Methane Activation with Rhenium Catalysts I: Bidentate Oxygenated Ligands

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Supplementary Information

We include the final enthalpy and structure for all of the species mentioned in the manuscript

H_2O
enthalpy: -76.420439

H	0.0000000000	0.0000000000	0.0000000000
O	0.0000000000	0.0000000000	0.9649402977
H	0.9364263498	0.0000000000	1.1977829378

H_3O^+
enthalpy: -76.826901

H	-0.0045442479	0.0506371675	0.0097874810
O	0.0009675559	-0.0048540933	0.9898456944
H	0.9039479992	-0.0049061809	1.3748902028
H	-0.5730395918	-0.7186930040	1.3428065642

CH_4
enthalpy: -40.474452

C	0.0000000000	0.0000000000	0.0000000000
H	0.6304893456	-0.6304893456	0.6304893456
H	-0.6304893456	0.6304893456	0.6304893456
H	0.6304893456	0.6304893456	-0.6304893456
H	-0.6304893456	-0.6304893456	-0.6304893456

Re(III) Systems

$Re(acac)_2$ System
$(acac)_2Re(OH)(OH_2)$
enthalpy: -764.436157

Re	-1.3157900604	0.5207450887	0.0034036131
C	-3.7535799467	0.0851705933	1.6158203748
H	-4.7957695018	-0.2416305790	1.6753312228
C	-1.2801639624	3.4328816645	-0.7323820737
H	-1.8230734534	4.3761169561	-0.8562304022
C	0.9054373913	2.2852221670	-0.8980110348
C	0.0971376742	3.4153448477	-0.9934716251
H	1.9670775946	2.3823905991	-1.1445327118
H	0.5649498298	4.3436787973	-1.3025668962
C	-1.8351280418	1.0669073320	2.8434141304
C	-3.1514673803	0.6018243332	2.7635958189
H	-1.4678489526	1.4425555814	3.8022747343
H	-3.7506768530	0.6444782093	3.6665203923
O	-0.9728317375	1.1202842807	1.8892656217
O	-3.2044308162	-0.0704929490	0.4594290316
O	-1.9930894512	2.4389291526	-0.3569758315
O	0.5462826180	1.0934854632	-0.5550281318
O	-1.7087353132	-0.4213699925	-1.9487191538
H	-1.2717786284	-1.2498318250	-1.6125863483
O	-0.6945473743	-1.3872656628	0.0947354554
H	0.1680329811	-1.5099489201	0.5092407192
H	-2.6592635880	-0.6034678013	-2.0065264189

$(acac)_2Re(OH_2)(OH_2)^+$
enthalpy: -764.874356

Re	-1.3957213839	0.6558550594	-0.1288464626
C	-4.0319605684	0.0484993196	1.0815709256
H	-5.1155745375	0.0072548855	0.9562235569
C	-0.5917448491	3.4419602017	0.4511196596
H	-0.9046926608	4.4445641175	0.7490207273
C	1.2724614152	1.9459231865	-0.1571680216
C	0.7654675955	3.1763619133	0.2513974399
H	2.3474285700	1.8350539433	-0.3111503655
H	1.4672134334	3.9864656062	0.4110272896
C	-2.1071105604	-0.2518728068	2.5944785764
C	-3.4779956931	-0.2452283331	2.3246325769
H	-1.7577621037	-0.5192169875	3.5936894688
H	-4.1528630567	-0.4997852523	3.1333285288
O	-1.1618844954	0.0248925977	1.7608325693
O	-3.3772998863	0.3646787133	0.0095528769
O	-1.5639067875	2.6058503764	0.3080123370
O	0.5807868190	0.8772583433	-0.3977612280
O	-1.8016775572	1.3962204543	-2.1693625634
O	-1.0586426415	-1.4856706675	-0.5550266015
H	-0.5866721425	-1.9025934624	0.1849879313
H	-2.2742736952	2.2442878781	-2.1322174248
H	-0.5729407271	-1.7125562373	-1.3615163194
H	-2.2966111303	0.8232241509	-2.7729757845

$(acac)_2Re(OH)(H)(CH_3)^‡$ metathesis transition state
enthalpy: -728.428553

Re	.0031557378	.0007522295	-.0010313188
C	-.0069444209	-.0126270712	2.3369979850
H	1.1743822239	.0070108044	1.5940383353
O	2.0089561830	-.0098365184	.6397813593
C	-.0172968005	2.8382368524	-.9401158234
H	-.0762822219	3.9052972743	-.6975150981
C	-2.7618985119	-.9565401782	-.4827751470
H	-3.8150005879	-.7000583738	-.6219360033
C	-1.0611774191	-2.7388864691	-.3385582448
C	-2.3740068744	-2.2964020280	-.5172964901
H	-.8449063731	-3.8087685747	-.3849405060
H	-3.1409097719	-3.0424218118	-.6945653309
C	.1050580566	1.1656096424	-2.7650735448
C	-.0153661161	2.4789249559	-2.2860409010
H	.1511434186	1.0190217406	-3.8508008694
H	-.0766460898	3.2766740644	-3.0179781886
O	.1764631738	.0963940310	-2.0754758065
O	.0731616809	2.0652720215	.0836029666
O	-1.9818656758	.0554088361	-.2926855756
O	-.0352369342	-1.9913849615	-.1073629612
H	2.4233351988	.8599429599	.5396403066
H	-.9712467443	-.5300815235	2.2840011453
H	.5803644391	-.6081866442	3.0507265145
H	-.1720723742	.9861194970	2.7468512576

$(acac)_2Re(OH_2)(CH_3)$
enthalpy: -728.465669

Re	-1.3146859254	.4706674151	-.0562847559
C	-3.2997676062	-1.3987085442	1.0030489983
H	-4.3370430426	-1.5855986281	1.2896372267
C	-2.2360534768	3.3078187881	.3281133587
H	-2.6835280418	4.1938039372	-.1356768770
C	-1.2951608453	2.3431266498	2.4089537685
C	-1.9085823238	3.3777121324	1.6771714270
H	-1.0677646698	2.5388609859	3.4668233954
H	-2.1266703449	4.3039958959	2.1977962738
C	-.9935214993	-2.3018834918	.8848808789
C	-2.3485100507	-2.4133242634	1.1781826636
H	-.3336836706	-3.1473920054	1.0928007831
H	-2.6943027535	-3.3533215291	1.5949053494
C	-1.6180652384	-.0744854584	-2.0934157870
H	-2.1861806145	.7038981570	-2.6177982664
H	-.6888941857	-.2450451502	-2.6720638150
H	-2.1923776416	-1.0080086807	-2.1742926225
O	-.4018826468	-1.2665774046	.3679267567
O	-3.0776596202	-.2148639438	.5450094529
O	-2.0691595728	2.3186330105	-.4826373964
O	-.9696259670	1.1987890163	1.9709825716
O	.7268666225	1.0671107338	-.6712581147
H	.7820413316	.8844245673	-1.6244283730
H	1.3123983431	.4275399801	-.2353616253

$(acac)_2Re(OH)(H)(CH_3)^{\ddagger}$ oxidative addition transition state
enthalpy: -728.445327

Re	-1.2722467471	.4614252478	-.0413524511
C	-3.7185082657	.1658583867	1.7009022963
H	-4.7471140977	-.1990180805	1.8072401498
C	-1.2162981795	3.3691592815	-.8203397209
H	-1.7590976810	4.2824536757	-1.0912398022
C	1.0180556135	2.3714217291	-.4096750295
C	.1768321008	3.4380719866	-.7510773977
H	2.0941497976	2.5718074854	-.3497045423
H	.6429490795	4.3953823785	-.9551706450
C	-1.8509228994	1.3245034509	2.8315072845
C	-3.1474816214	.7958147666	2.8051477684
H	-1.5223908204	1.8094526835	3.7608062162
H	-3.7512413426	.8876217683	3.7007589647
O	-.9932785442	1.3164657707	1.8953425823
O	-3.2095366312	-.0518621644	.5474191838
O	-1.9562935188	2.3515139432	-.5909512686
O	.6928885088	1.1648392470	-.1623767982
O	-.5777980548	-1.2366825206	.5647537759
H	.3883673343	-1.2692193505	.6201740868
C	-2.2795612552	-.4390941924	-1.8455442796
H	-1.7695218872	-.7337047622	-2.7648232687
H	-2.7230597947	-1.3220734411	-1.3850939333
H	-3.0501508997	.2967953825	-2.0812877150
H	-.7872450937	.2058448527	-1.5813189387

$(acac)_2Re(OH)(H)(CH_3)$ oxidative addition intermediate
enthalpy: -728.446947

Re	-1.2651996927	0.3999302670	-0.0920336516
C	-3.7095236326	0.0963819669	1.6946223815
H	-4.7083808332	-0.3407119361	1.8125858346
C	-1.2798553553	3.3282146472	-0.9631342654
H	-1.8573577453	4.2075506401	-1.2750041690
C	0.9479875802	2.4284827974	-0.4356956786
C	0.0984898223	3.4784814623	-0.7860907367
H	2.0179138813	2.6444697536	-0.3363231488
H	0.5355011122	4.4567498713	-0.9481615635
C	-1.9571642440	1.4739651985	2.7378359559
C	-3.1985650591	0.8269384385	2.7642876206
H	-1.6664554887	2.0493845312	3.6282135667
H	-3.8055984747	0.9139956664	3.6577909276
O	-1.1197180232	1.4828912268	1.7865791024
O	-3.1775144137	-0.1367085702	0.5557203081
O	-1.9583907571	2.2626151101	-0.8111264683
O	0.6425754385	1.2066795949	-0.2289020192
O	-0.7131680987	-1.1630228451	0.9180761777
H	0.0306034290	-1.6575954744	0.5509999949
C	-2.3237141522	-0.2425493004	-1.8938961288
H	-1.8565738704	0.0966497379	-2.8205152571
H	-2.4170219900	-1.3305563531	-1.9070627499
H	-3.3123973362	0.2079846712	-1.7900151177
H	-0.4618376098	-0.3886087390	-1.2660144602

$(acac)_2Re(OH)(H)(CH_3)^{\ddagger}$ reductive elimination transition state
enthalpy: -728.415762

Re	-1.3142492116	.4907675633	-.1248975690
C	-3.7183293664	.0557702109	1.6105981608
H	-4.7290058186	-.3582085477	1.6991693649
C	-1.3898124848	3.3320932925	-1.1039733207
H	-2.0022404477	4.2074351637	-1.3442689191
C	.8698308982	2.3822890843	-.9323101670
C	-.0051771152	3.4229934116	-1.2508163849
H	1.9467182365	2.5525288704	-1.0306836835
H	.4154317202	4.3593464436	-1.5983272421
C	-1.9186640189	1.3054202436	2.7890960891
C	-3.2072838250	.7348920122	2.7072887660
H	-1.6509274107	1.7813809541	3.7442729562
H	-3.8422489019	.8118200931	3.5828944763
O	-1.0312391253	1.3321163806	1.8928800837
O	-3.1619501891	-.1779186249	.4722019272
O	-2.0484247676	2.3126855610	-.6991024085
O	.5514839422	1.2148115336	-.5135941512
O	-.5525449242	-1.3200405666	.6806282060
H	-1.2257441146	-2.0095256242	.5721071098
C	-1.9664174417	-.1475074048	-2.0802701442
H	-1.2336050606	.1080386039	-2.8546485392
H	-2.1613149279	-1.2238127808	-2.1491343880
H	-2.9032644934	.3770464207	-2.2962349629
H	-.4647495006	-.8633479964	-.6391423935

$(acac)_2Re(CH_3)(H)(CH_3)$ oxidative addition intermediate
enthalpy: -692.482418

Re	-1.2758376333	0.3697336368	-0.0707534154
C	-3.7125824243	0.1421951900	1.6682079503
H	-4.7270910606	-0.2584459328	1.7678785033
C	-1.3547851738	3.4057442658	-0.7684356255
H	-1.9054642197	4.3477560424	-0.9074485458
C	0.8735446316	2.3425554028	-0.8288852941
C	0.0408815595	3.4465009964	-0.9500034098
H	1.9474592154	2.4846137393	-0.9889343611
H	0.4936583852	4.3985762840	-1.2018511636
C	-1.9325582760	1.4961214441	2.7415969533
C	-3.2119162062	0.9067563390	2.7149038115
H	-1.6748764734	2.0819795747	3.6363342028
H	-3.8562691817	1.0646653427	3.5723098669
O	-1.0357871357	1.4265174981	1.8544362784
O	-3.1380594303	-0.1694961772	0.5609896748
O	-2.0545622582	2.3997465841	-0.4634679610
O	0.5439494753	1.1302667355	-0.5528407433
C	-2.1252384254	0.0826819698	-2.0351546741
H	-1.3834029695	0.2658312544	-2.8197978625
H	-2.5395926195	-0.9183445779	-2.1753003306
H	-2.9309555371	0.8182439257	-2.1175813627
H	-0.6968354635	-0.8847858791	-0.9111100599
C	-0.4989515654	-1.2526438068	1.1194457669
H	-0.9488471409	-2.2179121806	0.8716095990
H	0.5852806811	-1.3331668962	0.9890056517
H	-0.7090475431	-1.0210489791	2.1686325601

Re(acac)(cat)$^-$ *cis* System
$(acac)(cat)Re(OH)(OH_2)^-$
enthalpy: -879.490291

Re	-.8825611199	.0554843774	.0992874654
C	-1.7721881144	2.5773721470	-1.2026625773
H	-2.5976647627	3.2192905908	-1.5298532010
C	.6903384684	2.2742303905	-1.1162752409
C	-.4611679905	2.9952201893	-1.4481222802
H	1.6716559569	2.6956096735	-1.3582462736
H	-.3263266875	3.9540584991	-1.9426630949
O	-2.1364471638	1.4651767388	-.6433348307
O	.7222680371	1.1245251885	-.5051684056
O	-.4371323148	-1.0761395466	-1.8817836070
H	.0058579249	-1.6662634122	-1.1909177724
O	.3066780471	-1.5769963944	.4436888450
H	-.1892211884	-2.1887367059	1.0048960287
H	.2871678873	-.5337359462	-2.2319724987
O	-1.0709345432	.8269891759	1.9442512257
O	-2.4782012059	-1.0326627029	.7623788985
C	-2.2115234416	.4591819503	2.5585685824
C	-2.6437548358	.9975477797	3.7709411559
C	-2.9698858676	-.5621247593	1.9206849055
C	-3.8286980252	.5284512432	4.3594908301
H	-2.0481070651	1.7768275844	4.2405482623
C	-4.1439601524	-1.0241987296	2.5195364683
C	-4.5722733956	-.4753992986	3.7385481557
H	-4.1659793300	.9541760166	5.3028207669
H	-4.7126174605	-1.8059556434	2.0211284397
H	-5.4915173011	-.8358583119	4.1969219520

(acac)(cat)Re(OH_2)(OH_2)
enthalpy: -879.929110

Re	-0.8799386858	0.1027205654	0.1254289845
C	-1.8375888073	2.3640868222	-1.4766877867
H	-2.6874013753	2.8994150773	-1.9052384850
C	0.6256475731	2.3089100265	-1.1620406497
C	-0.5499610931	2.8738578825	-1.6590695491
H	1.5781641682	2.8072389018	-1.3602952321
H	-0.4584127027	3.7948325673	-2.2256587603
O	-2.1649846570	1.2914047068	-0.8230756328
O	0.7104445405	1.2183345580	-0.4658190149
O	-0.9463483148	-0.9486096880	-1.8889642607
H	-1.8536735698	-0.7796845063	-2.1924924860
O	0.7401811958	-0.9971543779	1.2097211881
H	1.5539840417	-0.5700137930	0.8952546936
H	-0.8864151298	-1.9036487474	-1.7420760362
O	-0.9850233962	0.7281463223	2.0278268500
O	-2.3731137599	-1.0603023351	0.7477597258
C	-2.1380400916	0.3171892646	2.6360627819
C	-2.5633961808	0.7847651552	3.8754728730
C	-2.8765926040	-0.6727680303	1.9473040765
C	-3.7349937883	0.2588903481	4.4338823675
H	-1.9829883619	1.5487347007	4.3849929942
C	-4.0374776001	-1.1966022585	2.5127931636
C	-4.4633718589	-0.7231879550	3.7590000225
H	-4.0786707365	0.6222716298	5.3985344044
H	-4.5927117282	-1.9591275859	1.9739654124
H	-5.3715171789	-1.1236328096	4.2014038519
H	0.5214527647	-0.5607520029	2.0649118307

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ metathesis transition state
enthalpy: -843.485742

Re	-1.3564765890	0.1454625665	0.0893405290
C	-1.3416544991	2.9744451578	-0.7178942410
H	-1.9108477646	3.8615915420	-1.0114726623
C	0.9127694763	2.0234498748	-0.2766543663
C	0.0488974798	3.0665258039	-0.6285444861
H	1.9887627627	2.2160541952	-0.2208888201
H	0.4957208537	4.0341574946	-0.8425357237
O	-2.0727425759	1.9197428105	-0.4973125852
O	0.5531769263	0.8085028234	0.0105898533
O	-0.4918433554	-1.8154481483	0.3565862323
H	0.4393732868	-1.6331362251	0.5554852901
C	-1.0495243190	-0.8983602853	-2.0539645912
H	-1.8537403483	-1.5465133686	-2.4151726312
H	-1.2842371850	0.1177903610	-2.3993457906
H	-0.1041177298	-1.1641031540	-2.5483243194
H	-0.6610457264	-1.5290989578	-0.8252403415
O	-3.2510471433	-0.5248651337	0.3084393847
O	-1.6524956331	0.6304239409	2.0390455547
C	-3.7969717657	-0.1677344531	1.4841658369
C	-5.1323984983	-0.3955789842	1.8208855831
C	-2.9325148414	0.4733206133	2.4173911655
C	-5.6197961940	0.0126861624	3.0723279041
H	-5.7767091946	-0.8880973534	1.0963781243
C	-3.4277799429	0.8737148631	3.6598314984
C	-4.7736639624	0.6430698914	3.9848227265
H	-6.6633092336	-0.1637161455	3.3271453225
H	-2.7527346698	1.3613009854	4.3594468307
H	-5.1547965451	0.9607021120	4.9538027815

(acac)(cat)Re(OH_2)(CH_3)$^-$
enthalpy: -843.511278

Re	-1.0029579612	-0.1180403025	-0.5432919313
C	-2.1191030295	2.6821472382	-0.1423388953
H	-2.9740695661	3.3722093609	-0.1229544581
C	0.3536338023	2.4952394919	0.0636467216
C	-0.8428989328	3.2167019936	0.0815463056
H	1.2938926608	3.0258347181	0.2505857189
H	-0.7749527085	4.2844640082	0.2769067851
O	-2.4017796742	1.4509762091	-0.4000221973
O	0.4856090367	1.2081935183	-0.1324595931
O	-0.4433435206	0.6573101963	-2.6614753581
H	0.0416320380	-0.1394313923	-2.9328126006
H	0.2459076430	1.2711296229	-2.3490732090
C	0.5006038007	-1.6108270441	-0.9441989109
H	0.6088067460	-1.8827142605	-2.0157219503
H	1.4888813177	-1.2721632385	-0.6002362881
H	0.2720302646	-2.5537089927	-0.4300343000
O	-2.5344743329	-1.3823249999	-0.9833084530
O	-1.4108951338	-0.7913005754	1.2977040568
C	-3.1281116697	-1.8771361316	0.1127119372
C	-2.5264954231	-1.5435865860	1.3586900691
C	-4.2686935817	-2.6834762362	0.0937710574
C	-3.0767113774	-2.0135065206	2.5511121469
C	-4.8160113871	-3.1523961561	1.2987774433
H	-4.7181758059	-2.9320934400	-0.8650142604
C	-4.2261851054	-2.8196643606	2.5183076508
H	-2.6005440638	-1.7441511919	3.4911569873
H	-5.7072182968	-3.7774422211	1.2769241354
H	-4.6558590315	-3.1823151448	3.4504693949

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ oxidative addition transition state
enthalpy: -843.511696

Re	-0.0390752319	0.0200607378	-0.0430428930
C	0.0276053195	0.0253776057	2.2728585588
H	1.0832873459	0.0124484723	1.1784570503
O	-0.3282538204	-1.9168616451	0.0818694719
C	-0.6630566975	2.9931617565	0.1095001261
H	-0.3425890299	4.0423204495	0.0114119274
C	-2.6012432783	1.5094115200	0.5885702210
C	-2.0088545361	2.7716802916	0.4311114307
H	-3.6801310183	1.4928162195	0.8080567261
H	-2.6480058496	3.6419997926	0.5442701846
O	0.2465565321	2.1286000808	-0.0893088906
O	-2.0516719344	0.3686452919	0.5161801080
H	0.1635122443	-2.3501936213	-0.6301486997
H	0.8968263600	-0.1397843597	2.9203543889
H	-0.3973434282	1.0004251192	2.5288704968
H	-0.6936239182	-0.7738106065	2.4560999419
O	-0.6757604618	0.1634620869	-1.9821986427
O	1.7328649200	-0.2678994008	-1.0433279116
C	0.3060861078	0.0839899276	-2.8859431991
C	1.6129997780	-0.1554420315	-2.3759625779
C	0.1122664297	0.2111825573	-4.2647526119
C	2.6922147569	-0.2641482288	-3.2572207873
C	1.2041784059	0.1033993244	-5.1393219339
H	-0.8934971044	0.3948201312	-4.6360382168
C	2.4854138160	-0.1334240966	-4.6392571734
H	3.6839345418	-0.4452101683	-2.8487668729
H	1.0470876022	0.2068025302	-6.2116690076
H	3.3308709333	-0.2152324318	-5.3201632031

(acac)(cat)Re(OH)(H)(CH_3)$^-$ oxidative addition intermediate
enthalpy: -843.511755

Re	-1.3978401492	-0.0916271714	-0.4150486958
C	-1.4260882767	2.8635862501	0.3474685189
H	-1.9144973977	3.7341968318	0.8150315533
C	0.7141181196	2.0813874743	-0.6752997806
C	-0.0978863866	3.0483127004	-0.0682074047
H	1.7415317882	2.3993027809	-0.9172811084
H	0.3472295582	4.0213642002	0.1161258416
O	-2.1473254916	1.8286308287	0.2569259068
O	0.4390753030	0.8872562450	-1.0024525216
O	-0.3536955391	-1.7151733929	-0.7675098782
H	0.3483780705	-1.7010255391	-0.0988009620
C	-1.9675198638	0.7968063415	-2.3321591673
H	-1.6035255443	0.1977994004	-3.1742124567
H	-3.0522236173	0.9078292892	-2.4324922832
H	-1.5118156968	1.7925711816	-2.3886330252
H	-2.4046000880	-0.9747821687	-1.3413343022
O	-0.4049318708	-0.0573316646	1.4296847853
O	-2.8483717850	-0.7717671753	0.8055810293
C	-1.2035182155	-0.3847589470	2.4511115939
C	-2.5311827905	-0.7669805686	2.1149880894
C	-0.8141741035	-0.3679535664	3.7936687712
C	-3.4356457551	-1.1193362377	3.1167450356
C	-1.7302900233	-0.7234514769	4.7959771246
H	0.2039507429	-0.0740992436	4.0386083265
C	-3.0319538857	-1.0953057866	4.4611866188
H	-4.4454097557	-1.4059370649	2.8334909855
H	-1.4192255173	-0.7054771933	5.8390733210
H	-3.7409848530	-1.3670487144	5.2408630182

