.CO^{+}

A
Gas phase Energy: -1235.32769960196 hartrees
Solvation Energy:-1235.36582789793 hartrees
Zero Point Energy: 224.462 kcal/mol
Coordinates:

Rh1	-2.4779481380	1.5602359803	-0.1295882483
N2	-2.4880292132	3.6595136204	-0.3135097190
N3	-4.5565025636	1.6544799386	-0.1364199194
N4	-2.6565091214	1.5176761424	-2.3928498321
N5	-5.1701680894	2.4871797369	-1.0207867375
N6	-3.3601665159	4.2159964686	-1.2021413268
N7	-3.5454350154	2.3930205411	-2.9355189030
B8	-4.3491271822	3.3440654437	-2.0250710024
C9	-1.7910192866	4.6621675803	0.2494623996
C10	-5.5044063896	1.0405775137	0.5907087593
C11	-2.1603448453	0.7853931355	-3.4018395850
C12	-3.5991713464	2.2115877005	-4.2745448361
C13	-3.2016697241	5.5561724282	-1.1935203595
C14	-6.5055274192	2.3893074844	-0.8466405133
H15	-5.0759877011	4.0384704902	-2.6680635163
C16	-6.7630093360	1.4768829460	0.1696160413
C17	-2.7248543043	1.1902140567	-4.6177064930
C18	-2.2066575210	5.8857183037	-0.2812879091
H19	-1.0558659721	4.4674831493	1.0154284565
H20	-5.2342001299	0.3521294176	1.3772361183
H21	-1.4302792266	0.0094923938	-3.2179459472
H22	-4.2518155109	2.8193265736	-4.8835089439
H23	-3.8079257345	6.1796476039	-1.8334685657
H24	-7.1758193841	2.9765810507	-1.4563660120
H25	-7.7239758308	1.1741514074	0.5551570994
H26	-2.5247281083	0.7957275065	-5.6017228423
H27	-1.8400221277	6.8690270161	-0.0311230490
O28	-2.6203580747	-1.4909359579	-0.1092744229

C29	-2.5522379829	-0.3545843562	-0.0844062567
C30	-0.2254963927	1.6223407778	-0.7919121609
C31	-0.2105202446	1.6018104336	0.5760767877
H32	-0.0689875324	0.7134816193	-1.3622274870
H33	-0.0470066577	0.6808969371	1.1224126728
H34	-0.1480354115	2.5098018477	1.1614843588
H35	-0.2007097200	2.5531279498	-1.3462706675
C37	-2.9761333007	1.7290833457	4.7601336789
C38	-3.4246251248	2.7716600102	3.9491114171
C39	-3.2593901205	2.7185165593	2.5603117512
C40	-2.6271870614	1.6194135916	1.9708095595
C41	-2.1874341793	0.5679637372	2.7853977027
C42	-2.3621146537	0.6239202602	4.1728658774
H43	-3.1074538157	1.7751904661	5.8364875846
H44	-3.9142204062	3.6352127642	4.3898814096
H45	-3.6382138906	3.5340933661	1.9574286457
H46	-1.6940888900	-0.3068960598	2.3719704060
H47	-2.0114840110	-0.2013297651	4.7856532758

B
Gas phase Energy: -1235.35686996163 hartrees
Solvation Energy:-1235.39346266770 hartrees
Zero Point Energy: 225.727 kcal/mol
Coordinates:

Rh1	-2.4656899658	1.3982983512	-0.2831912900
N2	-2.3952002512	3.5122331228	-0.2670937690
N3	-4.4997416537	1.6226132820	-0.1344321573
N4	-2.7023165094	1.5629049179	-2.5257067651
N5	-5.1217387751	2.5091093259	-0.9561986094
N6	-3.2670907892	4.1754169507	-1.0778070261
N7	-3.5801273641	2.5104408604	-2.9550583941
B8	-4.3085544401	3.4086623352	-1.9379666816
C9	-1.6867331177	4.4397691972	0.4006452444
C10	-5.4311142949	1.0279032477	0.6290045860
C11	-2.2558346515	0.9210086080	-3.6138861769
C12	-3.6736508820	2.4644681533	-4.3043754850
C13	-3.0973880275	5.5049347648	-0.9185316727
C14	-6.4466855414	2.4723956706	-0.7008750663
H15	-5.0387899480	4.1751643915	-2.4894772635
C16	-6.6892145346	1.5392896676	0.3004382542
C17	-2.8390871767	1.4588941717	-4.7695686386
C18	-2.0921823391	5.7203728035	0.0152548439
H19	-0.9328903936	4.1514540641	1.1177168302
H20	-5.1560980563	0.2828814656	1.3606309321
H21	-1.5462131716	0.1114326477	-3.5180708833
H22	-4.3233582097	3.1462803154	-4.8327699751
H23	-3.7034398814	6.2015148518	-1.4782005737
H24	-7.1214429954	3.1138088185	-1.2478441510
H25	-7.6397069643	1.2682860591	0.7328482614
H26	-2.6776936002	1.1579425403	-5.7930360024
H27	-1.7108442238	6.6655968593	0.3685029174
O28	-2.7846527656	-1.6309799934	-0.3813037595
C29	-2.6371682126	-0.5012461767	-0.3308879426
C30	-2.2704694824	1.3767465860	1.8266072885
H31	-2.7979134393	0.5022576025	2.2110331086
H32	-2.7625143443	2.2839333092	2.1764592190

C33	-0.7718082449	1.3158085575	2.1557783699
H34	-0.5933329835	0.7805206135	3.0945561718
H35	-0.3568327553	2.3213996797	2.2831297191
C36	0.9605234497	-0.6718693156	-1.2871592333
C37	0.5150163101	0.6382991032	-1.3866849158
C38	-0.0106208559	1.2995149267	-0.2504012400
C39	-0.0797882395	0.6250305072	1.0019931936
C40	0.3785610594	-0.6955393003	1.0799752059
C41	0.9042766341	-1.3283536541	-0.0466495195
H42	1.3751577783	-1.1801085118	-2.1514838040
H43	0.5909258232	1.1795865962	-2.3240866826
H44	-0.1038041763	2.3815532033	-0.2853112434
H45	0.3292463603	-1.2254802560	2.0266323568
H46	1.2747199473	-2.3458684549	0.0376807331

D
Gas phase Energy: -1467.60739236050 hartrees
Solvation Energy:-1467.64355565603 hartrees
Zero Point Energy: 289.508 kcal/mol
Coordinates:

Rh1	-2.5286056571	1.8957535413	-0.3116533711
N2	-2.9487160974	3.9578079061	-0.4853845224
N3	-4.5389194349	1.6559181346	0.0156969278
N4	-3.0499480705	1.6964816439	-2.5462038823
N5	-5.4134221130	2.3335542106	-0.7771378118
N6	-3.9938071193	4.3268098672	-1.2784099566
N7	-4.1403392127	2.4085340444	-2.9412987453
B8	-4.9201015377	3.2660566501	-1.9291648289
C9	-2.4243381368	5.0805547758	0.0353208700
C10	-5.2469202549	0.9264702314	0.8944486405
C11	-2.6798271528	0.9438217887	-3.5911249700
C12	-4.4432310485	2.1070627250	-4.2264178321
C13	-4.1147979632	5.6715515171	-1.2541829029
C14	-6.6690136240	2.0276043959	-0.3888140225
H15	-5.8549233472	3.7969251001	-2.4490330958
C16	-6.6103229739	1.1329279832	0.6730994170
C17	-3.5272093296	1.1727250555	-4.6849740142
C18	-3.1261716295	6.1957267261	-0.4313268986
H19	-1.5923207139	5.0402255438	0.7228287936
H20	-4.7526339565	0.3075792371	1.6269117751
H21	-1.8259977234	0.2864700027	-3.5149592315
H22	-5.2823735709	2.5775952723	-4.7172316038
H23	-4.8957703088	6.1581054723	-1.8192905679
H24	-7.5139483662	2.4683211261	-0.8965422411
H25	-7.4351978111	0.6931274977	1.2116301203
H26	-3.4794376845	0.7234131037	-5.6648257896
H27	-2.9440607123	7.2328473822	-0.1966256560
O28	-2.1389649031	-1.1244627304	-0.1674207787
C29	-2.2468251779	0.0109582811	-0.1932120847
C30	-2.2467410534	2.2179831893	1.7658626522
H31	-3.1427437937	2.7670232212	2.0603412583
H32	-1.3943958386	2.9023109053	1.8105723615
C33	-2.0083668145	1.0176890846	2.6863511775
H34	-1.1423298987	0.4358569308	2.3527842698
H35	-2.8684954943	0.3386934395	2.6681972242
C36	-1.3320935581	2.4419408805	6.7172147522

C37	-2.6347480222	2.2650400658	6.2453407122
C38	-2.8515692149	1.7956802100	4.9501340206
C39	-1.7717601410	1.4931164141	4.1094768236
C40	-0.4695161806	1.6752230890	4.5929300731
C41	-0.2488036217	2.1447336082	5.8882253898
H42	-1.1624878199	2.8029311286	7.7269381789
H43	-3.4813010393	2.4868629389	6.8881187252
H44	-3.8688003809	1.6529340058	4.5921257697
H45	0.3802710052	1.4311247094	3.9584858615
H46	0.7667145694	2.2706928343	6.2516250765
C47	0.5299790439	1.4229668019	0.0663645361
C48	-0.0698927096	2.4774907077	-0.6625043457
H49	0.5261516706	1.4526899625	1.1501559417
H50	-0.3455234378	3.3921493721	-0.1516508716
C52	1.2225938982	0.3921722823	-2.0024955778
C53	1.1597975672	0.3768876894	-0.6050593912
H54	1.7334402636	-0.4111745556	-2.5250941830
H55	1.6201935752	-0.4317539417	-0.0470470658
C56	0.6446707909	1.4372342305	-2.7358554161
C57	0.0030389557	2.4792931355	-2.0728330462
H58	0.7141445244	1.4439643885	-3.8188836770
H59	-0.4279728802	3.3044464248	-2.6290952508

E

G
Gas phase Energy: -1313.96206651892 hartrees
Solvation Energy:-1314.00038333931 hartrees
Zero Point Energy: 260.140 kcal/mol
Coordinates:

Rh1	-2.4939252439	1.7716565382	-0.2518727541
N2	-2.7630887268	3.8318615943	-0.5867266294
N3	-4.5432978541	1.6679229812	0.1300382603
N4	-3.1182475681	1.4550299534	-2.4441868343
N5	-5.3866741771	2.3644870770	-0.6755244783
N6	-3.8369130077	4.2242860024	-1.3285907758
N7	-4.1546110216	2.2314316909	-2.8598343562
B8	-4.8579528578	3.1944042078	-1.8815372559
C9	-2.1027816187	4.9431552042	-0.2174023161
C10	-5.2850747092	1.0180237708	1.0432217309
C11	-2.7704133288	0.6800005706	-3.4820368556
C12	-4.4495604185	1.9448060614	-4.1491449039
C13	-3.8411690125	5.5707865701	-1.4224589917
C14	-6.6550832424	2.1516805079	-0.2657911296
H15	-5.7612830946	3.7605222125	-2.4188287116
C16	-6.6370037055	1.2978486652	0.8304481805
C17	-3.5836980500	0.9550502892	-4.5895073876
C18	-2.7469754740	6.0724943561	-0.7290487469
H19	-1.2164038081	4.8890839301	0.3965392255
H20	-4.8193844684	0.4014105149	1.7974013127
H21	-1.9648461245	-0.0357280886	-3.3942533466
H22	-5.2502945663	2.4626597387	-4.6561495063
H23	-4.6207881213	6.0756704658	-1.9731624114
H24	-7.4780730851	2.6227041415	-0.7824023874
H25	-7.4806242312	0.9313342707	1.3941677755
H26	-3.5470145783	0.4979363468	-5.5661204531

H27	-2.4602599327	7.1053004919	-0.6065031674
O28	-2.2754714285	-1.2468934007	0.1492491487
C29	-2.3366687092	-0.1149476415	0.0292836948
C30	-2.2892823471	2.2437638994	1.8458496661
H31	-3.2818248999	2.6339257635	2.0686939669
H32	-1.5794003356	3.0683418776	1.8987144727
C33	-1.8985975904	1.1243948538	2.8094479320
H34	-0.9298248559	0.6896845479	2.5390687619
H35	-2.6338144824	0.3113698614	2.7777414554
C36	-1.6968881222	2.7955806060	6.7950473232
C37	-2.9213243203	2.3705902518	6.2745676394
C38	-2.9827087585	1.8205837600	4.9945381016
C39	-1.8228380917	1.6848918658	4.2193570511
C40	-0.6002045494	2.1169835298	4.7496715512
C41	-0.5356840340	2.6663163214	6.0304931551
H42	-1.6473588315	3.2196333236	7.7931689860
H43	-3.8264837907	2.4621000669	6.8672202776
H44	-3.9383750606	1.4842065307	4.5982703064
H45	0.3097201905	2.0084515580	4.1634091347
H46	0.4205264665	2.9863268596	6.4332601891
C47	-0.1571556301	2.0249415524	-0.0550802466
H48	0.1885435001	1.1800945638	0.5302011171
H49	-0.0256699738	3.0012058841	0.3930092957
C50	-0.4565688136	1.8973642108	-1.3847643122
H51	-0.3612274193	0.9435810769	-1.8909966801
H52	-0.6083637696	2.7662224143	-2.0147488258