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ reductive elimination transition state
enthalpy: -843.473177

Re	-0.0329914977	0.0083592911	-0.0262332166
O	0.1160294726	0.0688211187	2.1380458880
H	1.0571211446	-0.2021140056	1.2726509606
C	1.9256742180	0.5860856537	-0.7876385271
C	-0.9766692168	1.0160579099	-2.6899070342
H	-1.2123368212	0.8423712375	-3.7506280573
C	-1.0783233150	2.6837029754	-0.8484981816
C	-1.2615503127	2.2944241341	-2.1766052675
H	-1.3719166533	3.7083408337	-0.5800903358
H	-1.6827729713	3.0251497159	-2.8602138542
O	-0.4863972446	0.0198225066	-2.0800024366
O	-0.6143579136	1.9899551682	0.1203597560
H	-0.5427141459	-0.6265988893	2.3089950911
H	2.4430590068	1.3238967164	-0.1581979371
H	2.5806343952	-0.2922361719	-0.8633154759
H	1.8381074826	1.0126471996	-1.7993021160
O	-1.9574396188	-0.7930162912	0.4537276307
O	0.2743936403	-1.9588185429	-0.2319439051
C	-2.0232863371	-2.1061695090	0.2560695017
C	-0.8059637635	-2.7524905457	-0.1198757661
C	-3.1820404864	-2.8810972087	0.4025358492
C	-0.7740377851	-4.1300200819	-0.3389881487
C	-3.1393593376	-4.2644286845	0.1777216408
H	-4.1064795572	-2.3855333392	0.6904261050
C	-1.9458146017	-4.8874929665	-0.1912374751
H	0.1672255031	-4.5930786230	-0.6255147746
H	-4.0478240228	-4.8539292327	0.2911993175
H	-1.9203037179	-5.9610350446	-0.3678208403

(acac)(cat)Re(CH_3)(H)(CH_3)$^-$ oxidative addition intermediate
enthalpy: -807.547331

Re	-1.3343156251	-0.1120128489	-0.3958500735
C	-1.1670194675	2.9491702715	0.3423164591
H	-1.5217701407	3.8572968933	0.8647936637
C	0.7216764712	2.0521278974	-1.0174486427
C	0.0804381152	3.0666620622	-0.3096784942
H	1.6897054130	2.3125891702	-1.4734031214
H	0.5864759758	4.0254877800	-0.2489745609
O	-1.9260971386	1.9520481710	0.3921629462
O	0.3553786650	0.8469095601	-1.2206422585
C	-2.4177742226	0.7155772456	-2.0972116948
H	-2.0612668705	0.3347374759	-3.0617713271
H	-3.4891773488	0.4934139426	-2.0227543476
H	-2.2930759742	1.8053901993	-2.0899585917
H	-1.9484051783	-1.2405786071	-1.3913672120
O	-0.4565796406	-0.0564670046	1.5246213652
O	-2.8317679884	-0.7750756333	0.7326377229
C	-1.3229279753	-0.3530115508	2.4855760279
C	-2.6281914921	-0.7431558883	2.0648905316
C	-1.0386042699	-0.3132243757	3.8572920288
C	-3.6069042135	-1.0763137950	2.9999587228
C	-2.0295291554	-0.6477495559	4.7909908519
H	-0.0414634971	-0.0175377619	4.1749120082
C	-3.3053842020	-1.0260160267	4.3697073823
H	-4.5931710436	-1.3680985756	2.6471110162
H	-1.7978732702	-0.6096356675	5.8543141076
H	-4.0703940794	-1.2810542849	5.1004206259
C	-0.0496879316	-1.8220305658	-0.5886994258
H	-0.5251703638	-2.7273152226	-0.1941421879
H	0.2552347345	-2.0080574424	-1.6246180079
H	0.8352585533	-1.5968346637	0.0161003303

Re(acac)(cat)$^-$ *trans* System
(acac)(cat)Re(OH)(OH_2)$^-$
enthalpy: -879.485269

Re	-1.1485706226	0.3272943796	-0.0961578581
C	-1.2689691629	3.2333476397	0.2207081988
H	-1.8260583187	4.0944158543	0.5978218455
C	0.7630030089	2.4123126845	-0.9367905616
C	-0.0421959861	3.4285707089	-0.4128431804
H	1.7213427008	2.6680693421	-1.3981234555
H	0.3190532118	4.4504597849	-0.4960882251
O	-1.8661703427	2.0872368734	0.4185510265
O	0.4852297030	1.1416947022	-0.9115844163
O	-2.0246255481	0.0755650098	-1.9675793679
O	-0.6755703788	-1.7334632115	-0.9200293716
H	-1.2748916275	-1.3777025238	-1.6556698783
H	-2.9835641061	0.0929067860	-1.8513095839
H	-1.2732733378	-2.2344675042	-0.3401630474
O	-0.3471916464	0.0576035708	1.7890867338
O	-2.6667065153	-0.7110232896	0.7921026200
C	-1.2498690465	-0.4038276366	2.6594721179
C	-2.5045844813	-0.8314780625	2.1299882399
C	-1.0177781941	-0.5186406214	4.0350975790
C	-3.4784698240	-1.3594631964	2.9764182741
C	-2.0080524631	-1.0449697302	4.8775563418
H	-0.0582823389	-0.1909213239	4.4282169242
C	-3.2312234825	-1.4645733664	4.3549777172
H	-4.4257938923	-1.6788273793	2.5472209572
H	-1.8169023166	-1.1227252681	5.9466164541
H	-3.9980658676	-1.8710800846	5.0116375801

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ metathesis transition state
enthalpy: -843.484232

Re	-1.2112870178	0.3558544390	-0.0081980996
C	-1.3077942878	3.1892996490	-0.8362241955
H	-1.9135616175	4.0834657350	-1.0165757810
C	0.9593344086	2.1869706358	-0.8656380541
C	0.0714199882	3.2532644638	-1.0424919386
H	2.0274108885	2.3466351218	-1.0454210025
H	0.4859168621	4.2059455094	-1.3618130249
O	-1.9874320303	2.1499075062	-0.4538648663
O	0.6402063968	0.9891478531	-0.4848203823
O	-1.3899402222	-0.7006701490	-1.9034855129
H	-2.3331640230	-0.9118421885	-1.9629436894
C	-0.3355582996	-1.8617324879	0.2199412708
H	0.6356224407	-2.1436126541	-0.2018581885
H	-0.1341621548	-1.4852096662	1.2319358073
H	-0.9694139813	-2.7465982509	0.3494618302
H	-0.9161420332	-1.3884324718	-1.0010862745
O	-3.0536470428	-0.2734206486	0.5583929517
O	-1.1310229182	0.8488516822	1.9684668107
C	-3.3718906396	0.1275525428	1.8044583047
C	-4.6351663265	-0.0420610093	2.3725026443
C	-2.3331766758	0.7488872793	2.5585824239
C	-4.8846690377	0.4069205730	3.6788386383
H	-5.4131522749	-0.5203354781	1.7818384525
C	-2.5944059132	1.1899233172	3.8584359330
C	-3.8708539881	1.0197817050	4.4152683623
H	-5.8740016797	0.2774239475	4.1133461446
H	-1.7921425949	1.6645313317	4.4187980183
H	-4.0671428023	1.3721481042	5.4264403823

(acac)(cat)Re(OH_2)(CH_3)$^-$
enthalpy: -843.513282

Re	-0.9704366897	-0.0915297551	-0.6188546764
C	-2.0201599042	2.6401793795	-0.6804211918
H	-2.8657869154	3.2921549924	-0.9116318233
C	0.2622661002	2.4442687936	0.2652707475
C	-0.8591224175	3.1805476291	-0.1211092373
H	1.1056948644	2.9549310454	0.7391341970
H	-0.8415391452	4.2536033994	0.0527833427
O	-2.2323302560	1.3779564530	-0.9423690645
O	0.4042189224	1.1549645497	0.1300994520
C	-0.1752880798	0.0436986238	-2.5997483257
H	-0.7843140855	-0.5433971132	-3.3015773320
H	-0.1891153328	1.0875181212	-2.9496096694
H	0.8650174446	-0.3092017149	-2.6734189589
O	0.2751791632	-1.8834049183	0.0191703230
H	-0.1712473425	-2.5563215766	-0.5212283301
H	-0.2844465911	-1.8268768335	0.8472177818
O	-2.2807863419	-1.5484679573	-1.1915015341
O	-1.6926218799	-0.8925261058	1.3277885901
C	-3.0884781364	-2.0186046476	-0.2188900616
C	-2.7789088183	-1.6592584674	1.1292828127
C	-4.1811632311	-2.8482893184	-0.4823030857
C	-3.5862755728	-2.1431539676	2.1635265824
C	-4.9815331658	-3.3216871268	0.5684649517
H	-4.3962544223	-3.1078315745	-1.5164755636
C	-4.6856768364	-2.9692733879	1.8846057034
H	-3.3392382402	-1.8618852733	3.1848985531
H	-5.8354093079	-3.9604955607	0.3501694875
H	-5.3073751454	-3.3322678677	2.7012595413

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ oxidative addition transition state
enthalpy: -843.504108

Re	-0.0156193539	-0.0043915261	-0.0152054417
C	0.0306126842	-0.0268425297	2.2770651925
H	1.0354195349	0.0040527562	1.2730032339
O	0.4575599233	1.9199338091	-0.2399241663
C	-1.7620517975	0.2272867743	-2.4700996748
H	-1.9075848057	0.1387535681	-3.5589787914
C	-2.9164380120	0.7688265199	-0.3311876790
C	-2.8899229358	0.5970859349	-1.7168847090
H	-3.8824303026	1.0631222579	0.1078479026
H	-3.8169387188	0.7643257501	-2.2571855024
O	-0.5909194494	-0.0208869792	-2.0629579367
O	-1.9712155913	0.6301425600	0.5133423445
H	1.4107316934	2.0207909250	-0.3610716666
H	0.8670779957	0.1436714858	2.9685686957
H	-0.7261487814	0.7372226361	2.4648220513
H	-0.3691436272	-1.0248614092	2.4666628915
O	-0.4734797335	-1.9903078504	0.0457305421
O	1.7030606213	-0.8240124384	-0.8371444911
C	0.4271014467	-2.7820911359	-0.5588834998
C	1.6043319408	-2.1349306824	-1.0472359494
C	0.2709284432	-4.1600954201	-0.7173074219
C	2.5870953256	-2.8996067409	-1.6885417343
C	1.2649283112	-4.9120597092	-1.3638904327
H	-0.6330213663	-4.6292311105	-0.3347649613
C	2.4130682265	-4.2826511601	-1.8463187816
H	3.4787090448	-2.3982839766	-2.0583392195
H	1.1344695305	-5.9855194439	-1.4890662840
H	3.1824372164	-4.8652490249	-2.3509097236

(acac)(cat)Re(OH)(H)(CH_3)$^{-}$ oxidative addition intermediate
enthalpy: -843.515990

Re	-1.3375611281	0.1221409805	-0.2686213955
C	-1.2470873794	3.1973734129	0.5014855289
H	-1.6743672166	4.0927727916	0.9911128429
C	0.6967155467	2.3770929397	-0.8050808570
C	-0.0085754705	3.3810500597	-0.1446493380
H	1.6599971892	2.6731785057	-1.2517757371
H	0.4340265523	4.3720977095	-0.1180871072
O	-1.9228758000	2.1446046490	0.5933883740
O	0.4024381155	1.1499268669	-0.9663046290
O	-2.1639245771	0.9846596342	-1.8633126403
H	-2.7037400001	0.3681338056	-2.3697233592
C	0.0905577910	-1.4670327452	-0.5609774024
H	0.3402647254	-1.5971770863	-1.6195267084
H	0.9858389400	-1.1644825293	-0.0100509888
H	-0.2702697461	-2.4185116995	-0.1577206645
H	-1.9119544782	-1.1281515802	-1.1303868304
O	-0.5684150163	-0.0576610858	1.6425074853
O	-2.9623553749	-0.4682349085	0.7589170813
C	-1.4993769365	-0.2534317773	2.5747816711
C	-2.8185297589	-0.4761282227	2.0933375820
C	-1.2566504607	-0.2682213204	3.9527207936
C	-3.8654355338	-0.7086013635	2.9867094523
C	-2.3149415008	-0.4973786322	4.8431168462
H	-0.2436061892	-0.0980048081	4.3091400159
C	-3.6093452891	-0.7153311514	4.3656607130
H	-4.8655779535	-0.8757983267	2.5946891621
H	-2.1229615623	-0.5028989426	5.9147076191
H	-4.4260288190	-0.8885519539	5.0638329131

(acac)(cat)Re(OH)(H)(CH_3)$^{-‡}$ reductive elimination transition state
enthalpy: -843.479087

Re	-0.0263989392	0.0013707403	-0.0380452949
O	0.0615398273	-0.2334797836	2.1849141967
H	1.0010783298	0.0997228204	1.3303886405
C	1.6059493019	-1.2872233103	-0.4882846891
C	-3.0422980172	0.5582922305	0.5841766424
H	-3.9010660885	1.2244750080	0.7878500284
C	-2.4205495111	-1.8363438862	0.2484820991
C	-3.3436101929	-0.8117058496	0.4838515542
H	-2.8268597996	-2.8594633308	0.2163716859
H	-4.3820959247	-1.1028603659	0.6117506275
O	-1.9183017354	1.1232032556	0.4796678879
O	-1.1655419123	-1.7617874750	0.0539433432
H	-0.2442789484	0.6368667166	2.4835782780
H	1.8499760248	-1.9657281999	0.3404594308
H	1.3280978719	-1.9018911552	-1.3563657054
H	2.5113040752	-0.7230081213	-0.7478082327
O	-0.2883056158	0.3271352943	-2.0056847930
O	0.8807162265	1.8180814714	-0.2541519408
C	0.2393582481	1.4662782292	-2.4765515758
C	0.8573705376	2.2979884903	-1.5045582042
C	0.1826199200	1.8693202321	-3.8116059847
C	1.3965614153	3.5287838431	-1.8872372032
C	0.7314650018	3.1056593939	-4.1857301669
H	-0.2928117082	1.2166063106	-4.5399503388
C	1.3305807978	3.9289488937	-3.2306863817
H	1.8599727320	4.1586063293	-1.1314831332
H	0.6866387467	3.4210855071	-5.2265432502
H	1.7498690993	4.8890852196	-3.5261990361

Re(acac)(gly)$^-$ *cis* System
(acac)(gly)Re(OH)(OH_2)$^-$
enthalpy: -727.055841

Re	-.8930531083	.0226184021	.1200785745
C	-1.7527437814	2.6603406764	-.9694910120
H	-2.5696807439	3.3475271255	-1.2174746454
C	.6999733392	2.2670413817	-1.0459660840
C	-.4420609186	3.0431494781	-1.2672127649
H	1.6798371835	2.6674016219	-1.3286557431
H	-.2997846030	4.0231395131	-1.7181989380
O	-2.1327027764	1.5243208102	-.4576916657
O	.7252368976	1.0821986550	-.4945213648
O	-.5354893054	-.9837408316	-1.9809476895
H	-.0565429523	-1.5919550834	-1.3219181576
O	.3057301250	-1.6591070256	.2683791889
H	-.2458041946	-2.3202643449	.7101325592
H	.1639719313	-.3913741827	-2.2994050695
C	-2.2735965928	.4717913995	2.5191105619
C	-2.7678293755	-.9152809944	2.0967345224
H	-3.8586498747	-1.0151375238	2.2505496700
H	-2.2817828218	-1.6797078335	2.7384807915
H	-2.2568247433	.5869622765	3.6173551941
H	-2.9542334287	1.2378653747	2.1052231230
O	-2.4380431253	-1.1110048627	.7421960510
O	-.9686007411	.6336489874	2.0044033666

(acac)(gly)Re(OH_2)(OH_2)
enthalpy: -727.496667

Re	-0.9494653201	-0.1077215552	0.4301707815
C	-0.9372419662	1.9403235307	-1.6634208508
H	-1.5036114988	2.5137928156	-2.3997318486
C	1.2823022028	1.5834101063	-0.5864092795
C	0.4267802087	2.1995032236	-1.5046235005
H	2.3302550120	1.8911394435	-0.5469045399
H	0.8550402678	2.9683008503	-2.1402299038
O	-1.6497008983	1.0591175820	-1.0166873134
O	0.9419874153	0.6551582572	0.2595995415
O	-0.3215425814	-1.3395697111	-1.3636395987
H	0.5824441705	-1.0918770055	-1.6125268811
O	0.0178829443	-1.1874323338	2.1348217896
H	0.9545887502	-0.9390518918	2.0777642869
H	-0.8950067191	-1.0722990211	-2.0996425564
C	-2.8930193341	0.6197168125	2.4553234791
C	-3.6256279526	-0.0342297594	1.2751864870
H	-3.9540279621	0.7384563519	0.5618996112
H	-4.5161585488	-0.5824520798	1.6136824737
H	-2.9485334670	-0.0257751205	3.3459614886
H	-3.3427823858	1.5877052633	2.7179071698
O	-2.7261481284	-0.9209355125	0.6291619293
O	-1.5160827578	0.8029604308	2.1091202731
H	-0.4060547663	-0.5164748197	2.7314961510

(acac)(gly)Re(OH)(H)(CH_3)$^{-‡}$ metathesis transition state
enthalpy: -691.051329

Re	-1.3867927679	0.1311914001	0.1057241320
C	-1.3373417208	2.9906140050	-0.5910037729
H	-1.8941573780	3.8986360147	-0.8424309596
C	0.9156133235	1.9814748778	-0.2626062419
C	0.0576305324	3.0501597859	-0.5441026846
H	1.9967713583	2.1559334818	-0.2422150699
H	0.5159939665	4.0158911232	-0.7450062660
O	-2.0904448639	1.9432558661	-0.3821197129
O	0.5438166768	0.7592228193	-0.0083834676
O	-0.4895365719	-1.8505842461	0.2205200389
H	0.4426443514	-1.6408485853	0.3876220828
C	-1.1313966532	-0.8025210182	-2.1209554861
H	-1.9136088758	-1.4702942005	-2.4978473500
H	-1.4255963882	0.2161183199	-2.4084193431
H	-0.1883303208	-0.9980845423	-2.6533197205
H	-0.7018479298	-1.5045918028	-0.9153219012
C	-3.6862055481	-0.5574321785	1.6677095201
C	-2.9532830783	0.5675544917	2.4077220687
H	-4.7825697654	-0.4165507042	1.7062286484
H	-3.4613938619	-1.5205643071	2.1653808810
H	-3.0763291381	0.4814903160	3.5022188198
H	-3.3824904175	1.5380364168	2.0950074033
O	-1.5889805414	0.4882868629	2.0666737959
O	-3.2415263133	-0.5718356212	0.3317765192

(acac)(gly)Re(OH_2)(CH_3)$^-$
enthalpy: -691.072766

Re	-1.0775960022	-0.0827088838	-0.4309257453
C	-1.7982952613	2.9185932194	-0.6808256186
H	-2.5134729651	3.7238370843	-0.8998171818
C	0.5840458955	2.4086210458	-0.1023904307
C	-0.4860733347	3.2797239753	-0.3824393851
H	1.5674032946	2.8337242738	0.1237278276
H	-0.2589336671	4.3448350404	-0.3760512413
O	-2.2741653664	1.6984726901	-0.7904567112
O	0.5166417734	1.0986669368	-0.0192311416
O	-0.5100136935	0.6712160139	-2.5646575359
H	0.2189111639	1.2638748638	-2.3037313153
H	-1.3020455502	1.2431292443	-2.5491560908
C	0.2367340793	-1.7642397394	-0.5412702247
H	0.3447501240	-2.1139966592	-1.5801257135
H	1.2365199001	-1.4966375929	-0.1702496839
H	-0.1298655998	-2.6133821020	0.0525401245
C	-3.6180376673	-1.1788918113	0.1598079067
C	-2.8111488739	-1.3505420330	1.4487734962
H	-2.4851351790	-2.4045840565	1.5371535807
H	-4.1981676550	-0.2385605891	0.2170166529
H	-4.3397449825	-2.0060061456	0.0272316675
H	-3.4141081651	-1.1159018779	2.3440879604
O	-2.7097904037	-1.1381886559	-0.9155389724
O	-1.6838511764	-0.4982849991	1.3987242439

(acac)(gly)Re(OH)(H)(CH_3)$^{-‡}$ oxidative addition transition state
enthalpy: -691.074481

Re	0.0026966793	0.0000916482	-0.0000298784
C	-0.0102244174	0.0015960495	2.3243602144
H	1.0975755973	-0.0025040586	1.2493443303
O	-0.8485974566	-1.7755110529	0.2062038962
C	0.1206653362	3.0599531052	-0.1145230904
H	0.6862083467	3.9920992203	-0.2839665904
C	-2.1329023105	2.1484060120	0.4233853489
C	-1.2406634831	3.2064228693	0.1855727245
H	-3.1833221289	2.4270112964	0.6135309617
H	-1.6412657984	4.2157940241	0.2157707334
O	0.7965005043	1.9914120171	-0.2198844969
O	-1.8885456842	0.9069610711	0.4535094954
H	-1.2452995405	-1.9616539910	-0.6572283313
H	-0.8023146787	-0.7394233630	2.4525731196
H	0.8185012183	-0.2600195791	2.9923601394
H	-0.3635851285	1.0011080375	2.5958288926
C	0.5082308338	-0.1267435222	-2.8161137426
C	1.4942058580	-1.1065058696	-2.1795880333
H	2.4602117297	-1.1193126430	-2.7194772014
H	1.0673621996	-2.1293132599	-2.2499259162
H	0.1544349814	-0.4815130526	-3.8025720898
H	1.0214822226	0.8416479547	-2.9785322294
O	1.6964200596	-0.7320506032	-0.8428159167
O	-0.5758564943	0.0155000052	-1.9328077766

(acac)(gly)Re(OH)(H)(CH_3)$^-$ oxidative addition intermediate
enthalpy: -691.076369

Re	-1.4233174032	-0.0339263835	-0.3289696726
C	-1.1913858357	3.0290557590	0.0260459486
H	-1.5835482361	4.0006320604	0.3776234793
C	0.8470736721	1.9381317258	-0.9235236146
C	0.1311427448	3.0454896327	-0.4484229614
H	1.8861635794	2.1394004835	-1.2373794270
H	0.6530999452	3.9979021998	-0.4248075587
O	-1.9990322375	2.0631655632	0.1044008228
O	0.4767278401	0.7347469210	-1.0510064422
O	-0.4440949480	-1.7462969798	-0.3177477293
H	0.1036114222	-1.6265464885	0.4770585977
C	-2.0357840649	0.7298500136	-2.2953725373
H	-1.6988865411	0.0847466837	-3.1148495644
H	-3.1254618286	0.8265059528	-2.3661247400
H	-1.5932811609	1.7242585697	-2.4333869055
H	-2.3169766262	-1.0541572456	-1.2407532044
C	-1.4425873893	0.2154431940	2.5665731961
C	-2.6357789381	-0.6664374646	2.1913258721
H	-3.5129465797	-0.4697737301	2.8334361406
H	-2.3544349212	-1.7290095694	2.3242944016
H	-0.9978100443	-0.1190512922	3.5237916492
H	-1.7987536397	1.2531799691	2.7192465797
O	-2.9756091952	-0.4137304328	0.8473618662
O	-0.5078518733	0.1394402199	1.5282471809

(acac)(gly)Re(OH)(H)(CH_3)$^{-‡}$ reductive elimination transition state
enthalpy: -691.037771

Re	-0.0296761866	-0.0012465168	-0.0409376202
O	0.1572979215	-0.1924012734	2.1268586779
H	1.0278996019	0.2777179054	1.2815440631
C	1.9866637925	-0.3626284958	-0.8360384750
C	-0.5855477622	1.3756034846	-2.6688223822
H	-0.8843029494	1.2918667386	-3.7244499869
C	-0.0406428435	2.9389817827	-0.8298484455
C	-0.3619658816	2.6626531831	-2.1649059599
H	0.0638650287	3.9976722106	-0.5462174519
H	-0.4847969115	3.5019088093	-2.8430310468
O	-0.4924215117	0.2682177046	-2.0495377267
O	0.1319998069	2.1032738815	0.1148593914
H	-0.7330714714	0.2018603236	2.2318120028
H	2.5719215547	0.5673323908	-0.9269542143
H	2.5792786036	-1.0525377371	-0.2208438676
H	1.9099167127	-0.8025540731	-1.8413203023
C	-2.6550798114	-1.1405214610	0.3020919662
C	-1.6426688914	-2.2850095816	0.4798733869
H	-2.0189632988	-3.2287311478	0.0446598539
H	-1.4798330568	-2.4525417424	1.5598111533
H	-3.5402223388	-1.3103383383	0.9466039603
H	-3.0153034665	-1.1529916417	-0.7471285610
O	-0.4271131008	-1.9251227713	-0.1399886530
O	-2.0235523773	0.0691309084	0.6117675461

(acac)(gly)Re(CH_3)(H)(CH_3)$^-$ oxidative addition intermediate
enthalpy: -655.109069

Re	-1.3752026328	-0.0639904505	-0.3014274724
C	-1.3021592901	3.1010091267	-0.0802195080
H	-1.6986775221	4.0869304191	0.2347445194
C	0.7458535095	2.0177563310	-1.0330222203
C	0.0095609261	3.1237733244	-0.6022800134
H	1.7641854399	2.2325895223	-1.3987167355
H	0.5030168320	4.0905062288	-0.6538279091
O	-2.0735709577	2.1229556093	0.0636528187
O	0.4234877841	0.7878381657	-1.0692306570
C	-2.1616812485	0.5446955412	-2.2608545595
H	-1.7521505315	-0.0436268280	-3.0918616558
H	-3.2546467906	0.4561434558	-2.2948987488
H	-1.8985942852	1.5968841047	-2.4284119843
H	-2.0100476359	-1.2790118180	-1.1828358780
C	-1.4620979257	-0.1773478036	2.5944805093
C	-2.9141246263	-0.1061136047	2.1059316481
H	-3.2555505127	0.9432425157	2.1353379776
H	-3.5958739240	-0.7072879618	2.7334854544
H	-1.2190126256	-1.2369912550	2.8244832700
H	-1.3387149825	0.3918130952	3.5370975173
O	-2.9402902822	-0.5972770525	0.7816602775
O	-0.6499880229	0.3368903289	1.5866708454
C	-0.1396453447	-1.8132629584	-0.1897606396
H	-0.6807062860	-2.6750320909	0.2188368649
H	0.2599356072	-2.0916808026	-1.1726604686
H	0.6920399620	-1.5619819613	0.4780063960

Re(acac)(gly)$^-$ *trans* System
(acac)(gly)Re(OH)(OH_2)$^-$
enthalpy: -727.051310

Re	-1.1930138067	0.3633754225	-0.0339514151
C	-1.1643774125	3.2955275633	-0.0552774297
H	-1.6693025314	4.2209476745	0.2325183286
C	0.7835115919	2.2524191848	-1.1850276716
C	0.0427988346	3.3554139404	-0.7518755471
H	1.7302736292	2.4078526214	-1.7108438356
H	0.4396038987	4.3440989513	-0.9727369282
O	-1.8138264476	2.2062830621	0.2903601024
O	0.4579924270	0.9988004181	-0.9854436979
O	-2.0722637972	0.0015084857	-1.9365072639
O	-0.9146601874	-1.8029954937	-0.6978023018
H	-1.4133671437	-1.3911130305	-1.4947989907
H	-1.4790258112	0.3956547964	-2.5921750784
H	-1.6418104160	-2.1001524089	-0.1195244495
C	-1.3733826207	0.2545313300	2.7753876257
C	-2.4618860057	-0.7330542270	2.3315242294
H	-3.3941292970	-0.5887216583	2.9080192438
H	-2.1150046864	-1.7665560677	2.5363180134
H	-0.9652036360	-0.0229357540	3.7649057030
H	-1.8258589479	1.2604059430	2.8695274291
O	-2.7036834470	-0.5547889365	0.9512971986
O	-0.3603391193	0.2486917890	1.8030144829

(acac)(gly)Re(OH)(H)(CH_3)$^{-‡}$ metathesis transition state
enthalpy: -691.047229

Re	-1.2146771032	0.3650925508	-0.0307168928
C	-1.3655767636	3.1308334579	-1.0523782341
H	-1.9873330305	3.9940960072	-1.3114139350
C	0.9305252715	2.1831533736	-0.9939608155
C	0.0114990640	3.2077356663	-1.2555705776
H	1.9951948062	2.3603043640	-1.1801235249
H	0.4033579660	4.1432468710	-1.6488261347
O	-2.0380980829	2.1016055341	-0.6066881494
O	0.6388558228	1.0108214481	-0.5137395043
O	-1.3787010177	-0.7752701401	-1.8989902914
H	-2.3220243596	-0.9952260892	-1.9192953480
C	-0.3181109537	-1.8464100790	0.2723388642
H	0.6455705592	-2.1577831450	-0.1477467753
H	-0.0991407825	-1.4098586788	1.2558687710
H	-0.9562108225	-2.7184535476	0.4582186427
H	-0.8961623068	-1.4136345740	-0.9636573861
C	-3.4615114915	0.4283180320	1.6575918203
C	-2.2793853003	0.5766404161	2.6257283559
H	-3.8144700171	1.4327689891	1.3605433206
H	-4.3073484976	-0.0912967264	2.1448120667
H	-2.1515406105	-0.3746524211	3.1814148196
H	-2.4889229060	1.3597370096	3.3787975159
O	-3.0287071140	-0.2890955580	0.5229093017
O	-1.1038476052	0.8817855651	1.9108962872

(acac)(gly)Re(OH_2)(CH_3)$^{-}$
enthalpy: -691.075779

Re	-1.1137742984	0.2794230313	0.0498227472
C	-1.4818415102	3.3073950888	-0.4383618211
H	-2.0739773626	4.2295404276	-0.3520501583
C	0.5739404991	2.2900505854	-1.4367808274
C	-0.2981422143	3.3609193956	-1.1777423718
H	1.4733087602	2.4768813736	-2.0343096475
H	-0.0290796909	4.3236676223	-1.6096261275
O	-1.9966964768	2.2504442126	0.1360837356
O	0.4471310243	1.0582410842	-1.0033166580
O	-2.0647070854	0.5834227315	-2.0629090981
H	-1.2872540000	0.9909526951	-2.4872854027
C	-1.3899642950	0.2980481548	2.8466114466
C	-2.4948068997	-0.6534875558	2.3799196638
H	-3.4233494941	-0.5057187758	2.9627734160
H	-2.1660094977	-1.6981531048	2.5498108324
H	-0.9749937503	0.0056068591	3.8272101060
H	-1.8094698560	1.3162245694	2.9445782450
O	-2.7263443225	-0.4151873651	1.0133337125
O	-0.3631668178	0.2737415040	1.8733825634
C	-0.3769919069	-1.6685759731	-0.4391037897
H	-0.4042390006	-2.3480256167	0.4246032931
H	-0.9745645509	-2.1330713906	-1.2404318446
H	0.6635541193	-1.6110974246	-0.7900353501
H	-2.5846164837	1.3388693203	-1.7342532229

(acac)(gly)Re(OH)(H)(CH_3)$^{-‡}$ oxidative addition transition state
enthalpy: -691.066645

Re	-0.0005608141	0.0080870921	-0.0376819211
C	0.0743764276	-0.0132794461	2.2997643452
H	1.0074017076	-0.0221308940	1.3163621499
O	-0.5118065484	-1.9288070199	0.0557349237
C	0.0415413242	-0.1724107346	-3.0792184098
H	-0.4848292581	-0.0487985400	-4.0407020345
C	2.2000947383	-0.7970803193	-2.0324618424
C	1.3774411065	-0.5861037823	-3.1471664365
H	3.2315377076	-1.1291557288	-2.2434216898
H	1.8038284626	-0.7597553815	-4.1309152405
O	-0.6535131783	0.0884748944	-2.0522833678
O	1.9219049148	-0.6569601878	-0.8039264693
H	-1.4399233659	-1.9839315960	0.3206847655
H	0.3941814149	-0.9472359163	2.7705278653
H	0.5100110255	0.8403443385	2.8290770288
H	-1.0166462123	0.0631609618	2.3320366332
C	-0.8062506464	2.7582109706	-0.2019146229
C	-1.8652224129	2.0749932707	0.6750066920
H	-2.8678295071	2.5145934727	0.5108025018
H	-1.5989187432	2.2662348840	1.7369430707
H	-0.6174746909	3.7964557498	0.1323393276
H	-1.1825430125	2.8074835089	-1.2430110400
O	-1.8782248864	0.7087498475	0.3683336994
O	0.3696192664	1.9939491671	-0.1293375302

(acac)(gly)Re(OH)(H)(CH_3)$^{-}$ oxidative addition intermediate
enthalpy: -691.078452

Re	-0.0773207252	0.0457626074	-0.1061655502
C	0.0688933618	-0.3023629101	2.0130993190
H	1.3905416879	0.3896092751	0.5031381391
O	0.5472661310	1.7522202792	-0.9486739911
C	-2.5954805543	0.5896490157	-2.1005674424
H	-3.1523608416	0.4400136166	-3.0479086900
C	-2.8147351396	1.5228863568	0.1983308911
C	-3.3148977834	1.2295306159	-1.0758677851
H	-3.5053682675	2.0587914240	0.8731124020
H	-4.3375465728	1.5269514039	-1.2899054970
O	-1.4032070479	0.1850454739	-2.0859755233
O	-1.6799199534	1.2662876951	0.6973781019
H	-0.0748035132	1.8928542467	-1.6770204031
H	0.2993715404	0.6215204375	2.5548062485
H	-0.9065916524	-0.6871031797	2.3255520672
H	0.8379560805	-1.0486379146	2.2397611876
C	-0.9030526771	-2.6170347060	-0.8449143276
C	0.6118864336	-2.5904440739	-1.0490274971
H	0.9159968490	-3.1203669576	-1.9686695824
H	1.1064197309	-3.0931644433	-0.1953103470
H	-1.2399021589	-3.6123318304	-0.4990077237
H	-1.4004252302	-2.4151093240	-1.8124281884
O	1.0173223448	-1.2438427258	-1.1273229028
O	-1.2072921993	-1.6378818568	0.1088727540

(acac)(gly)Re(OH)(H)$(CH_3)^{-‡}$ reductive elimination transition state
enthalpy: -691.039630

Re	-0.0384780838	-0.0081378791	-0.0214430414
O	0.0820429096	0.0728561793	2.2183946589
H	0.9985767531	-0.3094961183	1.3016955108
C	1.8650212044	-0.8006619939	-0.6939803759
C	-3.0951776302	-0.2692767604	0.5239973821
H	-4.0973534280	0.1630039788	0.7015308789
C	-1.8596704676	-2.4224404429	0.3361993207
C	-3.0232835202	-1.6741943894	0.5348678689
H	-1.9638445038	-3.5186880451	0.3685242513
H	-3.9448508374	-2.2215914866	0.7126094276
O	-2.1616315926	0.5597157870	0.3303936261
O	-0.6746386234	-2.0043826790	0.1190227359
H	0.1716323494	1.0336531955	2.3178346131
H	2.0828060614	-1.7927329690	-0.2738897053
H	1.8040940243	-0.8813152394	-1.7871508598
H	2.7129880312	-0.1451104710	-0.4457956585
C	-0.5700085813	1.5756755401	-2.2768343451
C	0.3820096218	2.4378344955	-1.4340947457
H	0.0718628674	3.4984731131	-1.4215224615
H	1.3965762919	2.3897886103	-1.8718545368
H	-0.4576187988	1.7948477672	-3.3552325138
H	-1.6104111973	1.8272630554	-1.9918043550
O	0.3873033019	1.9188581694	-0.1202309566
O	-0.2591356699	0.2310759021	-2.0209575616

Re(V) Systems

Re(acac)(cat)$^+$ *cis* System
(acac)(cat)Re(OH)$(OH_2)^+$
enthalpy: -879.169147

Re	-.8059595395	-.0280147135	.1813099225
C	-1.8053392474	2.3410098456	-1.4187955480
H	-2.6993256644	2.8068006659	-1.8364237804
C	.5996630120	2.3642032964	-1.0489540331
C	-.5658011219	2.9328491672	-1.5830561096
H	1.5666147974	2.8581678468	-1.1636182332
H	-.4963656518	3.8736907879	-2.1152459077
O	-2.0341316984	1.2377276953	-.7675058918
O	.6228368901	1.2600696816	-.4009320693
O	-.5196691004	-.9287379247	-1.8285165934
H	-1.3077604457	-1.3035669125	-2.2495951116
O	.3089682968	-1.3960092744	.7607068238
H	.9761292632	-1.8067625652	.1855026769
H	-.0018910591	-.4674782665	-2.5056574809
O	-1.0967057511	.7997182942	1.8903433629
O	-2.4688802863	-.9264712549	.6916059589
C	-2.2657137242	.5184434983	2.4883423060
C	-2.7095924585	1.1116358331	3.6743979524
C	-3.0385005672	-.4570962021	1.8084486975
C	-3.9444546773	.7037722118	4.1613935122
H	-2.1020563263	1.8563796347	4.1767707891
C	-4.2833151398	-.8568176284	2.3033467250
C	-4.7184962258	-.2680063219	3.4851477664
H	-4.3273632741	1.1388778403	5.0787206118
H	-4.8684386640	-1.6035433645	1.7781352055
H	-5.6774503096	-.5590899904	3.9018886483

(acac)(cat)Re(OH_2)(OH_2)$^{2+}$
enthalpy: -879.566541

Re	-0.8516261234	0.0825728605	0.1202481857
C	-1.9024918059	2.5143687923	-1.2634766410
H	-2.8166979863	3.0428260459	-1.5356197932
C	0.5259307599	2.4157448114	-1.1692838656
C	-0.6436315059	3.0410470626	-1.5692261318
H	1.5080562255	2.8391966118	-1.3745781948
H	-0.5848131746	3.9858858115	-2.0982485057
O	-2.1028278117	1.4024758226	-0.6307354737
O	0.5442040682	1.2931640159	-0.4953753152
O	-0.9106593905	-1.3093642098	-1.4435752905
H	-0.2158215384	-1.9670069758	-1.6250425223
O	0.8305333523	-1.1066156599	0.8383762073
H	1.7053077186	-0.8368106708	0.5048089231
H	-1.7709765074	-1.6625110826	-1.7367964363
O	-0.9668709855	0.5454393285	2.0017113060
O	-2.4358460574	-0.8917524084	0.6950957591
C	-2.1340489661	0.3163448529	2.6114093020
C	-2.5078440327	0.7652983877	3.8763032551
C	-2.9837964663	-0.5583539222	1.8461502793
C	-3.7464572750	0.3344707393	4.3424013876
H	-1.8697701968	1.4264311682	4.4521133017
C	-4.2239949986	-1.0033858718	2.3432140432
C	-4.5892455388	-0.5390379592	3.5915690326
H	-4.0872701453	0.6705911189	5.3171700371
H	-4.8475505114	-1.6734530637	1.7615027945
H	-5.5382579499	-0.8428470165	4.0213779803
H	0.9052194300	-1.1618489389	1.8083661972

(acac)(cat)Re(OH)(H)(CH_3)$^{+‡}$ metathesis transition state
enthalpy: -843.141613

Re	-1.3579046461	0.1651584340	0.1132642191
C	-1.1601060876	3.0231950480	-0.8176214594
H	-1.7722627010	3.8853648437	-1.0810012389
C	0.9985536228	1.9931390711	-0.4267383717
C	0.2248779534	3.0897873914	-0.8121682295
H	2.0876462330	2.0443926811	-0.4138901600
H	0.7131207973	4.0175729317	-1.0849063950
O	-1.8414533809	1.9595012835	-0.5032281052
O	0.4959605066	0.8667222970	-0.0498778385
O	-0.5152516324	-1.6307794153	0.5545589790
H	0.2803278335	-1.6359307708	1.1088488187
C	-1.3816577501	-1.0905274719	-1.8009805199
H	-0.7360082029	-1.8793394981	-2.2281694061
H	-2.4191245844	-1.3809979163	-1.9500649618
H	-1.1213542356	-0.1912725275	-2.3751496116
H	-0.7327908230	-1.5473125173	-0.7456539233
O	-3.2349530450	-0.2787723207	0.2227844197
O	-1.6734779925	0.3534444808	2.0149059191
C	-3.8458070498	-0.0934692438	1.3981091341
C	-5.2130703677	-0.2628753053	1.6420391275
C	-2.9526957674	0.2925742912	2.4256133863
C	-5.6578107735	-0.0177081334	2.9350636064
H	-5.8798707354	-0.5740902747	0.8454789909
C	-3.4011935074	0.5310181275	3.7241214674
C	-4.7660381188	0.3766808067	3.9572095568
H	-6.7107570352	-0.1347783405	3.1691308672
H	-2.7104877299	0.8286284339	4.5049885642
H	-5.1552973716	0.5570711536	4.9541250748

(acac)(cat)Re(OH_2)(CH_3)$^+$
enthalpy: -843.186321

Re	-.8906639672	-.1692274291	-.4786059133
C	-2.2586869085	2.4988089883	-.5434423413
H	-3.1705357159	3.0444178355	-.7950625182
C	.0440763577	2.5728796969	.2658365142
C	-1.1493377273	3.2007114546	-.0856865408
H	.8900039817	3.1352720526	.6609099941
H	-1.2252893503	4.2755707216	.0262207717
O	-2.3632891741	1.2148889933	-.6961812028
O	.2251422355	1.2982816962	.1794788246
O	-.4460304202	.8231043793	-2.4641765833
H	-1.0932987451	.5992601865	-3.1499179417
H	.4351417318	.7035397657	-2.8477923740
C	.3543610762	-1.6513828321	-1.2364411208
H	.8151028161	-1.4776020274	-2.2109074795
H	1.1383432394	-1.5414718540	-.4545699355
H	-.0427729270	-2.6667539262	-1.1871420526
O	-2.4168891045	-1.3255408675	-.9738520442
O	-1.3224876646	-.9256598053	1.2395739598
C	-3.1328827632	-1.7499496281	.0594774464
C	-2.5025304934	-1.5571871043	1.3211691520
C	-4.3769729157	-2.3952297375	-.0274351831
C	-3.0764069298	-2.0232933159	2.5079091217
C	-4.9459349399	-2.8422160003	1.1542352796
H	-4.8539940496	-2.5334024033	-.9913784647
C	-4.3053743537	-2.6594854305	2.4061693340
H	-2.5750573704	-1.8727084996	3.4577771072
H	-5.9056930486	-3.3480985957	1.1260297031
H	-4.7926330563	-3.0247791786	3.3043861288

(acac)(cat)Re(CH_3)(H)(CH_3)$^{+‡}$ OHM transition state
enthalpy: -807.182200

Re	0.0170582357	-0.0038482742	0.0296201858
C	0.4810859954	0.4925616892	2.1644771547
H	1.2954174482	-0.1368353197	1.2016738204
C	2.2285312505	-0.5416404672	0.0596621515
C	-2.6114296895	-1.1901544111	-0.8889536716
H	-3.5752533117	-0.9394598269	-1.3361419304
C	-1.0763957918	-2.8381181408	0.0087053611
C	-2.2861691917	-2.5088456854	-0.5964116062
H	-0.8564717183	-3.8718995784	0.2824187384
H	-2.9996340305	-3.2924884965	-0.8200392470
O	-1.8561761002	-0.1690369742	-0.6418738038
O	-0.1398049170	-1.9945354457	0.2890358125
H	1.3076868283	0.1594717431	2.8040393475
H	0.3708770304	1.5720952449	2.2269051531
H	-0.4245712190	-0.0345875243	2.5006334791
O	-0.2603746866	1.9407480777	0.0114534643
O	0.6024722150	0.4881068817	-1.7820228258
C	-0.3649129282	2.4910072943	-1.1898739220
C	-0.8397827716	3.7868396296	-1.4610764623
C	0.1262454726	1.6507233341	-2.2268975580
C	-0.8200242728	4.2008388252	-2.7796522815
H	-1.2065380162	4.4153940882	-0.6564751375
C	0.1589802794	2.0868305830	-3.5582378105
C	-0.3265191693	3.3599002820	-3.8135680321
H	-1.1851235405	5.1902059868	-3.0373269575
H	0.5460892592	1.4452431756	-4.3411648572
H	-0.3266248827	3.7319015080	-4.8333928683
H	2.2232117269	-1.1031789283	-0.8735086847
H	2.8195861323	0.3682957284	-0.0574449065
H	2.6434829999	-1.1748664915	0.8504958874

(acac)(cat)Re(CH_3)(H)(CH_3)$^+$ oxidative addition intermediate
enthalpy: -807.193385

Re	-1.2224928490	0.0900093302	-0.2032672370
C	-0.6893703307	3.1560289338	-0.3895728876
H	-0.9437227680	4.1553039036	-0.0191900082
C	0.6571093635	1.7883375909	-1.8778147780
C	0.2614911176	3.0234921094	-1.4302898223
H	1.4101229927	1.6888249160	-2.6598844728
H	0.7065164053	3.9144906790	-1.8565807779
O	-1.2797312002	2.1915169481	0.1723969735
O	0.2105851968	0.6385683347	-1.4258248830
C	-2.8557011682	0.6316898726	-1.4956273335
H	-2.3634893655	0.9247411291	-2.4309943993
H	-3.5604180625	-0.1752102474	-1.6735203095
H	-3.3451441721	1.4883171080	-1.0293253991
H	-1.6097630807	-1.0994651498	-1.2291320448
O	-0.8323942974	0.0271624353	1.7267650708
O	-2.8118120197	-0.7583140336	0.6479641690
C	-1.6457539885	-0.5529594460	2.5811615445
C	-2.8215032729	-1.0285166318	1.9301481874
C	-1.4596484780	-0.7069962844	3.9637142454
C	-3.8428707460	-1.6861844276	2.6461348435
C	-2.4722261904	-1.3527658977	4.6507307651
H	-0.5652691808	-0.3376678569	4.4519249461
C	-3.6474422471	-1.8368614953	4.0030627335
H	-4.7304502313	-2.0444326179	2.1370252346
H	-2.3728216374	-1.5005790502	5.7215658134
H	-4.4030727372	-2.3351274622	4.6014556729
C	-0.0699412956	-1.7458324362	-0.1978734249
H	-0.6305999390	-2.5361881497	0.3069192100
H	0.2633976365	-2.0749158063	-1.1794236402
H	0.7857461915	-1.4463842014	0.4178770184

Re(acac)(cat)$^+$ *trans* System
(acac)(cat)Re(OH)(OH_2)$^+$
enthalpy: -879.162920