TS1
Gas phase Energy: -1235.31051278440 hartrees
Solvation Energy:-1235.34799500711 hartrees
Zero Point Energy: 224.081 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-300.22 cm^{-1})
Coordinates:

Rh1	-.0153096274	-.0560543866	.0674744578
N2	-.0253135604	-.0399648710	2.1932961163
N3	2.1476273770	.1091266811	.1987853514
N4	.2141068344	-2.1753882150	.3048067375
N5	2.7837789646	-.6723837885	1.1090141884
N6	.9400478229	-.7652552163	2.8251074585
N7	1.1701368905	-2.6184905503	1.1648538869
B8	1.9764674861	-1.6136017104	2.0286326015
C9	-.8206819756	.4795718483	3.1453082965
C10	3.0760152536	.8497105182	-.4223791001
C11	-.3521011721	-3.2509376775	-.2643025579
C12	1.1935982597	-3.9689380814	1.1397620723
C13	.7488504494	-.6909817839	4.1589186048
C14	4.1116186097	-.4193903196	1.0612711814
H15	2.6994493954	-2.1934783388	2.7812411241
C16	4.3433896575	.5473140535	.0923409499
C17	.2381240750	-4.4162934209	.2364795772
C18	-.3652995561	.0996145970	4.4103520398
H19	-1.6682677364	1.0972696635	2.8885721594
H20	2.7903129741	1.5610368522	-1.1839448394
H21	-1.1439542581	-3.1382163285	-.9909184263
H22	1.8835738550	-4.5135500046	1.7669380271
H23	1.4164054278	-1.2062284650	4.8331947087

H24	4.7916725194	-.9413076058	1.7180546065
H25	5.2915111019	.9721462545	-.1986776070
H26	.0004412083	-5.4368729914	-.0197555491
H27	-.7870619745	.3617456939	5.3680328027
O28	.2097803093	-.5469653006	-2.9251734211
C29	.1020801010	-.3115291062	-1.8142402662
C30	-2.1653332516	-.0927217612	.0766798586
C31	-2.0934340533	1.3278569224	.0078439053
H32	-2.5328097993	-.6195172536	-.7995496946
H33	-2.3669183622	1.8236624294	-.9152390006
H34	-2.2611521098	1.9227332530	.8973122839
H35	-2.4195441054	-.5553183046	1.0248635844
C36	1.0288483884	4.6630616855	-.5400474897
C37	.8882020827	4.1325951554	.7451303829
C38	.3109091737	2.8769521802	.9330513492
C39	-.1227098317	2.1192243674	-.1699225201
C40	-.0072465858	2.6803803330	-1.4582692014
C41	.5742482492	3.9347369582	-1.6424450844
H42	1.4768125347	5.6417752681	-.6805202882
H43	1.2326047650	4.6949161806	1.6076397823
H44	.2300937799	2.4838382417	1.9382933007
H45	-.3890841077	2.1559824238	-2.3294286479
H46	.6586736129	4.3451851055	-2.6440592492

TS2
Gas phase Energy: -1467.56444955423 hartrees
Solvation Energy:-1467.59994975125 hartrees
Zero Point Energy: 286.356 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -1313.22 25.66 28.57 33.92 48.31 52.85
Coordinates:

Rh1	-.0935335799	-.0527878994	.0553671918
N2	.0459693883	-.0141959321	2.1547418610
N3	2.0679360693	.0975310884	.0963389793
N4	.1779418679	-2.1741274512	.2052529064
N5	2.7489200361	-.7160123709	.9474358616
N6	1.0056766336	-.7800291618	2.7466876163
N7	1.1250823146	-2.6441278752	1.0609569249
B8	1.9757055523	-1.6600670518	1.9020028345
C9	-.5880419120	.6648336709	3.1258533495
C10	2.9703660544	.8275833003	-.5765101146
C11	-.4298571395	-3.2294340971	-.3553595877
C12	1.1077761157	-3.9957562030	1.0350255748
C13	.9663080343	-.5779969569	4.0804587844
C14	4.0743223845	-.4895796161	.8109209106
H15	2.7269967569	-2.2524083043	2.6155839442
C16	4.2620007295	.4899342528	-.1556535262
C17	.1303208770	-4.4126406378	.1406819651
C18	-.0393997759	.3369884950	4.3684236989
H19	-1.4017286190	1.3334567397	2.8881246650
H20	2.6553004700	1.5521936852	-1.3143249708
H21	-1.2301075747	-3.0875248076	-1.0675605184
H22	1.7889013435	-4.5619774858	1.6527718755
H23	1.6544344382	-1.0990408651	4.7291626389
H24	4.7862664088	-1.0372198514	1.4103639728
H25	5.1966325436	.9011214999	-.5039594183

H26	-.1387576191	-5.4255894432	-.1152710346
H27	-.3330998419	.7107818655	5.3367936208
O28	.0515456849	-.2759975466	-2.9856406778
C29	-.0434303251	-.1707373192	-1.8550217942
C30	-.4036025656	2.2399083984	.0420500809
H31	-.0524877043	2.4521045902	-.9670443702
H32	.3948569260	2.3941963978	.7644878788
C33	-1.6159595760	3.1503580688	.3670986200
H34	-1.9753007857	2.9602038830	1.3838108652
H35	-2.4496563158	2.9446974834	-.3102244731
C36	-.3458388823	7.2610340850	-.0539444673
C37	-.9974458891	6.6175646098	-1.1080948567
C38	-1.4108722006	5.2923574547	-.9687973100
C39	-1.1833663848	4.5968517187	.2265207808
C40	-.5267056974	5.2508516786	1.2783219801
C41	-.1119583212	6.5751565172	1.1405556536
H42	-.0270265381	8.2933582777	-.1602164941
H43	-1.1897473136	7.1487505231	-2.0356241458
H44	-1.9283146610	4.7997646109	-1.7890566742
H45	-.3505631770	4.7250507965	2.2142561576
H46	.3871277832	7.0732890951	1.9662232035
H47	-1.3813606397	1.0705836204	.1682679749
C48	-4.9947207348	-.6974911311	-.1738806585
C49	-4.2791093180	-1.0153664731	.9840080653
C50	-2.9235382945	-.7013194169	1.0874478795
C51	-2.2662188500	-.0687515242	.0194113893
C52	-2.9952507469	.2510876334	-1.1416753955
C53	-4.3522065996	-.0602499347	-1.2364057889
H54	-6.0505834176	-.9393871716	-.2440431956
H55	-4.7767606285	-1.5115599604	1.8114823177
H56	-2.3833335585	-.9649235593	1.9881402060
H57	-2.5204148317	.7778683533	-1.9646715455
H58	-4.9026097050	.2015855159	-2.1347168635