Re	-1.2340748017	0.3234150206	-0.1351955661
C	-1.3357101534	3.2553719662	0.0183588142
H	-1.9052773960	4.1611062500	0.2401839915
C	0.8383850829	2.3266145067	-0.7035237679
C	0.0045140099	3.3829458806	-0.3913400055
H	1.8693594874	2.5245217279	-0.9997238087
H	0.4123444124	4.3846423569	-0.4613979188
O	-1.9921333157	2.1710394558	0.1925131892
O	0.5277810325	1.0556134690	-0.6951554233
O	-2.1423612633	0.2464655844	-1.7649914231
O	-0.2836137434	-1.5329040341	-0.8174297429
H	-0.5809386839	-2.3891999726	-0.4748634681
H	-1.8932982748	-0.4353089822	-2.4133061099
H	0.6825271042	-1.4855750829	-0.7224063952
O	-0.4606137787	-0.0715664101	1.6351817558
O	-2.7740507259	-0.2473625301	0.9780236216
C	-1.2094801281	-0.5631073601	2.6030348048
C	-2.5846928941	-0.6464875365	2.2100325095
C	-0.7918727062	-0.9414432524	3.8892346932
C	-3.5701417105	-1.0831856840	3.1159251425
C	-1.7723983758	-1.3788797348	4.7611431467
H	0.2507837749	-0.8652791886	4.1769990840
C	-3.1420257708	-1.4517812740	4.3768997344
H	-4.6096269323	-1.1352495699	2.8126725034
H	-1.4981433155	-1.6662529212	5.7710715624
H	-3.8672605809	-1.8076533939	5.1017083324

(acac)(cat)Re(OH)(H)(CH_3)$^{+‡}$ metathesis transition state
enthalpy: -843.144587

Re	-1.2144110104	0.3480879157	-0.0208471895
C	-1.2125268583	3.2772551526	-0.7774871356
H	-1.8548562587	4.1566138396	-0.8319567661
C	0.9527117822	2.2216943374	-0.9994959128
C	0.1350640865	3.3422729300	-1.1084632551
H	2.0133610460	2.2658799710	-1.2482202199
H	0.5588968918	4.2836624301	-1.4359348320
O	-1.8125415540	2.1987708711	-0.3802992454
O	0.5392633028	1.0678918184	-0.5856346215
O	-1.5864920041	-0.9134945786	-1.5400770085
H	-2.5198277493	-1.1650288459	-1.6573159207
C	-0.0318059883	-1.5829324167	0.3887435099
H	0.1908493232	-2.4429652026	-0.2749840896
H	0.9425217676	-1.1247689276	0.5589162206
H	-0.4475932621	-1.9954399849	1.3079059846
H	-0.8486806105	-1.5171504288	-0.7313528719
O	-3.0398138787	-0.1017627859	0.4722766129
O	-1.1589392691	0.5417987222	1.9222823519
C	-3.4273523908	0.2128751457	1.7062685158
C	-4.7402350074	0.1394662169	2.1966999717
C	-2.3425148758	0.6058909699	2.5376251908
C	-4.9352788298	0.4843740899	3.5231346780
H	-5.5527190964	-0.1708463936	1.5490153333
C	-2.5472408137	0.9352123003	3.8808026305
C	-3.8532460846	0.8794953785	4.3505207534
H	-5.9344460636	0.4498736425	3.9448002442
H	-1.7154119370	1.2270756403	4.5119512096
H	-4.0542305527	1.1403908211	5.3848466183

(acac)(cat)Re(OH_2)(CH_3)$^{+}$
enthalpy: -843.201439

Re	-.9546563349	-.1588928922	-.5468943144
C	-2.0495391442	2.6225636582	-.6320046446
H	-2.9421385044	3.1979062507	-.8766626710
C	.2206175145	2.5054529554	.2021714706
C	-.9091749805	3.2402891709	-.1293397174
H	1.1203372901	2.9810456605	.5912396349
H	-.9086213402	4.3140904513	.0131519169
O	-2.1668178611	1.3498502414	-.8545997520
O	.2942744967	1.2151284685	.0796792060
C	-.2751315845	-.5649127179	-2.4839212132
H	.6270359416	-1.1788045566	-2.5748294532
H	-1.0601559522	-.9363581380	-3.1412065256
H	-.0032941576	.4667099620	-2.7725683063
O	.7217956582	-1.4203636968	.0053237948
H	1.1322192401	-1.9955615368	-.6575198377
H	.5315304082	-1.9351652897	.8075293480
O	-2.4483613836	-1.2401591756	-1.2219645562
O	-1.5635279268	-1.1544814185	1.0520786618
C	-3.2757119884	-1.7807842212	-.3381498640
C	-2.7647519213	-1.7442087157	.9826356142
C	-4.5108034494	-2.3850273609	-.6296483077
C	-3.4628730146	-2.3187835384	2.0464516251
C	-5.2065523629	-2.9395989545	.4306108762
H	-4.8854755037	-2.4008441375	-1.6471342879
C	-4.6881928935	-2.9054691215	1.7490353221
H	-3.0641704706	-2.2938291802	3.0544562541
H	-6.1676804804	-3.4113109961	.2549013870
H	-5.2669984995	-3.3526645057	2.5512239048

Re(acac)(gly)$^{+}$ *cis* System

(acac)(gly)Re(OH)$(OH_2)^{+}$

enthalpy: -726.751031

Re	-.8609935495	-.0318351068	.1879497227
C	-1.6706851658	2.3932475476	-1.4394767315
H	-2.5406182951	2.8722206801	-1.8907052633
C	.6978629829	2.3839140572	-.9105833481
C	-.4338030809	2.9864223981	-1.5024133405
H	1.6784744718	2.8629086037	-.9833459181
H	-.3271934187	3.9390668485	-2.0066015238
O	-1.9551486597	1.2525167937	-.8562786305
O	.6648067532	1.2830392081	-.2835351960
O	-.6917471592	-.9968723580	-1.8644317039
H	-1.5528837815	-1.2567888064	-2.2272253082
O	.3564167735	-1.3522934672	.5735348005
H	.6292021584	-2.0654811688	-.0255994897
H	-.1877296409	-.5725458095	-2.5749007163
C	-2.3743795048	.5085724516	2.4980911890
C	-2.8963035282	-.8192452803	1.9617852290
H	-3.9851377975	-.8981269734	2.0013795490
H	-2.4510994380	-1.6666470675	2.4974604645
H	-2.1857818133	.5102208843	3.5742424846
H	-3.0428841898	1.3408190357	2.2484479792
O	-2.4867778254	-.9098757419	.5745103698
O	-1.1021426352	.7792176950	1.8428985213

(acac)(gly)Re$(OH_2)(OH_2)^{2+}$

enthalpy: -727.151844

Re	-0.9542284398	-0.1053018198	0.3937733160
C	-0.8908885534	2.2099594916	-1.5128027466
H	-1.5510257736	2.7555921382	-2.1864241648
C	1.2409522626	1.8300032260	-0.4403543086
C	0.4406988101	2.5536491456	-1.3230783602
H	2.2866636710	2.0800541185	-0.2601861110
H	0.8545623997	3.3985803716	-1.8623927320
O	-1.4706114908	1.2107908942	-0.9027767284
O	0.7829919532	0.8135066616	0.2222770403
O	-0.5914136503	-1.5345478986	-1.1809773016
H	-1.3400362987	-1.8458732343	-1.7210639278
O	0.0877495863	-1.2880705221	1.8153034696
H	0.8668451808	-1.8520784877	1.6758931075
H	0.1412516437	-2.1654725286	-1.2729786258
C	-2.9874392414	0.7403770154	2.1176219977
C	-3.5267293745	-0.5922747851	1.5520326217
H	-4.5267030231	-0.5114080002	1.1171949793
H	-3.5081731568	-1.4164815293	2.2743151413
H	-3.2560623197	0.9041115277	3.1635894163
H	-3.3167233088	1.5813114375	1.4976685409
O	-2.5939732349	-0.9369536197	0.4969204071
O	-1.5547472416	0.6070920557	2.0282974962
H	0.0969411730	-0.9224667765	2.7211429722

(acac)(gly)Re(OH)(H)$(CH_3)^{+‡}$ metathesis transition state
enthalpy: -690.724525

Re	-1.4110525415	0.1495882712	0.1190314709
C	-1.2081563037	3.0352582736	-0.7121283130
H	-1.8581011562	3.8777286900	-0.9404357472
C	0.9617181872	2.0235973353	-0.3838557800
C	0.1659446469	3.1321570702	-0.7147482466
H	2.0511592448	2.0930564073	-0.3905223280
H	0.6341556843	4.0758376682	-0.9666018153
O	-1.8538004653	1.9262137000	-0.4379704499
O	0.4762037003	0.8838571790	-0.0578244481
O	-0.4244723231	-1.5913649614	0.3537339483
H	0.3657982527	-1.6186396427	0.9168009023
C	-1.3186983714	-0.9063872711	-1.9313676208
H	-2.3234045421	-1.2772915029	-2.1213674346
H	-1.1203879411	0.0303185867	-2.4642907094
H	-0.6064905819	-1.6223074580	-2.3845383289
H	-0.6076197825	-1.4387088198	-0.8939701231
C	-3.7456625138	-0.7362843467	1.5136755546
C	-2.9849796380	0.1825772983	2.4694424430
H	-4.8131845762	-0.5136677978	1.4413170411
H	-3.6101564778	-1.7950497436	1.7648355141
H	-3.0017419737	-0.1649627911	3.5051441697
H	-3.3673586208	1.2091014984	2.4099026358
O	-1.6238651280	0.1571862046	2.0036490240
O	-3.1502907795	-0.5283026139	0.2195510109

(acac)(gly)Re$(OH_2)(CH_3)^{+}$
enthalpy: -690.774715

Re	-1.2014845869	-.0182702361	-.4811432266
C	-1.4650210532	3.0114956037	-.2410906727
H	-2.2436360914	3.7693113097	-.3181934795
C	.7894420656	2.2863718246	.1957706094
C	-.1615099097	3.3191058638	.0527541710
H	1.8216735997	2.5303589983	.4630763462
H	.1288006624	4.3510092287	.2074340811
O	-1.8993436892	1.7867436712	-.4318866072
O	.5335532816	1.0524896677	.0436438031
O	-.8366226722	.1827812780	-2.6125615058
H	-1.5871161917	-.0379208957	-3.1876872218
H	-.0333046469	-.2098196885	-2.9899555497
C	.3907963058	-1.4323111129	-.5691770313
H	-.0558293484	-2.3912667478	-.8595733116
H	1.1546880120	-1.1479109635	-1.2980245358
H	.8431190733	-1.5239983305	.4176403271
C	-3.2094570820	-1.9684155334	.0147668407
C	-2.9520812023	-1.2141429973	1.3257056809
H	-3.0224098664	-1.8482550552	2.2124601773
H	-4.2686783096	-2.0775815850	-.2303515166
H	-2.7276013509	-2.9523906067	.0099738801
H	-3.6367418924	-.3621800353	1.4184469658
O	-2.5885832186	-1.1525853872	-1.0082056121
O	-1.5940662880	-.7449152675	1.2096836032

(acac)(gly)Re(CH_3)(H)(CH_3)$^{+‡}$ OHM transition state
enthalpy: -654.752094

Re	-0.0252555509	0.0136524818	0.0665238032
C	0.2252507792	0.1961853726	2.2947464853
H	1.2218301289	-0.1844130183	1.2901851108
C	2.2448298481	-0.2517563942	0.2319134772
C	-2.5516590409	-1.5529289905	-0.4960004796
H	-3.6119288945	-1.3728867947	-0.6638734454
C	-0.6360398336	-2.9996178817	-0.2180418607
C	-2.0045509934	-2.8104803399	-0.5057368701
H	-0.2125302052	-4.0062750520	-0.1811802460
H	-2.6364884310	-3.6670867422	-0.7055808115
O	-1.8610078037	-0.4560701383	-0.2577015338
O	0.1709521843	-2.0456914883	0.0238213953
H	0.9672497832	-0.2939124355	2.9354217935
H	0.1516251637	1.2559827180	2.5273644330
H	-0.7325481977	-0.3189188731	2.4528280674
C	-0.3931932240	2.6209977125	-1.0193170543
C	0.3768840770	1.8767308010	-2.1109599440
H	-1.4725928540	2.6570567737	-1.2102977238
H	-0.0320976898	3.6380328691	-0.8478564317
H	1.3690204294	2.3073911006	-2.2885624555
H	-0.1696801087	1.8592415979	-3.0608377303
O	0.5610586768	0.5174358895	-1.6865999353
O	-0.2277531282	1.8743975425	0.2103798877
H	2.3613111477	-0.8470130171	-0.6708376875
H	2.6579167772	0.7485185161	0.0999431273
H	2.7525180068	-0.7607011686	1.0600376933

Re(acac)(gly)$^+$ *trans* System
(acac)(gly)Re(OH)(OH_2)$^+$
enthalpy: -726.736814

Re	-1.2929504104	0.4066953421	-0.0448776578
C	-1.0210162729	3.3174277234	-0.2008401100
H	-1.5027151011	4.2891502851	-0.0755132260
C	1.0276323888	2.1009734052	-0.8568331052
C	0.2992506609	3.2750399528	-0.6286222618
H	2.0569947232	2.1843269903	-1.2167509207
H	0.7958331566	4.2200691324	-0.8147640872
O	-1.8099207314	2.3267098333	0.0947220265
O	0.6111294180	0.8987380751	-0.6977299690
O	-1.9700807543	0.0779114900	-1.7220970155
O	-0.5609519644	-1.7274748062	-0.5617946552
H	-0.5584136834	-2.3194985992	0.2057860978
H	-2.0891015742	-0.7554821086	-2.2034360032
H	0.3751178706	-1.6182240100	-0.8054544390
C	-1.2035254222	-0.3482722446	2.7375096601
C	-2.6212031049	-0.6292340062	2.2255224331
H	-3.3872473770	-0.4326718680	2.9809028613
H	-2.7176214714	-1.6647362624	1.8695318720
H	-0.7580388768	-1.1834791404	3.2844999422
H	-1.1649174096	0.5576617928	3.3515090422
O	-2.7721592668	0.2919347499	1.1530248533
O	-0.4292338486	-0.0957683087	1.5423114674

(acac)(gly)Re(OH)(H)(CH_3)$^{+‡}$ metathesis transition state
enthalpy: -690.723745

Re	-1.3143876643	0.4142747073	-0.0305149944
C	-0.9291246799	3.2374932340	-0.9976017648
H	-1.5113004752	4.1453697624	-1.1405690754
C	1.1092795003	1.9489745928	-1.0968754054
C	0.4103159516	3.1519162181	-1.2950179751
H	2.1728851387	1.8734769244	-1.3305623776
H	0.9275116920	4.0189555368	-1.6871192916
O	-1.6295715255	2.2311257949	-0.5219055340
O	0.5633610243	0.8865946052	-0.6404297245
O	-1.7182311544	-0.6942262941	-1.6797378685
H	-2.6556170230	-0.9218207914	-1.8030244326
C	-0.2553555016	-1.6414891328	0.2540182873
H	0.7014839299	-1.2233207213	0.5588456775
H	-0.7798216956	-2.1061610181	1.0877324883
H	0.0067644199	-2.4361307942	-0.4706728958
H	-0.9856154525	-1.4027508295	-0.8372892033
C	-3.3662464120	-0.0623693334	1.9134087362
C	-2.3142112860	0.8465708767	2.5521674740
H	-4.3838622923	0.3331124321	1.9801111815
H	-3.3539594830	-1.0834880531	2.3121117595
H	-2.1678285526	0.6466478084	3.6164665010
H	-2.5728775244	1.9024920557	2.4028542249
O	-3.0137303293	-0.1486815609	0.5160416834
O	-1.0944271161	0.5469079901	1.8559302480

(acac)(gly)Re(OH)(H)(CH_3)$^{+}$ oxidative addition intermediate
enthalpy: -690.718657

Re	-1.3893539851	.4029401606	-.0324578082
C	-.7123736511	3.3510776403	-.4688034905
H	-1.0286345563	4.3661803708	-.2145279498
C	.8311596005	1.8590267093	-1.5517180715
C	.3110035248	3.1314785241	-1.3967875989
H	1.7260239550	1.7003287630	-2.1572279811
H	.7675452239	3.9711037129	-1.9055609721
O	-1.2988396650	2.4280207184	.1852903705
O	.3694799787	.7783997878	-1.0060741560
O	-2.4829627476	1.0068842713	-1.4952849148
H	-2.8756647397	.3562689303	-2.0959381111
C	-.0837412170	-1.3720166640	.2827443270
H	.4946859523	-1.5853043229	-.6100280025
H	.5563332316	-1.0331678392	1.0985569501
H	-.7181027246	-2.2084084704	.5667352814
H	-1.3678847866	-.7880573962	-1.1386578558
C	-1.8364711838	-.4830507270	2.6892244866
C	-3.1078043067	-.9066214435	1.9224669540
H	-3.9856771067	-.3123563302	2.2007050134
H	-3.3449967647	-1.9685788607	2.0301491758
H	-1.1452404854	-1.3230339692	2.8199390709
H	-2.0628118487	-.0409940435	3.6628391147
O	-2.8535087826	-.6257152497	.5381285228
O	-1.2515284273	.5133180185	1.8641305215

(acac)(gly)Re(OH_2)(CH_3)$^+$
enthalpy: -690.771842

Re	-1.0793686665	-.1000053920	-.5511493169
C	-1.6763768177	2.8326555035	-.5760553441
H	-2.4768749719	3.5274227721	-.8240819498
C	.5361844543	2.3357872227	.2537135064
C	-.4582519580	3.2563441629	-.0713546456
H	1.5002768903	2.6456832872	.6564608786
H	-.2844036265	4.3146017198	.0799071350
O	-1.9752529140	1.5819665501	-.7985200921
O	.3767695964	1.0627613225	.1039534214
C	-.3882464584	-.4348380672	-2.5276820956
H	.4069087308	-1.1790792566	-2.6345224643
H	-1.2052166613	-.6536120283	-3.2135904034
H	.0474138713	.5529294307	-2.7497975282
O	.3361325903	-1.5999127181	-.0470763705
H	.7908733073	-2.1633336739	-.6905215160
H	.0280626406	-2.0995174827	.7325001015
C	-3.4659555706	-1.7372049479	-.3729672395
C	-3.1640730775	-1.2473874479	1.0376528073
H	-3.3856196240	-1.9998397216	1.8005105042
H	-3.7121956998	-.3259277797	1.2686410838
H	-4.4751244436	-1.4869691655	-.7148082859
H	-3.3179481975	-2.8172392975	-.4990701763
O	-2.5240423477	-1.0964532652	-1.2487009701
O	-1.7564895773	-.9815519530	1.0517134892

Re(cat)$_2$ System
($cat)_2$Re(OH)(OH_2)
enthalpy: -994.255315

Re	-0.9741974595	-0.1724753167	-0.2377287805
O	-1.6007713979	1.6533015324	-0.0323464195
O	-0.1676919355	0.7496756843	-1.7865453911
O	-1.0860237955	-1.6718803021	-1.9028914556
H	-0.3094584191	-2.1983603857	-1.6206278184
O	0.5253048871	-1.3726341124	-0.0317832743
H	0.8006044946	-1.4501286674	0.8950251731
H	-0.7749665220	-1.1285018420	-2.6489664217
O	-0.8558588629	-0.1628979516	1.7320335755
O	-2.7328748513	-0.8520757632	0.2376439822
C	-2.0728271035	-0.0892971850	2.3199981495
C	-2.3107811457	0.3005053852	3.6375120454
C	-3.1299014508	-0.4993213429	1.4881908812
C	-3.6261874357	0.2613134795	4.1023291967
H	-1.4879711965	0.6222220490	4.2676639168
C	-4.4420031975	-0.5473194191	1.9539876904
C	-4.6781872117	-0.1572189868	3.2729305742
H	-3.8390822767	0.5616293928	5.1242242899
H	-5.2422826326	-0.8695736645	1.2957560030
H	-5.6921224309	-0.1739312464	3.6616110278
C	-1.1697164451	2.6015296725	-0.8887173840
C	-0.3773299071	2.0786335979	-1.9213307157
C	-1.4672987300	3.9606310381	-0.8194963351
C	0.1200696793	2.8969674698	-2.9317902690
C	-0.9669555523	4.7830892629	-1.8306111447
H	-2.0768819521	4.3463448206	-0.0092095301
C	-0.1857619512	4.2590460325	-2.8707840397
H	0.7324714290	2.4816302659	-3.7254273086
H	-1.1875973407	5.8461632795	-1.8105469261
H	0.1935077117	4.9238673274	-3.6411276212

$(cat)_2Re(OH_2)(OH_2)+$
enthalpy: -994.674958

Re	-0.9686099370	-0.1316109664	-0.2926502550
O	-1.5061408678	1.0483339078	-1.7512691547
O	0.5543400303	1.0853297227	-0.3758056055
O	-1.6011754925	-1.5320848874	-1.8145461998
H	-2.0995278130	-2.3005306024	-1.4923592158
O	0.7143666395	-1.4916439585	-0.2541482016
H	0.6180218093	-2.2391422372	0.3582369290
H	-2.1149480437	-1.0836302290	-2.5091850873
O	-1.8208474881	1.0174102345	0.9505806857
O	-1.7725050940	-1.4164645503	0.9539905951
C	-2.5064168909	0.4873374851	1.9958674293
C	-3.1741544156	1.2187272622	2.9759448915
C	-2.4785877678	-0.9151203537	2.0003678262
C	-3.8206959781	0.4901093032	3.9716478640
H	-3.1804353436	2.3027755780	2.9509746509
C	-3.1248329660	-1.6429307112	2.9952973329
C	-3.7958173514	-0.9163022425	3.9799447988
H	-4.3536430200	1.0176564453	4.7558488326
H	-3.1030663235	-2.7272431400	2.9960077821
H	-4.3111545760	-1.4502018816	4.7719311855
C	-0.9331483497	2.2728606118	-1.6841235274
C	0.2422891832	2.2938238511	-0.8997366311
C	-1.3828254475	3.4159923891	-2.3472926448
C	0.9991064754	3.4582483375	-0.7581744818
C	-0.6294228337	4.5755183964	-2.1979659044
H	-2.2863731657	3.3871999469	-2.9464227420
C	0.5438255282	4.5962896220	-1.4153429523
H	1.8996139213	3.4614475744	-0.1538293164
H	-0.9501329331	5.4857954423	-2.6943283225
H	1.1027358103	5.5221674528	-1.3247658570
H	1.5406119631	-1.0172899923	-0.0540686183

$(cat)_2Re(OH)(H)(CH_3)^{\ddagger}$ metathesis transition state
enthalpy: -958.247240

Re	-0.0005073411	-0.0006775420	0.0123686467
O	-0.0365962933	-0.0097562746	2.0716473793
H	1.1460156261	-0.0176172671	1.6278240822
C	2.1957402056	0.1474239640	0.7622617427
O	-1.0313984057	0.4722100296	-1.5564500118
O	0.0091703126	1.9541152978	0.0831021631
H	-0.4641610360	-0.8361886412	2.3502719265
O	-1.2483001111	-1.4961345282	0.3166820879
O	0.8107070507	-1.4168717310	-1.0821032223
C	-1.2552965698	-2.3783194662	-0.7071062714
C	-2.2699794280	-3.2992376717	-0.9728985765
C	-0.0913736983	-2.3297972656	-1.5001920202
C	-2.0934694003	-4.1679384752	-2.0479265315
H	-3.1620315352	-3.3206968140	-0.3554847805
C	0.0845972707	-3.2059116819	-2.5731884759
C	-0.9313514033	-4.1216866591	-2.8380754723
H	-2.8684397271	-4.8919926533	-2.2817041300
H	0.9860516476	-3.1546300165	-3.1750121600
H	-0.8262098329	-4.8094701273	-3.6719838371
C	-1.2535046314	1.7777377278	-1.8199496881
C	-0.6507342008	2.6293192349	-0.8823736260
C	-1.9934792723	2.2793923544	-2.8877546921
C	-0.7660033255	4.0130856545	-0.9902415664
C	-2.1090080915	3.6666521959	-2.9966407796
H	-2.4537121694	1.6033167843	-3.6006678737
C	-1.5042299357	4.5200607517	-2.0622177294
H	-0.2961900748	4.6603976059	-0.2571793178
H	-2.6772474839	4.0904506841	-3.8193366004
H	-1.6131885440	5.5949999130	-2.1717631634
H	2.3909392007	0.9204606801	0.0152958365
H	2.6096756391	0.5591082981	1.6974497245
H	2.7046549271	-0.7775766641	0.4989834156

$(cat)_2Re(OH)(H)(CH_3)^{\ddagger}$ oxidative addition intermediate
enthalpy: -958.257519

Re	-1.1104985381	.0280186100	-.1457849745
O	-1.6806183047	1.8711069655	-.6844768834
O	.4122316056	.6996003681	-1.2011692355
O	.2625273350	-.8258382370	.9300237382
H	.8712532968	-1.3870720817	.4321611640
O	-1.5776825880	.7652290073	1.6667832831
O	-2.5971062698	-1.1142483873	.4636285462
C	-2.4032615042	.0626970167	2.4177943945
C	-2.7436926546	.3334368201	3.7522911176
C	-3.0058540099	-1.0152867092	1.7283684901
C	-3.6787033300	-.4939133823	4.3593759981
H	-2.2810232592	1.1647988761	4.2727742919
C	-3.9568655726	-1.8393148028	2.3442994551
C	-4.2798902534	-1.5682870419	3.6667068129
H	-3.9564430396	-.3115182844	5.3934630152
H	-4.4081822312	-2.6569357945	1.7923433354
H	-5.0054912296	-2.1914490981	4.1802603735
C	-.9571544995	2.4875060716	-1.6120911271
C	.2425790171	1.8090937515	-1.9256139947
C	-1.2688236974	3.7081163013	-2.2246352056
C	1.1426227793	2.3189369585	-2.8682978900
C	-.3688276636	4.2105993580	-3.1577984064
H	-2.1880075635	4.2253065114	-1.9712385808
C	.8218365613	3.5264210287	-3.4774380841
H	2.0581808569	1.7823767552	-3.0936611924
H	-.5885378840	5.1511048978	-3.6545287388
H	1.5002866401	3.9535565211	-4.2095198686
H	-.7343295578	-1.3541001890	-.9283343407
C	-2.2252290774	-.3474056520	-1.9865870060
H	-3.0968770263	.3058782949	-1.9118957894
H	-1.5929977545	-.0362473943	-2.8224013945
H	-2.5307592782	-1.3853289814	-2.0904809010

$(cat)_2Re(OH_2)(CH_3)$
enthalpy: -958.291168

Re	-1.2706510976	-0.1652411516	-0.3897346209
O	-1.7152203997	1.1321364067	-1.8280936544
O	0.4076159868	0.8493187203	-0.5607592968
O	-2.2081543184	-1.3362818871	-1.8964628389
H	-2.6340402365	-0.8846137684	-2.6385631387
O	-1.6255171337	1.0215522231	1.1063089186
O	-2.3015154069	-1.3082527332	0.8292608399
C	-2.2935512402	0.5407994782	2.1763040567
C	-2.5980296828	1.2529431921	3.3335502909
C	-2.7105762821	-0.7874758797	2.0060694792
C	-3.3407104762	0.5990932050	4.3200757691
H	-2.2632985755	2.2786379615	3.4487370791
C	-3.4559442728	-1.4376348919	2.9862127652
C	-3.7648227892	-0.7256463095	4.1485857602
H	-3.5924690969	1.1282051416	5.2345781525
H	-3.7750340792	-2.4646930082	2.8406421179
H	-4.3413929174	-1.2089653310	4.9319047631
C	-0.9561625054	2.2516001936	-1.7889050766
C	0.2345119533	2.0916502867	-1.0534072583
C	-1.2544664850	3.4581816714	-2.4216116035
C	1.1479595198	3.1415043095	-0.9315688076
C	-0.3423369100	4.5059693678	-2.2918726974
H	-2.1749741556	3.5666754704	-2.9865422516
C	0.8434996091	4.3500915326	-1.5556224037
H	2.0586367218	3.0022628089	-0.3579228574
H	-0.5551252322	5.4596091755	-2.7665105053
H	1.5319812250	5.1856303710	-1.4684555204
H	-2.2530738668	-2.2990912595	-1.9421736240
C	0.1377712119	-1.7582934451	-0.4925108695
H	-0.3088012032	-2.6985768065	-0.1524351184
H	0.4518829985	-1.8541761987	-1.5401533294
H	1.0268791979	-1.5220353144	0.0965693289

$(cat)_2Re(CH_3)(H)(CH_3)$ oxidative addition intermediate
enthalpy: -922.303015

Re	-1.1944890212	.0576946261	-.1902930911
O	-1.7180575808	1.9036326996	-.7774543409
O	.3604514084	.7044976278	-1.2134397073
O	-1.6408873119	.7742215594	1.6301421039
O	-2.5098541902	-1.2206088398	.5289134964
C	-2.3953294645	.0381067283	2.4332445007
C	-2.7203069057	.3260186040	3.7656006275
C	-2.8995006207	-1.1192056040	1.8030791626
C	-3.5492206954	-.5684082630	4.4333962171
H	-2.3326374422	1.2204831428	4.2412631502
C	-3.7315442833	-2.0178817236	2.4808335581
C	-4.0493758450	-1.7261470672	3.8019697610
H	-3.8185578819	-.3716554708	5.4670712970
H	-4.1088020213	-2.9005814083	1.9752688131
H	-4.6937569986	-2.3992667994	4.3591098977
C	-.9287444158	2.5462122746	-1.6261612237
C	.2748234026	1.8568940079	-1.8845300542
C	-1.1836844551	3.7884583887	-2.2224358042
C	1.2482741675	2.3808799710	-2.7431747871
C	-.2125311418	4.3055014651	-3.0724586215
H	-2.1090773562	4.3146738196	-2.0142127775
C	.9884258048	3.6128836107	-3.3315242362
H	2.1668652162	1.8334195966	-2.9262611861
H	-.3821259183	5.2665972697	-3.5491788116
H	1.7210842134	4.0515693351	-4.0019439327
H	-.6692786783	-1.3312489850	-.8592391434
C	-2.2702532249	-.4925013181	-1.9836525585
H	-3.1561771974	.1487132127	-1.9641359130
H	-1.6440888365	-.2338590111	-2.8422751096
H	-2.5537747522	-1.5418134035	-2.0113326530
C	.4361869144	-.8566324785	.8964616502
H	1.2457924820	-1.1945759973	.2541949099
H	.7786740773	-.0650566187	1.5691576192
H	.0270104286	-1.6869056516	1.4790914726

$(cat)_2Re(CH_3)(H)(CH_3)^{\ddagger}$ OHM transition state
enthalpy: -922.284685

Re	0.0005882290	-0.0003347433	0.0054763742
C	-0.0122648611	-0.0005917792	2.2733583865
H	1.1248300659	0.0141944718	1.2856780754
C	2.1998611649	-0.4435271396	0.3354886175
O	-1.0891745965	0.7901290796	-1.4209574115
O	0.4779081891	1.8906968927	0.1193791259
O	-1.5591649663	-1.1596035701	0.3943914811
O	0.2859589915	-1.5301078014	-1.2221069461
C	-1.9025093883	-1.9437581322	-0.6388050904
C	-3.1457412657	-2.5620901840	-0.8104694953
C	-0.8531203389	-2.1543653261	-1.5583296399
C	-3.3119566950	-3.3866842247	-1.9183301504
H	-3.9430647812	-2.3886498993	-0.0951801495
C	-1.0250026122	-2.9875953682	-2.6690879675
C	-2.2642182998	-3.5968357058	-2.8366074966
H	-4.2677755911	-3.8759808275	-2.0815817248
H	-0.2087030409	-3.1378776923	-3.3680278937
H	-2.4298230995	-4.2446090864	-3.6925452914
C	-1.0002149463	2.1172244881	-1.6216101508
C	-0.1067373961	2.7538522915	-0.7451346046
C	-1.6977890967	2.8450340693	-2.5848404459
C	0.1138507092	4.1270105389	-0.8052363505
C	-1.4776006180	4.2225023742	-2.6464809687
H	-2.3851031677	2.3408363281	-3.2560157168
C	-0.5852664935	4.8559017200	-1.7702462579
H	0.8084401529	4.5999179338	-0.1186437938
H	-2.0086501299	4.8123365712	-3.3878862114
H	-0.4341893265	5.9288555000	-1.8415476501
H	2.5812992758	0.1316866777	-0.5099504451
H	2.7871340922	-0.1700652667	1.2210156769
H	2.2885442133	-1.5113237662	0.1477884147
H	0.8436716118	0.2216548789	2.9228039715
H	-0.7472269425	0.7956403149	2.4036367175
H	-0.4374917509	-0.9660696192	2.5386389902

Re(cat)(gly) *cis* System

(cat)(gly)Re(OH)(OH_2)

enthalpy: -841.831584

Re	-1.2705108897	-0.1244913944	0.0301493907
O	-2.1855959007	1.4362352708	-0.7162198884
O	0.2770291029	0.9765727824	-0.6535030019
O	-1.9281429619	-0.7693099944	-2.1684036824
H	-1.4679205716	-0.1570610810	-2.7662718567
O	-0.4763959696	-1.8005675936	-0.2019642874
H	-0.7637522390	-2.3175876325	-0.9694520963
H	-2.8472794502	-0.4582729738	-2.1534751590
C	-1.8268059376	0.3026049214	2.7680949729
C	-2.8645233723	-0.6996850707	2.2857109301
C	-1.4443473794	2.2376343776	-1.5300549270
C	-0.0602488555	1.9602861492	-1.4929855499
C	-1.9657166210	3.2506847269	-2.3317732584
C	0.8220003716	2.7224875336	-2.2664236097
C	-1.0766611205	4.0028011812	-3.1051364327
H	-3.0335262866	3.4480545060	-2.3316667032
C	0.2987817848	3.7363010239	-3.0721792099
H	1.8863493430	2.5130170406	-2.2306282302
H	-1.4568648426	4.8031725340	-3.7329703973
H	0.9729793136	4.3294862261	-3.6837639480
H	-1.3751997387	0.0334144502	3.7287794548
H	-2.2590388817	1.3091064529	2.8485768373
H	-3.8501926949	-0.5272723264	2.7325070146
H	-2.5465482422	-1.7275143064	2.5138422726
O	-0.7712925618	0.3527327956	1.7851470251
O	-2.9598019933	-0.5390301093	0.8625655735

(cat)(gly)Re(OH_2)(OH_2)$^+$

enthalpy: -842.253685

Re	-1.1731124473	-0.0780766771	0.1035720083
O	-2.4284173188	1.1288829243	-0.7674753951
O	-0.0423799189	0.9051099954	-1.1583645355
O	-2.8361259157	-1.3544931747	-0.7017346640
H	-3.5060708231	-0.7095180327	-0.9985275846
O	0.2143710448	-1.5719058639	-0.6151743041
H	-0.0764177060	-2.1602392389	-1.3290666828
H	-3.2452277464	-1.8730386408	0.0116030717
C	-0.2513817958	0.5600041889	2.7264429110
C	-1.6384102222	-0.0401453026	2.9581154319
C	-1.9233510550	2.1654892022	-1.4708831064
C	-0.5403886623	2.0255043320	-1.7065307274
C	-2.6416496376	3.2550726579	-1.9604155784
C	0.1690082426	2.9732763567	-2.4484708174
C	-1.9318519044	4.1960478523	-2.7019504489
H	-3.7035748197	3.3550858056	-1.7654064680
C	-0.5495035883	4.0566881574	-2.9430509078
H	1.2333318722	2.8581481649	-2.6211368570
H	-2.4537835691	5.0595327758	-3.1015608832
H	-0.0351282508	4.8157117857	-3.5234790948
H	0.4866488294	0.2246687284	3.4605428414
H	-0.2766852304	1.6553397532	2.7126228026
H	-2.2739452168	0.5825347793	3.5930899346
H	-1.5888102258	-1.0531927865	3.3729162388
O	0.1524133014	0.0928206588	1.4326052172
O	-2.2357794077	-0.1354101164	1.6518832367
H	1.0590730858	-1.1630109062	-0.8778523532

(cat)(gly)Re(OH)(H)(CH3)‡ metathesis transition state
enthalpy: -805.819551

Re	-1.2608347754	-0.2004467683	-0.1491409247
O	-1.7041846738	1.6834341456	0.0101181188
O	-0.3037629640	0.6034928739	-1.6676958850
O	0.2166792359	-1.6222308825	-0.0712733255
H	0.2740480521	-1.9161182691	0.8540601456
C	-2.1045022208	0.2351797579	2.4877449288
C	-3.3703064884	-0.2745340605	1.7816234801
C	-1.2063780996	2.5549095187	-0.8935732898
C	-0.4062873945	1.9317276860	-1.8624477534
C	-1.4294840584	3.9293543295	-0.9092249720
C	0.1870912346	2.6690011434	-2.8842843946
C	-0.8330451910	4.6692427506	-1.9331000729
H	-2.0495262266	4.3932114262	-0.1495709006
C	-0.0378185358	4.0475710883	-2.9061776374
H	0.8029495931	2.1749020644	-3.6282409597
H	-0.9901255813	5.7429597547	-1.9750083859
H	0.4141145071	4.6479700438	-3.6896770320
H	-2.0301290142	-0.1087766752	3.5257257368
H	-2.0612983139	1.3300493970	2.4706473695
H	-4.1477139004	0.4973747903	1.7339998527
H	-3.7979193971	-1.1637217418	2.2628153376
O	-0.9771165604	-0.2708624390	1.7609781606
O	-3.0176248532	-0.6659687378	0.4439767018
H	-0.6928267052	-1.9914484109	-0.8286461227
C	-1.7880187024	-1.8816769088	-1.6780799807
H	-1.1183177973	-2.5113606126	-2.2851129312
H	-2.6375228897	-2.4530993431	-1.3095120444
H	-2.1297989498	-1.1047441442	-2.3668147802

(cat)(gly)Re(OH_2)(CH_3)
enthalpy: -805.868862

Re	-1.3218991813	-0.1200032849	-0.0832646371
O	-2.2117257996	1.1247312014	-1.3441775676
O	0.1450974932	1.0571272823	-0.6193781747
O	0.4220352867	-1.5094608497	-0.3319757552
H	0.1156949187	-2.4131701564	-0.4970203329
C	-1.6165418568	-0.6711954793	2.7626809066
C	-2.8215000836	0.1585395770	2.3361771708
C	-1.5050516958	2.1923058042	-1.7394192410
C	-0.1562705358	2.1513143204	-1.3449044235
C	-1.9984793548	3.2675306074	-2.4845075929
C	0.7325162389	3.1697693706	-1.6883334915
C	-1.1093794541	4.2834470293	-2.8333438060
H	-3.0429568762	3.2898709396	-2.7784350545
C	0.2387236488	4.2352804574	-2.4414539787
H	1.7702944731	3.1187692725	-1.3751328206
H	-1.4656964446	5.1276927259	-3.4166501870
H	0.9078056633	5.0417072116	-2.7274529210
H	-1.8915962585	-1.7329479320	2.8579173579
H	-1.1859599675	-0.3339898353	3.7131293629
H	-2.6662084223	1.2238571091	2.5573201219
H	-3.7565882036	-0.1660797265	2.8070995614
O	-0.6625220513	-0.5048176239	1.7215879701
O	-2.9345884841	-0.0235837843	0.9271102262
H	0.7290212761	-1.4774824536	0.5947949927
C	-2.2743271713	-1.5167012771	-1.3636432049
H	-1.6579631364	-1.7148984470	-2.2499644919
H	-2.3932753093	-2.4626664481	-0.8147290414
H	-3.2531806863	-1.1504184219	-1.6780440916

(cat)(gly)Re(OH)(H)(CH_3)‡ oxidative addition intermediate
enthalpy: -805.825704

Re	-1.2134026837	-0.1868725777	-0.0181984846
O	-1.8927419304	1.6858008546	-0.3206275458
O	0.1222384069	0.6298105096	-1.2311689820
O	0.2960748666	-1.1832691397	0.6383672356
H	0.7305363801	-1.7464006159	-0.0161224578
C	-2.4521302169	0.4738795012	2.4736802182
C	-3.2237432359	-0.7553557984	2.0036608962
C	-1.3280837266	2.3990283650	-1.2863908990
C	-0.1652307418	1.7914781888	-1.8195712433
C	-1.7504428349	3.6518948197	-1.7468009781
C	0.5856443084	2.4149800978	-2.8222585853
C	-0.9994124016	4.2642179560	-2.7457541276
H	-2.6390970022	4.1138820651	-1.3303261769
C	0.1538232874	3.6559637954	-3.2784624395
H	1.4750184142	1.9333878891	-3.2147669227
H	-1.3109833339	5.2332215315	-3.1248921542
H	0.7143267470	4.1657151833	-4.0561180785
H	-2.3439048498	0.5000236818	3.5649467867
H	-2.9456406932	1.3974101441	2.1341780707
H	-4.3131749681	-0.6508196178	2.0572205716
H	-2.9174041921	-1.6518808830	2.5589643712
O	-1.1858242362	0.3247216016	1.8818435229
O	-2.8459071205	-0.9399905074	0.6340262536
H	-1.0674361088	-1.4996131536	-0.9862929835
C	-2.4899762205	-0.4309623033	-1.8240412818
H	-1.8830444184	-0.1672561807	-2.6916236146
H	-2.9070467204	-1.4297745784	-1.9172552098
H	-3.2805039016	0.2994680632	-1.6584743155

(cat)(gly)Re(CH_3)(H)(CH_3) oxidative addition intermediate
enthalpy: -769.869424

Re	-1.3726994561	-0.0672210162	-0.0261608233
O	-1.8426194353	1.7982810046	-0.5190002644
O	0.1275299586	0.5526128644	-1.2029048868
C	-2.4437523169	-0.0379690820	2.7203746858
C	-2.6947532893	-1.4403631928	2.1717161378
C	-1.1279272886	2.4460228045	-1.4319422385
C	0.0219758699	1.7290436397	-1.8192453233
C	-1.4146127917	3.7033046058	-1.9781964167
C	0.9210596320	2.2518325760	-2.7582359019
C	-0.5168684650	4.2174244947	-2.9077162217
H	-2.3028105203	4.2453522932	-1.6717614882
C	0.6360638601	3.5024985993	-3.2935241656
H	1.8025639411	1.6873424582	-3.0436719888
H	-0.7071880621	5.1920841670	-3.3475571171
H	1.3109676825	3.9382148353	-4.0241578483
H	-2.0057769783	-0.0661979988	3.7267060983
H	-3.3773356780	0.5433587302	2.7664076930
H	-3.6859450173	-1.8356468571	2.4207474451
H	-1.9396574519	-2.1582819029	2.5241905291
O	-1.5502215590	0.5797399828	1.8221674677
O	-2.5840785882	-1.3392148086	0.7545624959
H	-0.9706754382	-1.4054138136	-0.8650186201
C	-2.6306469626	-0.4928807779	-1.7338075359
H	-2.1040085879	-0.1788888028	-2.6392965738
H	-2.9390699662	-1.5332219996	-1.7983603094
H	-3.4960959695	0.1563427972	-1.5668405669
C	0.3789259906	-1.0718462410	0.7566283288
H	0.0375826653	-1.9746211177	1.2681111722
H	1.0955172391	-1.3146790122	-0.0230896212
H	0.7927334948	-0.3593053985	1.4735612357

(cat)(gly)Re(CH_3)(H)(CH_3)‡ OHM transition state
enthalpy: -769.850269

Re	0.0042038378	-0.0002437749	-0.0009748583
C	-0.0077841232	0.0044675084	2.2746858480
H	1.1257975802	0.0149053329	1.2900438819
C	2.2015377668	-0.4669125024	0.3605596943
O	-1.0545240573	0.8356258729	-1.4306206928
O	0.5205318058	1.8897532277	0.1295485938
C	-2.0627898602	-1.7766113767	-0.7528705643
C	-0.9071190159	-2.0298254742	-1.7481357151
C	-0.9338149271	2.1633416548	-1.6185794641
C	-0.0349839331	2.7727644851	-0.7290428834
C	-1.6068316579	2.9133819950	-2.5817774944
C	0.2142057686	4.1418482025	-0.7772876768
C	-1.3577154318	4.2868640448	-2.6314045837
H	-2.2988451539	2.4303439703	-3.2636537526
C	-0.4604204308	4.8936357439	-1.7424390197
H	0.9124641190	4.5949943795	-0.0810525929
H	-1.8696368857	4.8932201364	-3.3728585327
H	-0.2855844176	5.9637069436	-1.8032633995
H	-2.5281584070	-2.7018419655	-0.3925991184
H	-2.8389655727	-1.1480770350	-1.2056837886
H	-1.1014688430	-1.5364676926	-2.7080501000
H	-0.7270563358	-3.0955642382	-1.9333124049
O	-1.5331502171	-1.0967341738	0.3916945479
O	0.2972305108	-1.4894933473	-1.1907638398
H	2.7984303252	-0.1456957646	1.2230483003
H	2.2708227285	-1.5442151807	0.2263639800
H	2.5751624494	0.0550350029	-0.5221940101
H	-0.4012155336	-0.9741341044	2.5410711733
H	0.8329633011	0.2733979951	2.9259578068
H	-0.7777814997	0.7704610749	2.3829442546

Re(cat)(gly) *trans* System
(cat)(gly)Re(OH)(OH2)
enthalpy: -841.834549

Re	-1.3554151293	-0.1311856107	-0.0729857066
O	-2.2493951667	1.2191185423	-1.1921146913
O	0.2034426073	0.8589500738	-0.7612929844
O	-2.0301846516	-1.3647978353	-1.4269820562
O	0.1564577513	-1.6697781279	-0.3304914729
H	-0.1968659047	-2.1556181071	-1.1012145567
H	-2.7832793469	-0.9900781371	-1.9110519345
C	-1.5493460664	0.1588108687	2.8141820397
C	-2.9305830692	-0.3058312387	2.3576119814
C	-1.4526309512	2.2172899278	-1.6368545032
C	-0.0776356364	2.0055634627	-1.4313549696
C	-1.9047072983	3.3647384068	-2.2868998904
C	0.8684654614	2.9196666869	-1.8871049877
C	-0.9557794922	4.2846694056	-2.7408084982
H	-2.9689085649	3.5202812955	-2.4318330311
C	0.4136141421	4.0650564458	-2.5464281075
H	1.9251508295	2.7377460440	-1.7181500580
H	-1.2879227040	5.1836723370	-3.2519387541
H	1.1323607720	4.7950701807	-2.9068706727
H	-1.1953823564	-0.3935125923	3.6924230663
H	-1.5417819401	1.2322631572	3.0479835104
H	-3.7411345363	0.2757078096	2.8111411221
H	-3.0926376673	-1.3698613109	2.5780220559
O	-0.6753397276	-0.0771790097	1.7193294109
O	-2.9632324309	-0.1345237561	0.9445486614
H	0.9589145679	-1.1923558613	-0.6058703458