TS3
Gas phase Energy: -1313.93019717026 hartrees
Solvation Energy:-1313.96749401223 hartrees
Zero Point Energy: 259.926 kcal/mol
Number and Magnitude of negative Eigen values: 1 (cm^{-1}) -349.77 26.50 32.27 35.08 60.29 63.81
Coordinates:

Rh1	-0.0552281935	-0.2696871572	-0.0165500322
N2	-0.1193972577	0.1528999112	2.0336000583
N3	2.1583453158	0.0519835705	0.1174122586
N4	0.3350317379	-2.2601711185	0.5560451516
N5	2.7792283290	-0.5097137042	1.1876198160
N6	0.8600964004	-0.3671464469	2.8206266566
N7	1.2472235886	-2.4823016964	1.5399416117
B8	1.9652453794	-1.2956636611	2.2385241407
C9	-0.9345919796	0.8716320024	2.8248818567
C10	3.1072823105	0.6412126652	-0.6267372743
C11	-0.1400137093	-3.4507811679	0.1576050579
C12	1.3388679795	-3.8120251228	1.7584242238
C13	0.6584487520	0.0268488822	4.0957474026
C14	4.1083952313	-0.2676517705	1.1171734160
H15	2.6730156458	-1.6934715118	3.1136511407

C16	4.3631540724	0.4695266555	-0.0304464199
C17	0.4716804310	-4.4695766062	0.8951199577
C18	-0.4785228686	0.8235487722	4.1448527084
H19	-1.7988003033	1.3779536158	2.4214386589
H20	2.8504687518	1.1611205577	-1.5394106329
H21	-0.8859545513	-3.5159371940	-0.6210378350
H22	2.0122718161	-4.1943322781	2.5111054413
H23	1.3355681530	-0.2878569803	4.8756973288
H24	4.7733998189	-0.6337833589	1.8853375270
H25	5.3169163899	0.8288406484	-0.3843000527
H26	0.3040258221	-5.5321354455	0.8131482241
H27	-0.9150186031	1.2972516606	5.0102110023
O28	0.2576436300	-1.0399031236	-2.9526093403
C29	0.1180263047	-0.7359677622	-1.8620601121
C30	-2.1457672872	-0.4337056981	-0.0597125347
C31	-2.0798655996	0.9359060838	-0.4933662304
H32	-2.4507549617	-1.1779904405	-0.7910570321
H33	-2.2283746731	1.1268881791	-1.5500744658
H34	-2.4975322190	1.7007123398	0.1522988726
H35	-2.4903079298	-0.6421912297	0.9490589275
C36	-0.3108959587	2.1295165505	-0.3870715688
H37	0.7513909688	1.9117789988	-0.4608196445
H38	-0.5104052418	2.5222365996	0.6064703795
C39	-0.7062721686	3.0751979317	-1.5189669091
H40	-0.5727538517	2.5861135046	-2.4904518879
H41	-1.7576627361	3.3709304393	-1.4400357880
C42	0.1895712893	4.2974113092	-1.4264201944
C43	1.8966699481	6.5105185417	-1.1708742769
C44	1.3707762628	4.3757525973	-2.1769239448
C45	-0.1255327893	5.3415814896	-0.5456063921
C46	0.7215536751	6.4422858061	-0.4192924513
C47	2.2183805117	5.4766083678	-2.0530554366
H48	1.6178286527	3.5807139075	-2.8775434297
H49	-1.0441598453	5.2988240788	0.0351717987
H50	0.4622248501	7.2480191407	0.2605576430
H51	3.1240925702	5.5312983440	-2.6494253989
H52	2.5548334186	7.3684562729	-1.0750918909

Ru.Tp.NH_3

A
Gas phase Energy: -1163.17280280227 hartrees
Solvation Energy:-1163.18196749761 hartrees
Zero Point Energy: 242.634 kcal/mol
Coordinates:

Ru1	-2.3882688522	1.5897181109	-0.1232154460
N2	-2.4500443355	3.7012854813	-0.3295111020
N3	-4.5551570304	1.6576104246	-0.1239890531
N4	-2.7068459247	1.5132507724	-2.3796272295
N5	-5.1863009958	2.5097640199	-0.9767476010
N6	-3.3620369086	4.2426164644	-1.1897350081
N7	-3.5917110913	2.3972814844	-2.9089632525

B8	-4.3652987333	3.3621287521	-1.9775002755
C9	-1.7764337957	4.7225295841	0.2143740834
C10	-5.5051142777	1.0534729509	0.6007319766
C11	-2.2291773541	0.7927087900	-3.4016421199
C12	-3.6697922061	2.2299613087	-4.2497193839
C13	-3.2492742423	5.5927103558	-1.1791351171
C14	-6.5239256415	2.4297771335	-0.7920687582
H15	-5.0978231412	4.0595039757	-2.6234394958
C16	-6.7755073959	1.5053126847	0.2117376478
C17	-2.8082847918	1.2054613604	-4.6130461664
C18	-2.2427427067	5.9451239043	-0.2946979436
H19	-1.0134009312	4.5370243813	0.9546217333
H20	-5.2288675019	0.3641174834	1.3851126548
H21	-1.4832125360	0.0299230144	-3.2270580895
H22	-4.3265342212	2.8501828517	-4.8413828931
H23	-3.8943166571	6.1971329274	-1.7989739981
H24	-7.1930645471	3.0350700709	-1.3852602186
H25	-7.7332952674	1.2105922572	0.6121942208
H26	-2.6210504871	0.8198645582	-5.6035869795
H27	-1.8984898030	6.9374223397	-0.0466261119
C28	-0.3008302082	1.5061059154	-0.8227451187
C29	-0.2772941035	1.6630091994	0.5604705491
H30	-0.0989749852	0.5331741607	-1.2690891038
H31	-0.0673102494	0.8184856423	1.2084271928
H32	-0.0695305158	2.6257006643	1.0132694221
H33	-0.1439563002	2.3504088585	-1.4865431962
C35	-3.1056194839	1.6721398848	4.7931955345
C36	-3.5540679744	2.7069102042	3.9686155381
C37	-3.3023065011	2.6825948970	2.5942073194
C38	-2.5868619267	1.6359966307	1.9725689949
C39	-2.1412107880	0.6146692754	2.8394111592
C40	-2.3950822642	0.6204905332	4.2165532093
H41	-3.3005930467	1.6895193896	5.8621324494
H42	-4.1070723194	3.5404218931	4.3969090150
H43	-3.6814109987	3.5004979347	1.9887559575
H44	-1.5409988394	-0.2102973405	2.4532639619
H45	-2.0242778340	-0.1933094452	4.8367171094
N46	-2.4643630156	-0.5869283352	-0.0320208736
H47	-2.8049723785	-0.8776172833	0.8834352721
H48	-3.1107767558	-0.9335418022	-0.7381979854
H49	-1.5670825050	-1.0463270994	-0.1821624630