(cat)(gly)Re(OH)(H)(CH3)‡ metathesis transition state
enthalpy: -805.818846

Re	-0.0006618227	-0.0021977559	0.0246326229
O	0.0835693225	-0.0887773743	2.0922280697
H	1.2582934749	-0.0679171973	1.6123396751
C	2.2468514225	0.2401758742	0.7269312372
O	-1.2914078379	-1.4521464381	0.3769010476
O	0.8748481212	-1.5258571382	-0.8652560472
H	-0.3962891370	-0.8718143774	2.4094812068
C	-0.5463256445	2.0291239660	-1.9727154841
C	-1.4054492302	2.4052104023	-0.7679627151
C	-1.1193186310	-2.5705761682	-0.3588021445
C	0.1063076668	-2.6166056970	-1.0489452526
C	-2.0273095555	-3.6268210442	-0.4369105930
C	0.4528023929	-3.7241585631	-1.8248568229
C	-1.6786541728	-4.7322969852	-1.2138228248
H	-2.9702288862	-3.5741462572	0.0977444542
C	-0.4541558622	-4.7811090872	-1.8988183254
H	1.4018323060	-3.7413439922	-2.3509591795
H	-2.3678767693	-5.5683303094	-1.2901362431
H	-0.2108688736	-5.6532282341	-2.4985641826
H	-0.0310210640	2.8933225740	-2.4067325069
H	-1.1418440014	1.5423608075	-2.7567059117
H	-2.4294926562	2.6795119850	-1.0450495437
H	-0.9576509895	3.2286675219	-0.1953281947
O	0.4168007219	1.1037576601	-1.4835937795
O	-1.4349579288	1.2419920117	0.0520821953
H	2.6624491822	0.7279521673	1.6215424444
H	2.8144393915	-0.6533396484	0.4722464854
H	2.3433670591	0.9778334855	-0.0720997438

(cat)(gly)Re(OH_2)(CH_3)
enthalpy: -805.869836

Re	-1.3512338998	-0.1150081306	-0.0480661230
O	-2.1303297404	1.1311736995	-1.3849782143
O	0.2175403307	0.9613926029	-0.6113627843
O	-2.5942042145	-1.3296181595	-1.4627622876
H	-3.0365875925	-0.6197540225	-1.9643053735
C	-1.5619563350	0.2717771393	2.7757518519
C	-2.8331708803	-0.4851978956	2.4049651269
C	-1.3486105566	2.1464960634	-1.8149379608
C	-0.0225911027	2.0504142289	-1.3568838709
C	-1.7609259735	3.2021668353	-2.6258923476
C	0.9198965837	3.0243911955	-1.6974498783
C	-0.8132968621	4.1685827792	-2.9704489188
H	-2.7894763496	3.2610715508	-2.9681283929
C	0.5095600655	4.0805408781	-2.5112108311
H	1.9382531267	2.9418594759	-1.3315462119
H	-1.1074364582	5.0027472228	-3.6009025973
H	1.2248002329	4.8485192225	-2.7912996240
H	-1.1185340972	-0.0668889321	3.7189836884
H	-1.7473641193	1.3535164132	2.8379085054
H	-3.7289741869	-0.0795560693	2.8894985394
H	-2.7416385619	-1.5508169533	2.6600441224
O	-0.6464325773	0.0032134058	1.7185521562
O	-2.9470218333	-0.3349046060	0.9965790902
H	-2.0438340796	-1.8234770347	-2.0878564613
C	0.0606989908	-1.6695564461	-0.3716012406
H	-0.3184280260	-2.5890910703	0.0928361118
H	0.1954332825	-1.8676036212	-1.4443958868
H	1.0277998370	-1.3979568932	0.0556904829

$Re(gly)_2$ System

$(gly)_2Re(OH)(OH_2)$

enthalpy: -689.402266

Re	-0.8471357866	-0.0762527386	0.1215019589
O	-0.7447260179	-1.9259710827	-1.1829070363
H	-0.6161955485	-1.4655163450	-2.0320619233
O	0.8007917688	-0.8498059840	0.7478110887
H	1.1936308852	-1.4193475546	0.0656638265
H	-1.6489064326	-2.2791694029	-1.1470061410
C	-2.3027731461	0.5171381996	2.4177936864
C	-2.8654665482	-0.8429285710	2.0213985616
H	-3.9605639494	-0.8657524345	1.9693618746
H	-2.5251496158	-1.6329728490	2.7038730357
H	-2.2960921448	0.6758098186	3.5023120469
H	-2.8637550254	1.3281466015	1.9354904318
C	-1.6404115406	2.1692753195	-1.5790817805
H	-1.7453575164	3.2546994141	-1.4649923787
H	-2.4420050985	1.8090965280	-2.2412131603
C	-0.2593976348	1.7725612811	-2.1018049150
H	0.5106788111	2.4806437925	-1.7663311826
H	-0.2340897819	1.7299019133	-3.1986308774
O	-0.9529214055	0.5089031397	1.9474516646
O	-2.3389914196	-1.1288689484	0.7079659922
O	-1.7846288896	1.5407715983	-0.3157376015
O	0.0170959308	0.4959952699	-1.5548138174

$(gly)_2Re(OH_2)(OH_2)^+$

enthalpy: -689.831440

Re	-0.9143759870	-0.1144890524	0.0219943692
O	-1.7623099836	-1.8878066465	-0.9503672821
H	-1.7868362323	-1.7916905316	-1.9166421328
O	0.7851941948	-1.4431722003	0.0758131303
H	1.2246644952	-1.6413834248	-0.7666341703
H	-2.6546451993	-2.0806725491	-0.6141776621
C	-1.0310591226	0.7378251108	2.6904296766
C	-2.1690392806	-0.2778316070	2.6185827530
H	-3.1356804801	0.1399363037	2.9152086367
H	-1.9762547529	-1.1791809292	3.2117416825
H	-0.5186169982	0.7481383264	3.6558860759
H	-1.3770352290	1.7477019243	2.4440043105
C	-1.5691786491	2.2108986442	-1.5539857622
H	-1.4522383690	3.2920933883	-1.4454985469
H	-2.5502728188	1.9876352063	-1.9883088298
C	-0.4272076366	1.5478470545	-2.3254955724
H	0.5283482142	2.0518969503	-2.1408196257
H	-0.6169187557	1.5164526785	-3.4025683198
O	-0.0863201698	0.3236468880	1.6764812629
O	-2.2561543149	-0.6979467535	1.2336500292
O	-1.5213735756	1.6234530058	-0.2407498180
O	-0.3713890463	0.2196367574	-1.8014603281
H	1.4406220094	-1.1515306657	0.7339939842

(gly)2Re(OH)(H)(CH3)‡ metathesis transition state
enthalpy: -653.389455

Re	-0.0719391347	0.1041300862	-0.0035141051
O	0.9346543443	0.0043753782	1.8573582100
H	1.6951880911	-0.5838905240	1.7242960683
C	-0.9073591024	2.8435791631	-0.0267449422
C	-2.0577913044	1.9987405752	-0.5759628923
H	-1.9973792236	1.9108059266	-1.6682096282
H	-3.0445738709	2.3886569693	-0.3043263170
H	-1.1893726622	3.4029889557	0.8744919680
H	-0.5224726362	3.5538149194	-0.7683164898
C	0.6693327006	-0.5676041381	-2.7168913054
H	1.0720981544	-0.0493720232	-3.5935849451
H	-0.0642267411	-1.3151660545	-3.0474767247
C	1.7542147798	-1.2032487550	-1.8534186222
H	2.6652478467	-0.5879950131	-1.8437194808
H	2.0136728100	-2.2123425333	-2.1971904099
O	0.1584488211	1.9559016877	0.3579244969
O	-1.9112277011	0.6865771813	-0.0194037527
O	0.0152021610	0.3831893440	-1.8838630535
O	1.2032954646	-1.2585604876	-0.5495531723
C	-1.0667435837	-1.6159456432	1.2645112869
H	-2.0476868909	-1.2425737395	1.5511694441
H	-1.1280886706	-2.1926585058	0.3382329304
H	-0.6917471522	-2.3231105685	2.0215453067
H	-0.0482257065	-0.8822662636	1.7056925017

$(gly)_2Re(OH_2)(CH_3)$
enthalpy: -653.436158

Re	-0.8731640308	-0.0847162147	0.1225693658
O	-0.6824040711	-2.0563809674	-0.9120585489
H	-1.6006173059	-2.3743429931	-0.9523301580
C	-2.3714147937	0.4109891834	2.4363945943
C	-3.0527416919	-0.8373342798	1.8861945320
H	-4.1303096716	-0.7041748720	1.7311699754
H	-2.8977143066	-1.7073035424	2.5395578930
H	-2.4113813062	0.4698727009	3.5309745150
H	-2.8226257477	1.3212113622	2.0154553928
C	-0.9886486032	2.4397966187	-1.2850036619
H	-0.0835947901	2.9550482946	-0.9357455833
H	-1.7329360809	3.1851670237	-1.5882792671
C	-0.6535481519	1.4328920490	-2.3789631609
H	0.0957177974	1.8200658726	-3.0810222092
H	-1.5583731624	1.1589761082	-2.9455390261
O	-1.0125775144	0.3226594791	2.0165009838
O	-2.4319568132	-1.1164234101	0.6183923089
O	-1.5368300339	1.6617058603	-0.2253505421
O	-0.1387932184	0.3152401397	-1.6838915616
H	-0.4270274287	-1.6928537410	-1.7817039521
C	1.0833953823	-0.5900913505	0.7209653419
H	1.4357998115	0.0571835803	1.5273296476
H	1.0301753385	-1.6194075026	1.1003723184
H	1.7569212642	-0.5688326248	-0.1405305828

$(gly)_2Re(OH)(H)(CH_3)^{\ddagger}$ oxidative addition intermediate
enthalpy: -653.395654

Re	-0.0812660004	-0.0473862863	-0.0206616225
O	-0.3610438259	0.8883418318	1.6546705266
H	0.4498975980	1.1604313892	2.1050136257
C	-2.7064662759	-1.1643303068	-0.3080206625
C	-1.9219028322	-2.2809624712	0.3660657439
H	-2.0773560861	-3.2730621400	-0.0737254135
H	-2.1475161920	-2.3220059802	1.4405722044
H	-3.7471063963	-1.1125486306	0.0336359338
H	-2.6832077085	-1.2681072237	-1.4030433399
C	0.5691588907	0.8202395583	-2.7179181363
H	0.0828885480	1.2143254668	-3.6181971728
H	1.3796566993	0.1462618132	-3.0281623327
C	1.1128646394	1.9472981225	-1.8157520441
H	0.5327819720	2.8738287223	-1.9260626463
H	2.1656498273	2.1715095496	-2.0282997298
O	-2.0243863580	-0.0033646786	0.1061283678
O	-0.5499356123	-1.9145067718	0.2064393968
O	-0.3872008055	0.1418686234	-1.9414724707
O	0.9691495529	1.5100657442	-0.4781197766
C	1.6299134461	-1.2690150877	-0.7699604312
H	1.2573249922	-1.6561033011	-1.7172665914
H	2.4873785519	-0.6098903657	-0.8989726709
H	1.8488579439	-2.0833129344	-0.0863744734
H	1.1808924994	-0.4004003925	0.9595114257

$(gly)_2Re(CH_3)(H)(CH_3)^{\ddagger}$ OHM transition state
enthalpy: -617.440600

Re	-0.0268028485	0.0528617035	-0.0297099254
C	0.4220972309	-0.0983944272	2.8079606386
C	1.7382418656	-0.4421349249	2.1015144953
H	1.8249319735	-1.5239406320	1.9397008303
H	2.6210764222	-0.0913480479	2.6490968555
H	0.5271516901	0.7489701488	3.4999302016
H	0.0254619906	-0.9529625304	3.3702899522
C	-0.2790467300	-2.7379508965	-0.7825944518
H	-0.6742120585	-3.6718477383	-0.3637986640
H	0.6198059587	-2.9677855284	-1.3738908529
C	-1.3179123897	-2.0077539281	-1.6332247544
H	-2.3303214082	-2.1288091835	-1.2217819261
H	-1.3178626425	-2.3512027605	-2.6746706599
O	-0.5356974594	0.2970723952	1.8141281622
O	1.7115296376	0.2018285757	0.8258045747
O	0.0571894408	-1.8589621009	0.2717010188
O	-0.9519869441	-0.6406293691	-1.5772113916
C	1.0756081092	1.4566967895	-1.4460448883
H	1.8533888060	1.8851065314	-0.8178392684
H	1.4775671853	0.6694497090	-2.0863349143
H	0.6400622160	2.2284414316	-2.0936177042
H	-0.3082660585	1.4687725788	-0.9642828118
C	-1.5304590890	1.7770452782	-0.1331016951
H	-1.7967561351	2.3101308494	-1.0537217788
H	-2.3926447592	1.1922771891	0.1875936160
H	-1.2463049827	2.4773411770	0.6512910330

$(gly)_2Re(CH_3)(H)(CH_3)$ oxidative addition intermediate
enthalpy: -617.422665

Re	0.1254684119	-0.1024391113	0.1288740995
C	0.0472986868	0.6021742947	2.9478111271
C	1.3889642374	1.1503225044	2.4713864390
H	2.2218765836	0.5246205569	2.8227299620
H	1.5743515513	2.1844319150	2.7862300987
H	-0.7253292989	1.3855427162	2.9602690833
H	0.1074951072	0.1525045756	3.9459399562
C	0.0271146720	-2.7396745548	-1.0897499639
H	-0.1700071363	-3.7902950784	-0.8458414464
H	0.8745092048	-2.6938095610	-1.7904590696
C	-1.2005344981	-2.0304508764	-1.6537155966
H	-2.1232478962	-2.3957541817	-1.1806228540
H	-1.3026823536	-2.1327971714	-2.7408503593
O	-0.2743171797	-0.3989595058	2.0081414155
O	1.3612787309	1.0875569581	1.0489763152
O	0.3232158376	-2.0367593758	0.0958521739
O	-1.0501676902	-0.6538326584	-1.3209268201
C	1.8816001322	-0.1317537242	-1.1650801453
H	2.4875777838	-0.9460901126	-0.7587233994
H	1.5640353747	-0.3580350097	-2.1843044455
H	2.4263205503	0.8076930670	-1.1250693240
H	0.2415939124	1.1457182384	-0.9053074474
C	-1.4979581866	1.3497675257	0.2468363012
H	-1.9403255707	1.5372574572	-0.7278496731
H	-2.2223736007	0.8747051918	0.9138642753
H	-1.1143936137	2.2717791483	0.6869194392

Protonated Species

$Re(acac)_2$ systems

Cis protonated
$(acac)_2Re(OH)(OH_2)^+$
enthalpy: -764.831706

Re	-1.3160991241	0.5360413501	-0.0187988842
C	-3.8423992708	0.0073099556	1.8899195786
H	-4.8548821681	-0.3665791585	1.9990065493
C	-1.2875785344	3.4152898162	-0.8841141157
H	-1.8496925675	4.3330423228	-1.0735570788
C	0.8952285217	2.2821934652	-0.8966020803
C	0.0950623718	3.4010524196	-1.0956196273
H	1.9669373904	2.3428638755	-1.0913695972
H	0.5719004817	4.3115325994	-1.4388068479
C	-1.8361143809	1.1270086175	2.8699359311
C	-3.1615584960	0.5873860821	2.9032307265
H	-1.4390476345	1.5833118452	3.7786360117
H	-3.6937579061	0.6755946344	3.8446610808
O	-1.0677655788	1.1598149155	1.8623069908
O	-3.3353824539	-0.1286518151	0.6133129364
O	-1.9874622473	2.4182691990	-0.4756004105
O	0.5089893655	1.1127303615	-0.4893367417
O	-1.4283006257	-0.1687483938	-2.0838499732
H	-1.1131153503	-1.0913170647	-2.0538462539
O	-0.9444186205	-1.3804527480	0.1623217626
H	-0.2518878962	-1.6871040019	0.7630134258
H	-2.2176510547	-0.1091691062	-2.6393703581
H	-3.6181322859	-0.9717739292	0.2218302089

$(acac)_2Re(OH)(H)(CH_3)^{+‡}$ metathesis transition state
enthalpy: -728.825430

Re	0.0011856072	0.0021595962	-0.0118420582
O	0.0121057323	-0.0051147258	2.0590406844
H	1.2077456353	-0.0015054663	1.5538652931
C	2.2141249438	-0.1975114335	0.6375408724
C	-1.4641503407	-2.8374870982	0.1359115173
H	-1.3702942305	-3.9108931001	0.2622429308
C	0.4260926035	0.7981582546	-2.8407210104
H	0.5407292777	0.4756874377	-3.8767716910
C	0.3452013511	2.6594572495	-1.2328377482
C	0.4864777772	2.1551787091	-2.5245203640
H	0.3976334083	3.7343265447	-1.0571988477
H	0.6452882517	2.8616527770	-3.3307323103
C	-2.9075712347	-0.8306930006	-0.2779460347
C	-2.6553967941	-2.2304065203	-0.0519574389
H	-3.9459363881	-0.5315526652	-0.4509678728
H	-3.5215712221	-2.8831133079	-0.0658152218
O	-2.0520286354	0.0876031030	-0.3225227348
O	-0.2700028979	-2.1664363378	0.1659256080
O	0.2356823557	-0.1598512694	-1.9932706074
O	0.1505446404	1.9598938094	-0.1599860107
H	-0.2328657034	0.8282482942	2.4894102335
H	0.4709999885	-2.7268424371	0.4456758055
H	2.5757121760	-1.2293016823	0.6447298904
H	2.5101071699	0.2732870913	-0.3067591956
H	2.7944200574	0.3601045559	1.3896038330

$(acac)_2Re(OH_2)(CH_3)^+$
enthalpy: -728.868903

Re	-1.2872562904	0.5548962465	-0.0438922221
C	-3.8948049301	0.0135809237	1.8013170562
H	-4.9303292103	-0.3083673409	1.8064388116
C	-1.3005967949	3.3647075803	-0.8870314125
H	-1.8789793903	4.2756910107	-1.0453673180
C	0.9017536130	2.2577405711	-0.9629891354
C	0.0726823212	3.3541719309	-1.1569493084
H	1.9670523166	2.3334621011	-1.1797270575
H	0.5220497805	4.2675741815	-1.5288675475
C	-1.9076170938	0.9445203300	3.0053728516
C	-3.2572620634	0.4453518411	2.9105208858
H	-1.5683685324	1.2797203723	3.9920324165
H	-3.8425043090	0.4456554747	3.8238778594
O	-1.0986888111	1.0502901595	2.0537415541
O	-3.2935606821	-0.0713994920	0.5689055518
O	-1.9832238012	2.3673707986	-0.4352975830
O	0.5343915245	1.0841231554	-0.5273636745
O	-0.4751867919	-1.4264294969	0.4224673027
H	0.3784589385	-1.4057668999	0.8822535946
H	-3.8940541332	-0.3591384093	-0.1377654183
C	-1.7909312060	-0.2228885450	-1.9514190663
H	-1.5412385983	0.5179713971	-2.7223188916
H	-1.2594195266	-1.1472237951	-2.2277353619
H	-2.8655708700	-0.4321116445	-2.0825771042
H	-0.3705263617	-1.9923939503	-0.3596845933

$(acac)_2Re(OH)(H)(CH_3)^+$ oxidative addition intermediate
enthalpy: -728.842998

Re	-1.1220151368	0.5094347893	-0.3192740763
C	-3.8846155054	0.4095709777	2.3940194296
H	-4.8632994974	0.1039146114	2.7594834297
C	-1.6177254169	3.4746711140	-0.9041620575
H	-2.3799896260	4.2351496835	-1.0962318973
C	0.7129438160	2.9142719638	-0.5560682894
C	-0.2815581434	3.8543332360	-0.7960990520
H	1.7551701723	3.2294963861	-0.4660669470
H	-0.0121732026	4.8976326351	-0.9015316109
C	-1.5397512963	1.0604626097	2.9340727414
C	-2.8606073167	0.6131942055	3.2631479373
H	-0.8877512003	1.2872036229	3.7905696945
H	-3.0747341063	0.4668955361	4.3156754358
O	-1.0503135731	1.2435562653	1.7997347420
O	-3.7706690075	0.5848699252	1.0744361575
O	-2.0696760658	2.2798623855	-0.8003956704
O	0.5444789768	1.6453014086	-0.4279442342
O	-1.3175145169	-1.1681259499	0.4840977981
H	-1.2086570731	-1.9919359239	-0.0180947992
H	-4.6150871499	0.4333418806	0.6257529262
C	-2.2480835517	-0.0755950213	-2.0251277035
H	-3.2879970149	0.1303905193	-1.7436626298
H	-1.9897322597	0.5398467730	-2.8887924015
H	-2.1314650924	-1.1296013894	-2.2793699404
H	-0.1788040589	-0.2099987859	-1.4276251286

Trans protonated

$(acac)_2Re(OH)(OH_2)^+$
enthalpy: -764.834822

Re	-1.2896724642	0.4819177996	-0.0053891817
C	-3.7948472925	0.1961758809	1.5881067830
H	-4.8574668519	-0.0565584778	1.6360283683
C	-1.3723191896	3.3913999073	-0.7823575411
H	-1.9774320345	4.2932543613	-0.9023004521
C	0.8430535876	2.3382748214	-0.9867212357
C	-0.0217090881	3.4241834069	-1.1301972557
H	1.8951798852	2.4507362322	-1.2573668884
H	0.3846193911	4.3505022679	-1.5190213696
C	-1.9118937592	1.1001327492	2.9966721224
C	-3.1967479099	0.7405049002	2.7789821097
H	-1.5510871181	1.4367033232	3.9624420594
H	-3.8550101633	0.8351983035	3.6362652948
O	-0.9439020303	1.0655964269	2.0232149337
O	-3.2099910857	-0.0594761310	0.5002924997
O	-2.0027071954	2.3726059500	-0.3044101788
O	0.5307080386	1.1699870577	-0.5350454895
O	-1.6583999069	-0.2146890839	-1.9828556889
H	-1.2260113678	-1.0928305132	-1.9856835515
O	-0.6840321862	-1.3702868171	0.1170518248
H	0.1021311300	-1.6116604668	0.6237960968
H	-2.5951576118	-0.3465504081	-2.2017247905
H	-0.0734336216	1.3704388668	2.3264008508

$(acac)_2Re(OH)(H)(CH_3)^{\ddagger}$ metathesis transition state
enthalpy: -728.847763

Re	-0.0076768879	0.0009498413	-0.0049367436
O	-0.0183673656	-0.0265176076	2.0464925556
H	1.2176199489	-0.0136286828	1.4910069478
C	2.1808143769	-0.1772487089	0.5715232536
C	-1.0575353814	-2.8003666483	-0.4366174351
H	-0.8553877293	-3.8760937127	-0.4429861624
C	0.4165627449	0.9905482919	-2.7858288616
H	0.5391352274	0.7296474300	-3.8385446067
C	0.3083228566	2.7609386824	-1.0776693810
C	0.4871377877	2.3267448207	-2.3917630949
H	0.3490180050	3.8267328340	-0.8471513854
H	0.6728278793	3.0743664675	-3.1541168024
C	-2.9092955658	-1.1457631313	-0.8128566813
C	-2.3749829026	-2.3875097789	-0.8456432996
H	-3.9476568800	-0.9556608086	-1.0650686529
H	-3.0454915608	-3.1810001707	-1.1574964889
O	-2.2023523600	-0.0366378772	-0.4523883608
O	-0.1188608996	-2.0680572703	-0.0350360843
O	0.2002647002	-0.0152086016	-2.0012538168
O	0.0734890809	1.9993629136	-0.0578391627
H	-0.2148852367	0.8170715653	2.4824565432
H	-2.7444172190	0.7672005153	-0.4190799849
H	2.5267351487	0.4691230738	-0.2393695995
H	2.7405845188	0.1928241719	1.4483071146
H	2.4679843532	-1.2151689786	0.4073481298

$(acac)_2Re(OH_2)(CH_3)^+$
enthalpy: -728.874478

Re	-1.2948329153	0.4891846875	-0.0506903813
C	-3.7459680684	0.1049132282	1.7196773584
H	-4.7619012160	-0.2971425413	1.7381317347
C	-1.3062223762	3.3454106421	-0.7653566059
H	-1.8728725441	4.2758979789	-0.8399043647
C	0.8799204287	2.2301638293	-1.0569868293
C	0.0371692625	3.3331652195	-1.1569396961
H	1.9266085876	2.3283590562	-1.3513484897
H	0.4560661785	4.2556107466	-1.5422815188
C	-2.0204051340	1.2061215483	3.1659525592
C	-3.2673542928	0.7381621472	2.9089486132
H	-1.7522264740	1.6284361473	4.1290203577
H	-3.9780074945	0.8140878128	3.7249524145
O	-1.0133407776	1.1639463706	2.2487904332
O	-3.1075174441	-0.0721054878	0.6373029411
O	-1.9767513080	2.3550896283	-0.2826024162
O	0.5493751732	1.0513028609	-0.6272107866
H	-0.2001431185	1.5680222585	2.5852352978
C	-1.7680152065	-0.1082739347	-1.9940766529
H	-1.8629171960	0.7689145919	-2.6450342693
H	-1.0038782020	-0.7655164034	-2.4303569814
H	-2.7326838704	-0.6296111761	-1.9886888450
O	-0.4489099552	-1.4974453647	0.3014974244
H	0.5108080271	-1.5209918141	0.1585287809
H	-0.8341619760	-2.2225477792	-0.2164165665

$(acac)_2Re(OH)(H)(CH_3)^+$ oxidative addition intermediate
enthalpy: -728.847763

Re	-1.1906097486	0.2746824127	-0.0915967785
C	-3.7081533890	-0.0709424441	1.7302965198
H	-4.7362549221	-0.4521994466	1.7436173420
C	-1.1350446083	3.2309933988	-0.8936515364
H	-1.7016042748	4.1575657742	-1.0295348932
C	1.0368350822	2.1166526447	-0.9429416812
C	0.2305100446	3.2170899029	-1.2003020715
H	2.1128146562	2.1848944420	-1.1196703151
H	0.6880678138	4.1158897437	-1.5952880200
C	-2.0269096657	1.0509991429	3.2146484055
C	-3.2237206247	0.4634727389	2.9702011668
H	-1.7634090197	1.3845511918	4.2154415783
H	-3.8994102840	0.3813995961	3.8141242596
O	-1.1118878538	1.2922198104	2.2602359808
O	-3.1177669733	-0.1728703739	0.6301513959
O	-1.8049694314	2.2461547728	-0.4327955886
O	0.6601488271	0.9751625424	-0.4670314926
O	-0.6366266843	-1.1645827715	1.0580174734
H	-0.1822584542	-1.9434594118	0.7104200280
H	-0.2621390460	1.5757183102	2.6302924857
C	-2.2868483082	0.0785245490	-1.9369469228
H	-3.1560658470	0.7312377161	-1.8414836375
H	-1.6607757692	0.3910239661	-2.7767907005
H	-2.6014056546	-0.9561339712	-2.0789672364
H	-0.5987087000	-0.7925204439	-1.1324553060

Cis cross protonated

$(acac)_2Re(OH)(OH_2)^{2+}$
enthalpy: -765.225863

Re	0.0171476407	0.1519757144	-0.0059323321
C	3.1533120820	-0.4574320849	0.2885119726
H	4.1697380915	-0.0986292539	0.1558555749
C	-1.7616309337	-1.6280108413	-2.0976659140
H	-1.8081633184	-2.1961887172	-3.0214454141
C	-2.8662537837	-0.7383507270	-0.0530647242
C	-2.8193799820	-1.4942619242	-1.2668545192
H	-3.8076202173	-0.6856597158	0.4983748736
H	-3.7340024722	-1.9961432066	-1.5658070612
C	1.5614351762	-2.1210657085	1.2426583028
C	2.8587636473	-1.5417426674	1.0362779196
H	1.5075970657	-3.0845130147	1.7583122782
H	3.6995569470	-2.0525124389	1.4949395590
O	0.4539774871	-1.6410077057	0.8747652207
O	2.2106716669	0.2622067584	-0.4107182228
O	-0.5373051522	-1.0522561046	-1.8487749394
O	-1.9024339917	-0.0908590153	0.4562505596
O	-0.7232573931	1.9304048952	-1.0442700689
H	-1.4579991395	2.3948156599	-0.6082009278
O	0.5078325455	1.2114798359	1.4726199265
H	0.0015843583	1.2007467983	2.3023971319
H	-0.1495345043	2.6136982002	-1.4233499521
H	2.5995665275	1.0789658428	-0.7655860304
H	0.1012869979	-1.2553684641	-2.5518562340

$(acac)_2Re(OH)(H)(CH_3)^{2+\ddagger}$ metathesis transition state
enthalpy: -729.207020

Re	-0.0206828986	-0.0109858393	0.0371215034
O	-0.0639676664	-0.0178407979	2.0369480701
H	1.1716650540	0.0246712819	1.6450060521
C	2.1564683780	-0.1602665487	0.7040038000
C	-1.4981974876	-2.8248166014	0.4419923891
H	-1.3827872650	-3.8633337657	0.7364578647
C	0.2624912384	1.1603105385	-2.9511646197
H	0.3776823811	0.9508700682	-4.0098626813
C	0.0796662324	2.7736164917	-1.0696768480
C	0.1527972978	2.4119860799	-2.4500450095
H	0.0706975688	3.8310052492	-0.7974227646
H	0.1674026715	3.2238525000	-3.1704946758
C	-2.9437545846	-0.8929049256	-0.1825365481
C	-2.7004226647	-2.2399392399	0.2635321997
H	-3.9742174677	-0.6074762311	-0.4161343732
H	-3.5700091160	-2.8688242891	0.4270764558
O	-2.0673784607	-0.0047794571	-0.3506947664
O	-0.2974733184	-2.1741569091	0.2239081155
O	0.2497767337	0.0361208311	-2.1542816371
O	0.0498234826	1.9614144974	-0.0922639972
H	-0.4322993346	0.7526907305	2.5046393747
H	0.4594639479	-2.7203362486	0.5011039530
H	0.4147653047	-0.7724010895	-2.6692066984
H	2.5393551929	-1.1713622558	0.5486811360
H	2.5707914760	0.5255394952	-0.0421584753
H	2.6517394518	0.1946889310	1.6316502302

$(acac)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -729.252906

Re	-0.0436773500	0.1539900988	-0.0379683974
C	3.1800360890	-0.4171396354	0.1044961105
H	4.1591031165	-0.0407017763	-0.1755166526
C	-1.6709294801	-1.6523747575	-2.0411158009
H	-1.6902570798	-2.2071053955	-2.9744066984
C	-2.8596819078	-0.8006999792	-0.0150563063
C	-2.7324532218	-1.5865305269	-1.2059077820
H	-3.8217846861	-0.8022361415	0.5034978776
H	-3.6101828976	-2.1494645072	-1.5080804778
C	1.7510582063	-2.0892266095	1.2689316138
C	3.0086577342	-1.5140204992	0.8748655222
H	1.7734376601	-3.0129289031	1.8576899433
H	3.9116259018	-2.0140239139	1.2102849857
O	0.6203760667	-1.6186682353	0.9849256013
O	2.1363434730	0.3144026314	-0.4121044641
O	-0.4710373559	-1.0277187696	-1.7911693350
O	-1.9682225427	-0.0576129862	0.4980712946
O	0.2372559503	1.2355343138	1.7601947980
H	-0.3929001937	1.0740997834	2.4838416730
H	2.4427538653	1.0755791810	-0.9353706903
H	0.1143552452	-1.0474043386	-2.5681310835
H	0.4248919503	2.1891176877	1.7353931938
C	-0.2776274348	1.9610686058	-1.0874778228
H	-0.8757639353	1.8237552562	-1.9987391083
H	-0.7956386842	2.7186837211	-0.4830241658
H	0.6726353561	2.4167181866	-1.4081503021

$(acac)_2Re(OH)(H)(CH_3)^{2+}$ oxidative addition intermediate
enthalpy: -729.225892

Re	0.3152396260	0.3897408131	0.0183513004
O	1.7790613330	-0.7698753626	0.0434026587
H	1.2534947159	1.3695164465	0.9192294905
C	1.0132983072	2.2167447879	-0.8861601311
C	0.4591363923	-1.4213461888	-2.7603563015
H	0.9953924383	-1.5432990298	-3.6972132466
C	-2.6206318902	1.7313981901	0.8720357824
H	-3.4833598529	2.3207883189	0.5730129497
C	-1.3659736461	0.4528446712	2.5736226383
C	-2.4956577280	1.1912790492	2.1049012741
H	-1.3819909906	0.0671868104	3.5977389460
H	-3.3112071440	1.3481938316	2.8031045673
C	-1.0397737570	-2.3029635512	-0.9979559047
C	-0.2608547185	-2.4151738885	-2.2018934181
H	-1.7213761050	-3.1287334813	-0.7599523476
H	-0.2964162803	-3.3590949686	-2.7358082725
O	-1.0244579681	-1.3384597669	-0.1971525604
O	0.5365275299	-0.1569210966	-2.2297793067
O	-1.6715719083	1.5770105973	-0.0970447548
O	-0.3057527626	0.2008360266	1.9359660497
H	2.5032047417	-0.6929250687	0.6895742609
H	1.1394648649	0.4035756633	-2.7492365859
H	-1.8643771229	2.1225614677	-0.8791840373
H	0.4576898745	2.3096045579	-1.8313656189
H	0.8314388905	3.1100696784	-0.2870446222
H	2.0867031000	2.1578413545	-1.0853472621

Trans diprotonated

$(acac)_2Re(OH)(OH_2)^{2+}$
enthalpy: -765.211516

Re	-1.2768160510	0.4708355152	0.0001631755
C	-3.9199499833	0.2217383818	1.8018134603
H	-4.9756188039	-0.0206711435	1.8478229988
C	-1.3922605410	3.2675489891	-1.0585514361
H	-2.0418219378	4.1125440758	-1.2900459218
C	0.8520743670	2.2842285467	-1.0299782324
C	-0.0410754472	3.3047587750	-1.3756795035
H	1.9209756512	2.3994964158	-1.2188397365
H	0.3562538005	4.1925642853	-1.8548990692
C	-1.9204307104	1.1197209681	3.0232559354
C	-3.2389472827	0.7469158960	2.8794223874
H	-1.5120308798	1.5109948976	3.9477502519
H	-3.8448027437	0.8867821302	3.7707977282
O	-1.0086348515	1.0461611549	1.9931208367
O	-3.3300721186	-0.0284798878	0.5873391643
O	-1.9778051013	2.2762832212	-0.4463662062
O	0.5374630804	1.1723799957	-0.4476717472
O	-1.3794697581	0.0173446208	-2.0740309495
H	-0.5696744220	-0.1446171129	-2.5857367283
O	-0.8176794905	-1.2975036332	0.4140582270
H	-0.1416136810	-1.8756711134	0.0223355595
H	-2.1455883405	-0.2770550898	-2.5894804214
H	-0.0955795096	1.2247909446	2.2874400469
H	-3.9602881383	-0.4372695600	-0.0291796196

$(acac)_2Re(OH)(H)(CH_3)^{2+\ddagger}$ metathesis transition state
enthalpy: -729.202554

Re	-0.0114466905	-0.0028671809	0.0857627799
O	-0.1141587912	0.0678082582	2.1042360036
H	1.1926047333	0.0060568493	1.6208829748
C	2.1361447649	-0.2934186171	0.7357594044
C	-1.4217532844	-2.8081906026	-0.4231013763
H	-1.2480255232	-3.8706764431	-0.5589982517
C	0.5103638092	0.6703600980	-2.7846792114
H	0.6199606205	0.2948353206	-3.8034982129
C	0.5057352459	2.5873581684	-1.2524306861
C	0.6426433327	2.0392037642	-2.5193907528
H	0.6139507324	3.6601676078	-1.0920975287
H	0.8538314933	2.7074414812	-3.3473492402
C	-3.0316271959	-0.9018260117	-0.7397007883
C	-2.6038258966	-2.2116456201	-0.8213699203
H	-4.0511003729	-0.6151360280	-0.9792804994
H	-3.3307866213	-2.8997230044	-1.2441580297
O	-2.2186108123	0.1152525802	-0.3541536400
O	-0.4194994401	-2.1482524738	0.2170517065
O	0.2581959969	-0.2320507179	-1.8936116700
O	0.2399123302	1.9209334811	-0.1566612165
H	-2.6909844413	0.9625809850	-0.2885399389
H	0.2155143097	-2.7553369843	0.6432245345
H	2.5251951399	0.0673955144	-0.2183080389
H	2.7249482111	0.2850599894	1.4719228311
H	2.3966293311	-1.3472682106	0.8444375221
H	-0.2646898438	0.9195530509	2.5523857290

$(acac)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -729.256742

Re	-0.0429003631	0.0261750169	-0.0585484930
C	3.2046803352	-0.0714780043	0.1112285423
H	4.0874719750	0.5564397247	0.1202163382
C	-0.7620614090	-0.1126338213	-2.9170813502
H	-0.4223638100	0.0130297995	-3.9464402357
C	-2.5706902888	-0.7185617867	-1.3752564889
C	-2.0902743193	-0.4606160224	-2.6500517071
H	-3.6016358389	-1.0387196255	-1.2228981569
H	-2.7693985109	-0.5726931609	-3.4879209994
C	2.3019921587	-2.4232058882	0.0192050771
C	3.2775484596	-1.4471636012	0.0830140032
H	2.5506292009	-3.4786892969	0.0166282025
H	4.2942932587	-1.8307178956	0.1044946605
O	0.9697179072	-2.1310928333	-0.0554757028
O	2.0185776343	0.6401494465	0.1527032317
O	0.1637921391	0.0625605631	-2.0276701243
O	-1.8759523505	-0.6347718436	-0.2668518459
O	-0.2981748709	-0.1541019320	2.0909541105
H	-1.0411900202	-0.6906283314	2.4175846435
H	0.4408291132	-2.9354976147	-0.1953403983
H	2.1832763329	1.6005440765	0.1373974518
C	-0.5837652174	2.0366791229	0.0662559714
H	-0.5973789964	2.4972953672	-0.9276124578
H	-1.5858735001	2.1261050890	0.5028044446
H	0.1065030509	2.6072334254	0.7051615464
H	-0.2111860807	0.6116367198	2.6835774662

$Re(cat)_2$ systems

Cis protonated

$(cat)_2Re(OH)(OH_2)^+$
enthalpy: -994.650852

Re	-0.9791394426	-0.2354611669	-0.3228736431
O	-1.9185620951	1.4624315501	-0.3202335655
O	-0.0070608295	0.8272938810	-1.6179623118
O	-0.9977488923	-1.5770894177	-2.1399520382
H	-0.2217915127	-2.1472864852	-1.9739453187
O	0.4865413270	-1.4047508819	-0.0831959945
H	0.8234001245	-1.4868823460	0.8256416552
H	-0.7744452499	-1.0453098002	-2.9231367010
O	-0.8348401715	-0.0526063637	1.6282246022
O	-2.8193373282	-0.9339513305	0.3805892832
C	-2.0030840800	0.0108064865	2.3174889523
C	-2.1164231463	0.4929105459	3.6220102313
C	-3.1477717939	-0.4671346870	1.6784803620
C	-3.3748128956	0.4839598730	4.2259785743
H	-1.2362801903	0.8656280930	4.1343884834
C	-4.4052277712	-0.4880688904	2.2481311852
C	-4.5054913035	0.0025742221	3.5544610744
H	-3.4780169901	0.8611405529	5.2382210751
H	-5.2730464339	-0.8646419595	1.7145029899
H	-5.4722650234	0.0081618723	4.0460626877
C	-1.4092591291	2.5088753795	-0.9747143349
C	-0.2770679403	2.1392989828	-1.7326414724
C	-1.8786049945	3.8262357206	-0.9527984424
C	0.4227372503	3.0706690404	-2.4998343502
C	-1.1833698404	4.7512798976	-1.7211807882
H	-2.7475734137	4.0954225657	-0.3629507458
C	-0.0501543456	4.3791379436	-2.4791778768
H	1.2984334721	2.7801220400	-3.0691249332
H	-1.5133579900	5.7847602232	-1.7385644017
H	0.4693644120	5.1378222333	-3.0555720104
H	-3.5041458543	-1.4375127754	-0.0856689671

$(cat)_2Re(OH)(H)(CH_3)^{+‡}$ metathesis transition state
enthalpy: -958.637200

Re	0.0711348483	-0.0020198522	0.0674867901
O	-0.0685413020	0.0262607225	2.0795156008
H	1.1814800155	-0.0476593826	1.7126494409
C	2.2278037751	-0.0019460338	0.8756851867
O	-1.0915241169	0.5824953731	-1.3580790229
O	0.1234634762	1.9254843106	0.2152091330
H	-0.5580840822	-0.7503126792	2.4042843300
O	-0.8060833062	-1.7113008487	0.2902624718
O	0.8009806941	-1.2410546604	-1.5791126569
C	-0.9628526552	-2.5143495923	-0.7961627142
C	-1.8997049300	-3.5451751762	-0.8731949586
C	-0.1132917700	-2.2687389269	-1.8782814904
C	-1.9608794044	-4.2932872009	-2.0485114981
H	-2.5596014197	-3.7357673295	-0.0338367985
C	-0.1544555470	-2.9971645834	-3.0508384126
C	-1.1049935288	-4.0230833560	-3.1238449038
H	-2.6867056563	-5.0953672856	-2.1323481484
H	0.5203465243	-2.7928832940	-3.8769124722
H	-1.1704949385	-4.6178333135	-4.0287709052
C	-1.3428411359	1.8940314664	-1.5225401629
C	-0.6346929623	2.6794555021	-0.5901985510
C	-2.1968483018	2.4669669263	-2.4644052783
C	-0.7689077056	4.0702071622	-0.5562764706
C	-2.3195469527	3.8535978629	-2.4354329810
H	-2.7432155843	1.8510509691	-3.1694630997
C	-1.6161885093	4.6413685270	-1.4982460923
H	-0.2241776166	4.6615781253	0.1710489908
H	-2.9784801776	4.3416523672	-3.1460127865
H	-1.7443407832	5.7187666291	-1.5130628876
H	1.2612107220	-0.8826569414	-2.3536112570
H	2.6350490120	0.2597201601	1.8715919736
H	2.6707047097	-0.9513700189	0.5756545383
H	2.5590181520	0.8215320987	0.2395521774

$(cat)_2Re(OH_2)(CH_3)^+$
enthalpy: -958.693263

Re	-1.0281499074	-0.0205695605	-0.2794856014
O	-2.0273886689	1.3740140563	-1.1663988110
O	0.4420967596	0.9377632474	-1.0078369080
O	0.3743254540	-1.5964406181	0.0909597870
H	0.2296574081	-2.5256283359	-0.1456624897
O	-1.3268149983	0.4751030840	1.5108285448
O	-2.8115577021	-1.3091448715	0.5696002777
C	-2.2801267129	0.0325013350	2.3759069231
C	-2.4191814392	0.5126288460	3.6762724887
C	-3.1483497053	-0.9356522015	1.8729550882
C	-3.4576666538	-0.0044980043	4.4509818378
H	-1.7380181448	1.2678643894	4.0522558542
C	-4.1831942206	-1.4557547560	2.6301498492
C	-4.3308546916	-0.9694773002	3.9352477245
H	-3.5921772485	0.3519694456	5.4667251995
H	-4.8515028103	-2.2120508964	2.2298808072
H	-5.1347565090	-1.3543088877	4.5539802279
C	-1.2579672183	2.4020707541	-1.6226645846
C	0.1212848884	2.1585021201	-1.5676558541
C	-1.7553875691	3.5849278300	-2.1643152485
C	1.0473615306	3.0718126825	-2.0487470664
C	-0.8288334462	4.5178805996	-2.6352952733
H	-2.8246074983	3.7640883103	-2.2026158122
C	0.5496821109	4.2655981700	-2.5821486633
H	2.1102876147	2.8593088230	-2.0070540955
H	-1.1839547802	5.4538056738	-3.0545701123
H	1.2442430022	5.0065028894	-2.9646603360
H	-3.5881623456	-1.4436077562	0.0056867975
C	-1.6827587058	-1.2261074465	-1.8949884795
H	-0.9555058547	-1.0418586986	-2.6971447277
H	-1.6861777080	-2.2941315612	-1.6550425348
H	-2.6606581757	-0.9095501247	-2.2648449878
H	1.3144069729	-1.3782324268	-0.0144199985

$(cat)_2Re(OH)(H)(CH_3)^+$ oxidative addition intermediate
enthalpy: -958.628160

Re	-1.0492942577	-0.3918568194	-0.7371929305
O	0.4497255087	-1.2106333333	-1.5492714798
H	-1.2081528633	-2.0220884593	-0.5391243612
C	-2.4617898674	-0.8045802602	-2.2902440183
O	-2.1686193240	1.2724642920	-0.4794802533
O	0.0663307858	1.0517954329	-1.5278540364
H	0.5213243904	-2.1760034210	-1.5349242656
O	-0.6285376135	-0.2810412100	1.1393062802
O	-2.9510758637	-0.9526897498	0.3311828394
C	-1.4912720678	-0.5800658849	2.1333942299
C	-1.1587092857	-0.5343329641	3.4898647219
C	-2.7775398246	-0.9455805546	1.7427438719
C	-2.1491518965	-0.8656816586	4.4138394799
H	-0.1575523391	-0.2492938202	3.7930576927
C	-3.7681843034	-1.2871482655	2.6423074697
C	-3.4356950493	-1.2356299256	4.0022104046
H	-1.9148688618	-0.8377538217	5.4729146607
H	-4.7574266188	-1.5808515907	2.3070150811
H	-4.1873040986	-1.4915558973	4.7412158516
C	-1.6578555725	2.4289045197	-0.8665303045
C	-0.3628957317	2.3009897016	-1.4480450511
C	-2.2864289478	3.6799852639	-0.7640449116
C	0.3389083856	3.4228038495	-1.9224562961
C	-1.5781696686	4.7778180721	-1.2219453153
H	-3.2742930729	3.7684750063	-0.3261256449
C	-0.2818438565	4.6518837075	-1.7936019531
H	1.3231520522	3.3060658568	-2.3615613545
H	-2.0206492031	5.7657983782	-1.1432066358
H	0.2269127908	5.5463829233	-2.1379102372
H	-3.5575026718	-0.2287966137	0.0781635444
H	-1.8167578940	-0.7451066235	-3.1751625823
H	-2.8879574264	-1.8026631988	-2.2003482657
H	-3.2338427044	-0.0376407977	-2.3507120891