D
Gas phase Energy: -1395.42389848699 hartrees
Solvation Energy:-1395.43311682084 hartrees
Zero Point Energy: 306.628 kcal/mol
Coordinates:

Ru1	-2.5811398059	1.9114260781	-.2303621754
N2	-2.9329633947	3.9663408848	-.5801776902
N3	-4.6164378714	1.7306730078	.0307972812
N4	-2.9916494877	1.5910021740	-2.4518179725
N5	-5.4554911979	2.3590290666	-.8403125103
N6	-3.9663016768	4.3014419685	-1.4045063897
N7	-4.0574570330	2.2790112109	-2.9398287864
B8	-4.8804829400	3.2053455521	-2.0087929069

C9	-2.3693187765	5.1109764556	-.1756335251
C10	-5.3824854915	1.1247971486	.9490139407
C11	-2.5086461992	.8667775190	-3.4694480342
C12	-4.2414783834	1.9865455819	-4.2502392341
C13	-4.0440380736	5.6503387251	-1.5097303163
C14	-6.7385650536	2.1421847799	-.4673092927
H15	-5.7776898858	3.7132112159	-2.6245747933
C16	-6.7402763702	1.3524154586	.6721314965
C17	-3.2655275983	1.0803745143	-4.6355848091
C18	-3.0357131156	6.2105079988	-.7420637873
H19	-1.5303776619	5.0880668335	.5043705258
H20	-4.9255765783	.5831340266	1.7640394561
H21	-1.6314333709	.2510000925	-3.3251174638
H22	-5.0460695275	2.4447807386	-4.8062670162
H23	-4.8102728524	6.1061737836	-2.1188492325
H24	-7.5496318006	2.5690835327	-1.0375673226
H25	-7.5948515404	1.0002497037	1.2290072729
H26	-3.1195628325	.6446874528	-5.6124171903
H27	-2.8165290176	7.2582070264	-.6050697319
C28	-2.3237568820	2.3017939212	1.8542943680
H29	-3.2374513589	2.7859560720	2.2297218053
H30	-1.5280071485	3.0543054110	1.9951334109
C31	-1.9926296309	1.1199321463	2.7945402672
H32	-1.1298504162	.5577328747	2.4091103561
H33	-2.8349488557	.4098256633	2.8207197746
C34	-1.1011542606	2.4344058128	6.8307049218
C35	-2.4236551221	2.2173380330	6.4366714825
C36	-2.7074649937	1.7774819132	5.1430870161
C37	-1.6818721037	1.5439471034	4.2160923304
C38	-.3602329679	1.7659811516	4.6279210020
C39	-.0686354035	2.2071089862	5.9188193193
H40	-.8785225234	2.7747886543	7.8382051616
H41	-3.2349442362	2.3885657739	7.1393536467
H42	-3.7404469112	1.6138314863	4.8431679078
H43	.4504360466	1.5896555829	3.9237592708
H44	.9644735891	2.3692862703	6.2150496589
C45	.7712864192	1.0028037294	-.1657885699
C46	-.0416003074	2.0021379529	-.7167618245
H47	.6028744802	.6747747985	.8568496267
H48	-.7458601304	2.5479619593	-.0463301378
C50	2.0294743801	.8899147139	-2.2278732879
C51	1.8003973349	.4406274837	-.9240146433
H52	2.8292325817	.4535099305	-2.8193198001
H53	2.4281434135	-.3376714017	-.4990170710
C54	1.2401995464	1.9104594697	-2.7661890503
C55	.2102376095	2.4725719483	-2.0104308047
H56	1.4253407478	2.2656474563	-3.7758391393
H57	-.4126860215	3.2581030373	-2.4234891437
N58	-2.3489888189	-.2577204201	-.0254433711
H59	-1.3758815023	-.5501123829	-.0955962523
H60	-2.7128220678	-.6184689288	.8512373347
H61	-2.8592049081	-.7017917021	-.7837212524

TS1

Gas phase Energy: -1163.13164772356 hartrees
Solvation Energy:-1163.14021504344 hartrees
Zero Point Energy: 242.104 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-345.15 cm^{-1})
Coordinates:

Ru1	-0.0860153711	-0.0769541750	0.1024465382
N2	-0.0500985118	-0.0874431541	2.2311860272
N3	2.1436973311	0.1596963261	0.2017580554
N4	0.3087300323	-2.1534168409	0.2750009111
N5	2.8062650494	-0.5967740111	1.1146994271
N6	0.9599484301	-0.7691300292	2.8451863540
N7	1.2556981483	-2.5895900261	1.1476139378
B8	2.0181525325	-1.5604721591	2.0275737693
C9	-0.8432795891	0.3834620201	3.2031359494
C10	3.0601017007	0.9181258460	-0.4093004021
C11	-0.2320488276	-3.2425802355	-0.2914369234
C12	1.3059651195	-3.9422015024	1.1296863439
C13	0.7936515560	-0.7175550298	4.1893365275
C14	4.1319332061	-0.3165252083	1.0752871747
H15	2.7637273079	-2.1325678152	2.7751482066
C16	4.3421246671	0.6520233884	0.1060630975
C17	0.3716241427	-4.4054848340	0.2149307875
C18	-0.3482124015	0.0162267440	4.4655086447
H19	-1.7268367808	0.9532344627	2.9561008304
H20	2.7531780914	1.6362247925	-1.1571457470
H21	-1.0398919488	-3.1370756989	-1.0017796095
H22	1.9969289810	-4.4712380754	1.7688809756
H23	1.4983881926	-1.2087694229	4.8433133755
H24	4.8193381159	-0.8222154055	1.7373223813
H25	5.2794109949	1.1048260830	-0.1798614177
H26	0.1498644618	-5.4306646472	-0.0395397943
H27	-0.7655044599	0.2505222129	5.4329027839
C28	-2.1751660359	-0.0752862241	0.0547738178
C29	-1.9216595054	1.3790363032	0.0510649623
H30	-2.6563584413	-0.4656006306	-0.8495186122
H31	-2.3474399301	1.9100166281	-0.7982880255
H32	-2.1699795932	1.9003138711	0.9739152498
H33	-2.6373278671	-0.4803874837	0.9560162854
C34	1.2079876557	4.5585075365	-0.6205344825
C35	1.0010224048	4.0660372418	0.6707183116
C36	0.2711872570	2.8963877346	0.8768301992
C37	-0.2518977642	2.1463353873	-0.1997018007
C38	-0.0732967977	2.6984777849	-1.4905298610
C39	0.6534464862	3.8682983966	-1.7030571617
H40	1.7707464599	5.4734425738	-0.7797578112
H41	1.4116774794	4.5957075406	1.5265971420
H42	0.1275049177	2.5370096642	1.8901688186
H43	-0.5431160667	2.2199298911	-2.3481246368
H44	0.7730408486	4.2514963245	-2.7137696797
N46	0.0093790986	-0.3524214119	-2.0597052482
H47	0.3435213798	-1.3013313022	-2.2210281087
H48	-0.8870885354	-0.2573670969	-2.5359334680
H49	0.6663857109	0.2879451621	-2.5008788254

TS2
Gas phase Energy: -1395.40402706882 hartrees

Solvation Energy:-1395.41382899416 hartrees
Zero Point Energy: 304.693 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-636.30 cm^{-1})
Coordinates:

Ru1	-0.2058792639	0.0665517529	0.1270971571
N2	-0.0954551277	-0.0256185578	2.2381156868
N3	2.0371446994	0.1526806965	0.1658697732
N4	0.1703439760	-2.1224720672	0.1844386217
N5	2.6877905506	-0.6449959804	1.0538081009
N6	0.8783928376	-0.7876718007	2.8160565737
N7	1.0934810505	-2.5943175936	1.0656531159
B8	1.8833531540	-1.6070465978	1.9644575215
C9	-0.8136712685	0.5115348941	3.2322174889
C10	2.9749337577	0.8577394484	-0.4790716246
C11	-0.3604992062	-3.1864784134	-0.4304201847
C12	1.1418105440	-3.9446486870	0.9976422523
C13	0.7641737185	-0.7181183826	4.1645299336
C14	4.0223382382	-0.4415434863	0.9631621868
H15	2.6287889806	-2.2116656905	2.6848534898
C16	4.2548851613	0.5181524269	-0.0118009479
C17	0.2247096462	-4.3702053340	0.0467174726
C18	-0.3063401845	0.1049182521	4.4764842847
H19	-1.6566038134	1.1467803921	3.0043747449
H20	2.6887875416	1.5826778800	-1.2285366636
H21	-1.1515586713	-3.0517596459	-1.1541636676
H22	1.8209761287	-4.4998229642	1.6275635406
H23	1.4520150059	-1.2596538966	4.7963789165
H24	4.7037088941	-0.9909760732	1.5956584783
H25	5.2054888973	0.9153323423	-0.3333733446
H26	0.0061437941	-5.3843291316	-0.2509881686
H27	-0.6702134604	0.3717674298	5.4567457814
C28	-0.1497000996	2.2672444091	-0.0565049123
H29	-0.2131805254	2.4714904453	-1.1358619311
H30	0.8743836969	2.4832560989	0.2607007026
C31	-1.0973748172	3.2597184049	0.6604059846
H32	-0.9993943192	3.1295827233	1.7447471554
H33	-2.1421912140	3.0346691819	0.4089279821
C34	-0.2430763608	7.3703185258	-0.4159198238
C35	-1.2161523403	6.6480959460	-1.1091275697
C36	-1.4953858514	5.3283414315	-0.7511741644
C37	-0.8108859279	4.7032054627	0.3006545909
C38	0.1618628458	5.4416387948	0.9889574223
C39	0.4451786054	6.7615253719	0.6359755564
H40	-0.0271189739	8.3994793487	-0.6887306818
H41	-1.7637943594	7.1145149998	-1.9240256213
H42	-2.2626466102	4.7745474601	-1.2882614553
H43	0.6972952520	4.9755662905	1.8132271953
H44	1.1993044497	7.3175403290	1.1864884338
H45	-1.3487128226	1.0732964130	0.4025042012
C46	-5.0058734221	-1.1046223653	-0.3109945189
C47	-4.2216518535	-1.6414306141	0.7141309347
C48	-2.8841026296	-1.2661670923	0.8597520110
C49	-2.2706899023	-0.3495536066	-0.0192071734
C50	-3.0951970772	0.1968209262	-1.0272398187
C51	-4.4350290724	-0.1754810708	-1.1802483964
H52	-6.0472739163	-1.3948205759	-0.4193278082

H53	-4.6547485558	-2.3589010330	1.4075788203
H54	-2.3017863311	-1.7007295287	1.6663979355
H55	-2.6971202009	0.9639522671	-1.6916670994
H56	-5.0329674115	0.2734344519	-1.9703493570
N57	-0.1560048780	-0.0165578024	-2.0511046640
H58	0.5624364203	-0.6769591460	-2.3414040598
H59	-1.0536533889	-0.3421324523	-2.4081186996
H60	0.0455775088	0.8813803496	-2.4896679399

Ir.acac-4CF_3

A
Gas phase Energy: -2296.25722552549 hartrees
Solvation Energy:-2296.26428076631 hartrees
Coordinates:

Ir1	-.2918829819	.0456952147	-.1798110977
O2	-1.9598650857	-.1248160490	-1.3660303005
O3	.8628740278	.2049990640	-1.9080867311
C4	2.1239268523	.3355790422	-1.8520807028
C5	2.9597976024	.3927694616	-.7310044743
C6	2.5208485505	.2873894548	.5897459028
O7	1.3387274554	.1456512673	1.0375431441
H8	4.0184804913	.5190322231	-.8992271238
C9	-.4015091931	2.1128231147	-.2784574538
C10	-1.1152048818	2.7041644432	-1.3305188367
C11	-1.1267962792	4.0941690157	-1.4891959289
C12	-.4290890401	4.9157043213	-.6020937609
C13	.2827639692	4.3344333231	.4486243410
C14	.2936824882	2.9452773607	.6119086567
H15	.8539707924	2.5199703907	1.4392224049
H16	.8329312628	4.9585023354	1.1483579689
H17	-.4398344211	5.9947011136	-.7277998723
H18	-1.6856034482	4.5306326695	-2.3130508148
H19	-1.6644135152	2.0856859999	-2.0315975810
O20	.1645818975	-2.1070789537	-.4879302008
C21	-.5180546641	-2.8012193692	-1.2849388435
C22	-2.2840260152	-1.1925992673	-1.9828948561
C23	-1.6768045587	-2.4469264021	-2.0037490729
H24	-2.1322350066	-3.2057153248	-2.6219351851
C25	-1.6071999698	.5447689703	1.5320548313
C26	-1.4019038435	-.8336349833	1.4960248896
H27	-1.0408373970	1.1667221291	2.2155074004
H28	-.6617569749	-1.2980939729	2.1403070105
H29	-2.1553074466	-1.4947377686	1.0779844448
H30	-2.5128118131	.9837142129	1.1275678450
C32	-3.5711437377	-.9773927604	-2.7985131771
F33	-3.9423369271	-2.0757332158	-3.4808929672
F34	-4.5799403535	-.6395670516	-1.9751776052
F35	-3.3996269311	.0228537531	-3.6780012205
C36	.0326888655	-4.2331169135	-1.4518608897
F37	-.7359362390	-4.9963778078	-2.2526064553
F38	1.2676030966	-4.1892453182	-1.9787159506
F39	.1102661458	-4.8363094950	-.2542329881

C40	2.7654479984	.4139583070	-3.2494619311
F41	4.0881563525	.6596216209	-3.1892341534
F42	2.5894203027	-.7524592731	-3.8934563143
F43	2.1924224026	1.3855696475	-3.9721550467
C44	3.5496458297	.3441957735	1.7290429348
F45	3.5753858226	-.8270922905	2.3858987821
F46	4.7911721668	.6050429695	1.2839298945
F47	3.2104980698	1.3065137076	2.6052257252

D
Gas phase Energy: -2528.51408039420 hartrees
Solvation Energy:-2528.51870950946 hartrees
Zero Point Energy: 242.243 kcal/mol
Coordinates:

Ir1	0.4442991922	-0.9079776468	-0.0610656697
O2	2.0978368782	-1.2536352343	1.4480618301
C3	1.8906710692	-1.9733787145	2.4568524751
C4	0.6926292000	-2.5701082542	2.8947296636
C5	-0.5471371640	-2.4295272048	2.2757339874
O6	-0.8802804617	-1.8174794490	1.2109996178
H7	0.7287028971	-3.1604277138	3.7974221662
O8	1.7784168159	0.0016823735	-1.3037150765
C9	-1.8470227719	1.2761809220	0.6065778091
C10	-0.4791086388	1.2914869362	0.1961955596
H11	-2.6240627030	1.4021879841	-0.1403244551
H12	-0.2249384466	1.6411362502	-0.7974670800
C13	-2.1714989244	1.1208257683	1.9335429844
C14	0.5353480467	1.1664558052	1.1746543121
C15	-1.1506988098	0.9992890403	2.9130617766
C16	0.1760225840	1.0265592127	2.5476623827
H17	-1.4257999623	0.8918899531	3.9579849334
H18	0.9613963917	0.9546028246	3.2929061296
H19	-3.2121016351	1.1037814217	2.2425236468
H20	1.5657311653	1.3810145178	0.9155204915
O21	0.9343915316	-2.7819411397	-0.6820749432
C22	1.8265237303	-2.9765968790	-1.5711520650
C23	2.5502970233	-0.6620659675	-2.0634562733
C24	2.6208512172	-2.0484887513	-2.2450858961
H25	3.3396985725	-2.4255045279	-2.9562516473
C26	-0.9382961121	-0.9772428835	-1.6433603644
H27	-0.3471363690	-1.3027882104	-2.5094934488
H28	-1.3386067310	0.0083857569	-1.8977663111
C29	-2.0911887062	-1.9683212438	-1.4137421809
H30	-2.7544518313	-1.5927010637	-0.6283013522
H31	-1.6895976754	-2.9190801191	-1.0498182581
C32	-4.2746933506	-2.6340501394	-5.0937916184
C33	-4.7408500184	-1.7036165224	-4.1637627398
C34	-4.0436836513	-1.4949829322	-2.9724488129
C35	-2.8737437214	-2.2101668296	-2.6878703808
C36	-2.4168109860	-3.1431873509	-3.6306694780
C37	-3.1089520290	-3.3545633295	-4.8226799023
H38	-4.8171732003	-2.8004278532	-6.0200709888
H39	-5.6503688635	-1.1432533923	-4.3627770614
H40	-4.4163726146	-0.7743929527	-2.2475403375
H41	-1.5133235517	-3.7110190728	-3.4189615108
H42	-2.7419115197	-4.0857223220	-5.5379220770

C44	1.9690511774	-4.4663944632	-1.9119661052
F45	2.9899034247	-4.7007904744	-2.7567243812
F46	2.1706440947	-5.1854663150	-0.7977137437
F47	0.8368846311	-4.9048824403	-2.4983363159
C48	3.5039717135	0.2450617189	-2.8525433284
F49	4.3092570499	-0.4551776866	-3.6737408551
F50	2.8006490240	1.1155193936	-3.5982684580
F51	4.2756602229	0.9451653079	-2.0022274164
C52	-1.7792402323	-3.0359571735	2.9661040331
F53	-2.5267976984	-3.7195249368	2.0872898519
F54	-1.4527317275	-3.8658357067	3.9759733885
F55	-2.5382538460	-2.0419874616	3.4793749606
C56	3.1427933868	-2.1572361140	3.3371375829
F57	2.9556945300	-3.0357823722	4.3430548038
F58	4.1787976932	-2.5850862036	2.5985504671
F59	3.4773719892	-0.9693970847	3.8842490387

TS1
Gas phase Energy: -2296.22185629287 hartrees
Solvation Energy:-2296.22551451105 hartrees
Zero Point Energy: 176.540 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-339.26 cm^{-1})
Coordinates:

Ir1	-0.0162347250	0.0767104063	0.0025134402
O2	-0.0797659482	0.0550155775	2.0454720230
O3	2.1569758737	-0.1283434702	0.0938438336
C4	2.8495761540	-0.1137701930	-0.9558628102
C5	2.4303926556	0.0237295617	-2.2942024276
C6	1.1094517683	0.1452647139	-2.7130129339
O7	0.0249415824	0.1557066891	-2.0392066044
H8	3.1933535486	0.0262512892	-3.0573301043
C9	-0.2702721871	-2.0871695814	-0.0381858951
C10	0.1030492109	-2.7685045863	1.1419213588
C11	0.6658426570	-4.0404849066	1.0833748847
C12	0.8525684545	-4.6719387673	-0.1494124889
C13	0.4683930612	-4.0227162671	-1.3275599623
C14	-0.0953755631	-2.7524327477	-1.2734384369
H15	-0.4059033520	-2.2638837764	-2.1913387364
H16	0.6038792031	-4.5111772915	-2.2882160522
H17	1.2881588920	-5.6659203943	-0.1923225046
H18	0.9626406901	-4.5386454958	2.0017927224
H19	-0.0261146288	-2.2803590366	2.1015861815
O20	0.4438901938	2.1082342830	-0.0465386680
C21	0.6250996057	2.7820190922	1.0102050817
C22	0.1982773106	1.0774150019	2.7523344148
C23	0.5361770699	2.3678063126	2.3471596421
H24	0.7382261174	3.0983836312	3.1153423401
C25	-2.0243789261	-1.2673202435	0.0791782921
C26	-2.0883958202	0.1831639434	-0.0575433797
H27	-2.4127308452	-1.8632048449	-0.7390436780
H28	-2.4309218348	0.5642171980	-1.0186896942
H29	-2.4878741246	0.7297340707	0.7966394760
H30	-2.2604296558	-1.6715919000	1.0581801730
C32	0.8174150020	0.2360549956	-4.2172780485
F33	0.0962975166	1.3333950275	-4.4939640131
F34	1.9371950117	0.2706805603	-4.9635141843

F35	0.0983022135	-0.8413333243	-4.6015831728
C36	4.3580907942	-0.2703422158	-0.6813384222
F37	5.0986909783	-0.2432044079	-1.8085410148
F38	4.7840846222	0.7221724921	0.1188857634
F39	4.5927542333	-1.4388984662	-0.0597048972
C40	0.9901873993	4.2455431035	0.7129563664
F41	1.1631073807	4.9683215396	1.8375863572
F42	2.1294874034	4.2996647652	0.0030612467
F43	0.0173361794	4.8257968134	-0.0094102107
C44	0.0919661576	0.7683058450	4.2516558226
F45	0.5518116156	1.7735964862	5.0180216765
F46	-1.1968209687	0.5491153617	4.5815813023
F47	0.7901381888	-0.3399429724	4.5493259435

TS2
Gas phase Energy: -2528.48755728834 hartrees
Solvation Energy:-2528.49199476710 hartrees
Zero Point Energy: 239.528 kcal/mol
Number and Magnitude of negative Eigen values: 1 (-436.22 cm^{-1})
Coordinates:

Ir1	0.0109688254	0.1086494736	0.0595921343
O2	-0.0984051649	0.5600503977	2.1486130148
C3	0.9288836597	0.5345215009	2.8843788324
C4	2.2642627737	0.2897336069	2.5307159633
C5	2.7030502554	0.0053207928	1.2395613869
O6	2.0386429563	-0.1246443183	0.1607725796
H7	3.0071289295	0.3331427342	3.3122539915
H8	0.5159187022	1.3395314935	-2.1346114527
O9	-2.0158800781	0.4072846760	-0.0368092588
O10	0.3492679531	2.2774936166	0.0261309851
C11	-0.6166508377	3.0878072775	0.0838617379
C12	-2.5652939191	1.5528707523	0.0430077277
C13	-1.9953424680	2.8231476019	0.1072279630
H14	-2.6668057335	3.6657029867	0.1681985484
C15	-0.2642855696	-1.8775282594	0.6298912639
H16	-0.7627566655	0.1940424977	-2.5950290419
C17	1.2803141036	-0.5746921236	-2.8210526874
H18	0.9590039636	-1.6231637219	-2.8474446492
H19	2.2067830574	-0.5381069634	-2.2420589260
C20	-1.4750889114	-2.2414856667	1.2325652457
C21	-1.6483608751	-3.5369567304	1.7260805291
C22	-0.6273199362	-4.4816459912	1.6122158555
C23	0.5732880669	-4.1249442397	0.9975391576
C24	0.7548938761	-2.8303898454	0.5023326567
H25	-2.2799677381	-1.5208606173	1.3189577162
H26	-2.5889298968	-3.8045789178	2.1996509768
H27	-0.7681523203	-5.4882891855	1.9948748109
H28	1.3744254242	-4.8523312817	0.8980643906
H29	1.6950872346	-2.5668030437	0.0287006251
H30	-0.1876390125	-0.9606967217	-1.0560604372
C31	0.2192390052	0.2888560810	-2.1241623994
C32	1.9633221657	0.8775289728	-6.8402001955
C33	1.0030544024	-0.1084272629	-6.6053657684
C34	0.7891194359	-0.5820457383	-5.3103655097
C35	1.5307859365	-0.0816524796	-4.2323194581
C36	2.4918587206	0.9077714799	-4.4801004083

C37	2.7078062484	1.3846691547	-5.7731401373
H38	2.1335434548	1.2448559993	-7.8480877675
H39	0.4234010560	-0.5124324657	-7.4305958552
H40	0.0444325293	-1.3550938959	-5.1338603722
H41	3.0789731948	1.3002399179	-3.6529563967
H42	3.4611281057	2.1476587270	-5.9480643807
C43	-0.1596999608	4.5595788266	0.1332962855
F44	-1.1943025149	5.4221345800	0.1723864834
F45	0.5955409158	4.7631124293	1.2254284239
F46	0.5809415651	4.8441743307	-0.9509548024
C47	-4.0980738301	1.4287690148	0.0366654661
F48	-4.7080760376	2.6071471106	0.2610555620
F49	-4.5121349340	0.9628677458	-1.1555098924
F50	-4.4937740724	0.5646428094	0.9856162799
C51	0.6075213147	0.8357397219	4.3604186253
F52	1.6967492252	0.7515205410	5.1496805948
F53	0.1054362921	2.0774415981	4.4727727640
F54	-0.3082169457	-0.0330003567	4.8149219879
C55	4.2010462409	-0.2275980396	0.9920730321
F56	4.3983497053	-1.4920843000	0.5717231661
F57	4.6449766662	0.6028958953	0.0343336255
F58	4.9414958337	-0.0321410684	2.0972056633