Trans protonated

$(cat)_2Re(OH)(OH_2)^+$
enthalpy: -994.657794

Re	-0.9970522933	-0.2230741490	-0.3116151051
O	-1.8673501657	1.5430588493	-0.3878486935
O	0.1634618636	0.8834910206	-1.4962274433
O	-1.3418058898	-1.2695820604	-2.1360091973
H	-2.1590907509	-1.7946195316	-2.1227228308
O	0.2779209752	-1.6157008520	-0.1556318146
H	0.7159637735	-1.7866723066	0.6926059177
H	-0.5957474057	-1.8727574835	-2.3130830573
O	-0.8021770029	0.2254619436	1.7738243562
O	-2.6129914918	-0.9853229644	0.4236533771
C	-2.0569798116	0.1196799597	2.4354349486
C	-2.3141782753	0.5994451305	3.7041067461
C	-2.9964340269	-0.5686650550	1.6673154619
C	-3.5962085746	0.3755938331	4.2212800882
H	-1.5580005900	1.1263905800	4.2793031657
C	-4.2669093884	-0.7931243694	2.1942752842
C	-4.5554680544	-0.3150665307	3.4744776916
H	-3.8388867684	0.7421169975	5.2129343534
H	-5.0038875705	-1.3241336143	1.6015273690
H	-5.5427319840	-0.4795863809	3.8934497726
C	-1.3201341922	2.5469809491	-1.0424562690
C	-0.1275702072	2.1431388674	-1.7190545931
C	-1.7972976442	3.8667878824	-1.1187175354
C	0.5920600776	3.0517480726	-2.5160880299
C	-1.0733282181	4.7475642938	-1.9006753826
H	-2.7046545310	4.1567969801	-0.6006407113
C	0.1063417550	4.3444756034	-2.5873099933
H	1.4927036419	2.7389622654	-3.0319344106
H	-1.4122032603	5.7734506986	-2.0032097756
H	0.6386140208	5.0801990609	-3.1818382793
H	-0.2438372029	0.9391132272	2.1177762148

$(cat)_2Re(OH)(H)(CH_3)^{+‡}$ metathesis transition state
enthalpy: -958.637894

Re	0.0325118347	-0.0209353984	0.0393154261
O	-0.0789200540	-0.0490562906	2.0567759123
H	1.1585478940	-0.0843582553	1.6602800429
C	2.1811629401	-0.0282094999	0.7818951707
O	-0.1055941863	0.5035047815	-1.8466200601
O	0.1641039803	1.9295353577	0.0659322675
H	-0.5584811204	-0.7476182861	2.5261691766
O	-1.9826980819	-0.8034730639	-0.3457121894
O	0.3483310723	-1.8514190043	-0.4411979774
C	-1.9259369111	-2.0296898709	-1.0362074410
C	-3.0083389789	-2.6571182790	-1.6229829881
C	-0.6277447617	-2.5452590369	-1.0917218798
C	-2.7611796518	-3.8593362025	-2.2970670603
H	-4.0060200350	-2.2316854692	-1.5726182777
C	-0.3887385515	-3.7384986434	-1.7734735311
C	-1.4676314222	-4.3881677344	-2.3731463316
H	-3.5870132217	-4.3788053550	-2.7714137692
H	0.6197214234	-4.1346394968	-1.8195256265
H	-1.3004458305	-5.3179082714	-2.9066474717
C	-0.0062405550	1.7719993667	-2.1936956326
C	0.1481925548	2.6214982668	-1.0574490295
C	-0.0745840318	2.3001798734	-3.4925086727
C	0.2475429657	4.0155364627	-1.1956184939
C	0.0313712875	3.6746856165	-3.6140203946
H	-0.1883278886	1.6462415618	-4.3497284041
C	0.1862464451	4.5208151955	-2.4821170611
H	0.3588511238	4.6504171757	-0.3239917845
H	-0.0023623893	4.1249078522	-4.6010571827
H	0.2557606190	5.5925441387	-2.6374173003
H	-2.7776225487	-0.6857784156	0.1958140763
H	2.5841879260	0.2173135731	1.7857628159
H	2.5961461236	-0.9873869540	0.4770621514
H	2.5393934329	0.7939394522	0.1612611097

$(cat)_2Re(OH_2)(CH_3)^+$

enthalpy: -958.685334

Re	-0.0001272988	-0.0018573637	0.0026239113
O	0.0006996461	0.0003287316	1.9339320273
O	1.8682998131	-0.0026410800	0.3483149451
O	0.5499905597	0.4505070275	-2.0173447272
H	0.3541396387	1.3329014119	-2.3724709512
O	0.4271955656	-2.2021083168	-0.1943299609
O	-1.6669260370	-0.9015955562	-0.2830331466
C	-0.6965928708	-3.0136313232	-0.2963413020
C	-0.7265560231	-4.3961693638	-0.3466256444
C	-1.8612544437	-2.2414534626	-0.3628707328
C	-1.9816909955	-5.0043633558	-0.4663120517
H	0.1831306319	-4.9869841800	-0.2925812908
C	-3.1100369586	-2.8480866260	-0.4852279283
C	-3.1536945513	-4.2410265396	-0.5385291685
H	-2.0414326223	-6.0870891916	-0.5025362178
H	-4.0065694564	-2.2398937484	-0.5308286590
H	-4.1123812392	-4.7400932040	-0.6317323038
C	1.1578789189	-0.3824167737	2.5049327636
C	2.2493074858	-0.3600789228	1.6122804234
C	1.3488716871	-0.7039967899	3.8499102173
C	3.5467828993	-0.6631183411	2.0163516970
C	2.6453013330	-1.0139133816	4.2573747487
H	0.5090127249	-0.7185740944	4.5358672813
C	3.7288069567	-0.9906376408	3.3595449858
H	4.3732570797	-0.6222835925	1.3148828042
H	2.8241998934	-1.2778599766	5.2948938264
H	4.7250678485	-1.2241360700	3.7204740002
C	-0.6846158243	2.0011102864	0.1088307541
H	-0.1089765000	2.6924133297	-0.5221654757
H	-1.7152065101	1.9701248077	-0.2764415466
H	-0.7029854911	2.3759116065	1.1335758319
H	1.4102735782	0.1553258380	-2.3537802733
H	1.2191610401	-2.6647585440	0.1202174723

$(cat)_2Re(OH)(H)(CH_3)^+$ oxidative addition intermediate
enthalpy: -958.658395

Re	-0.4444696755	0.0502877079	0.1396325185
O	1.0283598155	0.6482630836	1.1988863878
H	0.8216470340	-0.7563581107	-0.4309570659
C	-0.7101490547	-1.7130979713	-1.1334352609
O	-2.1659677886	0.5163932275	-0.8346819121
O	0.0938314733	1.2498625810	-1.3346380228
H	1.9359264863	0.3711128191	1.0131397736
O	-1.3544771035	1.5501357432	1.6874006330
O	-1.3484118366	-1.0470043161	1.3883478768
C	-2.1221112080	0.8224474640	2.6126075900
C	-2.8554053326	1.4021625558	3.6321077964
C	-2.1387643016	-0.5590135723	2.3860951843
C	-3.6264459509	0.5598184845	4.4426544163
H	-2.8402557493	2.4767520180	3.7832631805
C	-2.9207646807	-1.3951599032	3.1839242733
C	-3.6607540558	-0.8206650383	4.2167777750
H	-4.2137868218	0.9906650713	5.2467601341
H	-2.9272031462	-2.4629453479	2.9946898628
H	-4.2709339755	-1.4540000985	4.8519606853
C	-2.1103443789	1.2580809497	-1.9006014903
C	-0.7689884805	1.6952978623	-2.2022239743
C	-3.1976505688	1.6938471309	-2.6848272922
C	-0.5001354174	2.5614255773	-3.2854652594
C	-2.9082954781	2.5206477154	-3.7506675169
H	-4.2059269496	1.3710962385	-2.4527381762
C	-1.5762391654	2.9523228511	-4.0492834327
H	0.5143235993	2.8838309556	-3.4905917595
H	-3.7162479334	2.8631678935	-4.3897492516
H	-1.4216670943	3.6074671570	-4.9002478703
H	-0.5935894574	1.9786447537	2.1206074626
H	-0.4108032424	-1.4678418675	-2.1550545056
H	-0.1570261223	-2.5769844285	-0.7698904916
H	-1.7847981237	-1.8901756086	-1.0801710401

Cis cross protonated

$(cat)_2Re(OH)(OH_2)^{2+}$
enthalpy: -995.032562

Re	-1.1683529908	-0.0412970649	-0.2396592526
O	-2.1445205514	1.5369761167	-1.3844294804
O	0.2511510367	1.1750392727	-0.6315191260
O	-1.1513306991	-0.9324234143	-2.2712599381
H	-0.4025806464	-1.5126136771	-2.4929812838
O	-0.0625074957	-1.5027076342	0.0884022716
H	-0.4783559281	-2.3322961237	0.3972304694
H	-1.4816729548	-0.5155679225	-3.0821237802
O	-1.5461244245	0.7067209299	1.4140837582
O	-2.7502995659	-1.3862431468	0.5924017516
C	-2.3014647437	0.0749439135	2.3656388207
C	-2.4153283385	0.5509288805	3.6718884598
C	-2.9778580972	-1.0820085108	1.9570176953
C	-3.2175288511	-0.1737315962	4.5516805633
H	-1.8828975787	1.4459074637	3.9752256464
C	-3.7814342401	-1.8042876603	2.8145940648
C	-3.8916428562	-1.3291689132	4.1310782301
H	-3.3218376354	0.1630384190	5.5775697963
H	-4.3050274946	-2.6998845624	2.4940365721
H	-4.5137257947	-1.8735929925	4.8339942212
C	-1.2324653880	2.4838206251	-1.8985150901
C	0.0771361576	2.2238474480	-1.4470277076
C	-1.5451551975	3.5468609186	-2.7147275314
C	1.1301525071	3.0775222562	-1.8199577842
C	-0.4804927472	4.3881303318	-3.0880150169
H	-2.5600515763	3.7495405315	-3.0447986740
C	0.8346347947	4.1527617272	-2.6487717338
H	2.1338308625	2.8764144493	-1.4600428922
H	-0.6891228449	5.2442136125	-3.7216429656
H	1.6272703565	4.8260494383	-2.9573179540
H	-3.5546890565	-1.6918670736	0.1416090158
H	-3.0764692694	1.8057018980	-1.4474308652

$(cat)_2Re(OH)(H)(CH_3)^{2+‡}$ metathesis transition state
enthalpy: -959.011009

Re	0.0133733489	-0.0147371902	0.0260720213
O	0.0142636043	0.0062825216	2.0334288667
H	1.2914740177	0.0459395639	1.5211549402
C	2.2347068448	0.0016527937	0.5602934355
O	0.5424959196	0.6064453208	-1.9585036048
O	-0.2587253037	1.8464714971	0.0805020029
H	0.0527252210	-0.8523753154	2.4949915222
O	-1.6166029827	-0.7430680688	-0.4781651199
O	0.1743081097	-2.3474093287	0.1353137173
C	-1.9894919556	-2.0330523885	-0.6123003418
C	-3.2641072709	-2.4305165755	-1.0365611918
C	-0.9987398884	-2.9748653125	-0.2783513892
C	-3.5087986506	-3.7956571965	-1.1168024788
H	-4.0151973654	-1.6870073764	-1.2808718138
C	-1.2325296048	-4.3316146645	-0.3569525565
C	-2.5099234717	-4.7292104590	-0.7852989211
H	-4.4832755936	-4.1480217738	-1.4373887961
H	-0.4754759722	-5.0662385922	-0.0986694012
H	-2.7277184313	-5.7901514024	-0.8569955065
C	0.3098621369	1.9788612594	-2.1938569059
C	-0.1369306350	2.6175258916	-1.0276688904
C	0.5006245550	2.6438383670	-3.3842941433
C	-0.4181151099	3.9884293224	-1.0316025667
C	0.2083861494	4.0189840807	-3.3842092793
H	0.8500779586	2.1435545182	-4.2826868949
C	-0.2437964099	4.6771977463	-2.2290019063
H	-0.7628508039	4.4730406469	-0.1242695743
H	0.3379662194	4.5795944809	-4.3044220126
H	-0.4571774097	5.7399294661	-2.2705438162
H	0.9211208244	-2.9569554203	0.2493844216
H	1.0767490687	0.1655035937	-2.6407301120
H	2.5632417618	0.8972686408	0.0273730816
H	2.7713250558	0.0533550030	1.5292080310
H	2.6027457740	-0.9110636511	0.0866330372

$(cat)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -959.083666

Re	-1.0343073565	-0.0357673739	-0.2731812612
O	-2.0921975058	1.5530748907	-1.1150950047
O	0.3599534734	0.9389203967	-1.0680551745
O	0.3813452604	-1.5055655578	0.1405581409
H	0.2796853654	-2.4602965407	-0.0083982945
O	-1.4299412088	0.4413067283	1.4876191430
O	-2.7539931370	-1.4432749796	0.6418110488
C	-2.3461377759	0.0059186651	2.3683786239
C	-2.5240902767	0.5629395650	3.6435540412
C	-3.1305614259	-1.0732203907	1.9170831961
C	-3.5105126424	0.0052430076	4.4440281981
H	-1.9063827811	1.3928629911	3.9693272436
C	-4.1158479679	-1.6307950405	2.7079906000
C	-4.2932738692	-1.0721753355	3.9827281948
H	-3.6838108979	0.4020343542	5.4385369141
H	-4.7245736072	-2.4647012836	2.3719767339
H	-5.0575425464	-1.4880999530	4.6317299186
C	-1.2421010964	2.5586015539	-1.6694928919
C	0.0981325071	2.1822298171	-1.6129668578
C	-1.6718908638	3.7583405996	-2.1984997715
C	1.0858109439	3.0317504575	-2.0983632026
C	-0.6753805414	4.6123040370	-2.6911784212
H	-2.7212211901	4.0363405122	-2.2277743014
C	0.6774936182	4.2542038141	-2.6393663427
H	2.1299689588	2.7414434749	-2.0564680405
H	-0.9648799756	5.5682532073	-3.1145618206
H	1.4253748347	4.9374900113	-3.0275155665
H	-3.3214977825	-2.1161662105	0.2329877855
H	-2.9611555156	1.4976000850	-1.5496980088
C	-1.7179641661	-1.1606526889	-1.9203122962
H	-1.1296202699	-0.8127069366	-2.7800334562
H	-1.5344357295	-2.2332427558	-1.7970973478
H	-2.7764334977	-0.9951275398	-2.1431555238
H	1.3261454557	-1.2686565576	0.1397146360

Trans diprotonated

$(cat)_2Re(OH)(OH_2)^{2+}$
enthalpy: -995.044162

Re	-0.9923074560	-0.2768684594	-0.3643098813
O	-1.9711557305	1.3912450306	-0.5861727225
O	0.2071587537	0.8780471160	-1.4416801302
O	-1.1598931227	-1.1620987853	-2.3232010170
H	-1.1085312758	-2.1341855556	-2.3571978030
O	0.2122667422	-1.6623956809	-0.0915340917
H	0.6855272749	-1.8696867756	0.7341867338
H	-0.4670534294	-0.8229441595	-2.9210217960
O	-0.8357880458	0.2757859754	1.6914382101
O	-2.7380955973	-0.9707968510	0.5272016543
C	-2.0332621557	0.2076006827	2.4472193728
C	-2.1884334437	0.7387815074	3.7146130765
C	-3.0685464057	-0.4719633255	1.8206431030
C	-3.4299630644	0.5717011742	4.3404183743
H	-1.3777868936	1.2650773057	4.2111351469
C	-4.3005701174	-0.6457127430	2.4234205842
C	-4.4703120256	-0.1107937947	3.7055451297
H	-3.5782934554	0.9806944500	5.3340346240
H	-5.1070687834	-1.1770281247	1.9254817270
H	-5.4250178308	-0.2311448496	4.2058584100
C	-1.4132350626	2.4590339831	-1.1064712161
C	-0.1007226695	2.1447431703	-1.6234620558
C	-1.9682237305	3.7476109611	-1.2230749386
C	0.6652827288	3.1166030161	-2.2828371395
C	-1.1948783852	4.6905898786	-1.8670407877
H	-2.9583479951	3.9652122586	-0.8384164276
C	0.1041865879	4.3783952260	-2.3835480276
H	1.6498566585	2.8847328080	-2.6729541903
H	-1.5747984386	5.6990316529	-1.9952446482
H	0.6668757702	5.1681119253	-2.8721540026
H	-0.1632798126	0.8570528691	2.0835378189
H	-3.4593906287	-1.4698453635	0.1053814827

$(cat)_2Re(OH)(H)(CH_3)^{2+‡}$ metathesis transition state
enthalpy: -959.018188

Re	-0.0097629426	0.0007700825	-0.0514533433
O	-0.0086889255	-0.0210650529	1.9088255466
H	1.2511935171	-0.0420142407	1.5584860188
C	2.1388852263	-0.2551219438	0.5666590053
O	0.6180753877	0.4907868767	-1.8119502620
O	-0.0828396007	1.9702554692	-0.0678217506
O	-2.1584389523	-0.2597313462	-0.2267688460
O	-0.2821144299	-1.9424158030	-0.7104050861
C	-2.6113750512	-1.5077977626	-0.6990448097
C	-3.9413014320	-1.8361561653	-0.8991176998
C	-1.6024595682	-2.4238502742	-0.9704771732
C	-4.2308421305	-3.1156463784	-1.3860601224
H	-4.7349557248	-1.1246397942	-0.6884096039
C	-1.8699068576	-3.6917336580	-1.4540861693
C	-3.2109530464	-4.0307680509	-1.6608124559
H	-5.2659819988	-3.3944735986	-1.5514061906
H	-1.0729596811	-4.4010045282	-1.6601879056
H	-3.4546654618	-5.0186232228	-2.0361750857
C	0.8268231672	1.7440317860	-2.1456997208
C	0.4333473029	2.6313059212	-1.0764067648
C	1.3121711341	2.2299192462	-3.3729611737
C	0.5338532975	4.0259337241	-1.2188428249
C	1.4099293908	3.6016650937	-3.4879464974
H	1.5867026086	1.5530985659	-4.1742847539
C	1.0324162927	4.4846983305	-2.4232845786
H	0.2459355253	4.6927153318	-0.4139531803
H	1.7815966925	4.0346926943	-4.4112762121
H	1.1426872669	5.5535656515	-2.5782612887
H	-2.8728989575	0.3754100137	-0.0475345307
H	0.4119909892	-2.5148226000	-1.0874641636
H	2.5785484249	-0.1036722865	1.5869211262
H	2.4619873261	-1.2638795995	0.3069272465
H	2.6551483866	0.5113883897	-0.0143873200
H	-0.4716381705	0.5857324096	2.5134854121

$(cat)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -959.071348

Re	-0.8936709144	-0.1883606184	-0.2869006136
O	-1.7695031420	1.5198055208	-0.2794716155
O	0.1360327706	0.8346792521	-1.5173111592
O	0.7571713350	-1.4851300848	-0.2155671508
H	1.3611600138	-1.6540325042	0.5261724062
O	-0.8987286052	-0.0302338088	1.9883456883
O	-2.6797318857	-0.9404905076	0.4690198721
C	-2.1792877001	-0.0072941204	2.5598393927
C	-2.4845329711	0.4433738598	3.8326508683
C	-3.1748212045	-0.4957595155	1.7225930047
C	-3.8238955124	0.3897727692	4.2366097382
H	-1.7150008829	0.8278205185	4.4960765658
C	-4.5050575532	-0.5506111273	2.1002193085
C	-4.8199633655	-0.0992650560	3.3850524404
H	-4.0881930647	0.7393381830	5.2289889059
H	-5.2724805745	-0.9310031758	1.4319365034
H	-5.8513252640	-0.1294574957	3.7190656475
C	-1.3697451873	2.4823859661	-1.1112742703
C	-0.1978065215	2.0873611963	-1.8189243476
C	-1.9243544594	3.7545060626	-1.2689531117
C	0.4706188855	2.9562567521	-2.6899998550
C	-1.2674019358	4.6039688976	-2.1492695704
H	-2.8245787776	4.0470847237	-0.7406160697
C	-0.0882234021	4.2150646413	-2.8429801826
H	1.3728076110	2.6504662387	-3.2077437362
H	-1.6632884691	5.6010363614	-2.3147372823
H	0.3832920906	4.9283189340	-3.5112008795
H	-0.1985728215	0.1876205443	2.6241462162
H	-3.3204259484	-1.4548101118	-0.0554081701
C	-1.3835634758	-1.3703076721	-1.9768281866
H	-0.5983222704	-1.3648122263	-2.7373151906
H	-1.5352479171	-2.4013752598	-1.6240974925
H	-2.3128824766	-1.0210162338	-2.4402982599
H	1.1674300395	-1.7975750554	-1.0428226660

$Re(gly)_2$ systems

Cis protonated

$(gly)_2Re(OH)(OH_2)^+$
enthalpy: -689.834496

Re	-.0516675035	-.0327842251	.0557234567
O	2.3184868318	.3670160132	.2372138360
H	2.6192176600	1.0058427322	.9013239399
O	.6253975384	-1.3220094997	1.1877823876
H	1.5598266023	-1.4642045122	1.4045050405
H	2.6456507410	.6842787484	-.6183061904
C	-2.5040471508	-1.0938134140	-1.0602619993
C	-1.4889324914	-2.0993318819	-1.5710887525
H	-1.7116018118	-2.4880381681	-2.5662155426
H	-1.3358862913	-2.9251275809	-.8748745258
H	-3.3801075165	-1.5916212819	-.6340087803
H	-2.8398845867	-.4127389194	-1.8522142954
C	-.0305960269	2.6194772611	-.9953702820
H	-1.0737878994	2.8209840479	-1.2610269468
H	.6304364382	3.2652407497	-1.5800231694
C	.1693349547	2.7362109464	.5210387030
H	-.3443550741	3.5985306283	.9540989026
H	1.2381311980	2.8015129888	.7661113673
O	-1.9102188747	-.2952917704	-.0192895679
O	-.1922006665	-1.3991112863	-1.6029382163
O	.2704608402	1.2376820950	-1.3169154827
O	-.4266868200	1.5456956870	1.0442216356
H	-.0199247237	-.9741640553	-2.4592555246

$(gly)_2Re(OH)(H)(CH_3)^{+‡}$ metathesis transition state
enthalpy: -653.817783

Re	-.0014358716	-.0017482785	.0252276242
O	.0531976544	.1261821583	2.0539912431
H	1.3082483286	.0506923869	1.5322165814
C	2.2733692130	-.0261389219	.6654268094
C	-1.8067702552	-2.2702472867	-.5564805831
C	-.7013841284	-3.0085686625	.1845552385
H	-.5621901398	-4.0372615072	-.1562631016
H	-.8637553583	-2.9935671843	1.2634821520
H	-2.8027444180	-2.5141938005	-.1776235719
H	-1.7779361896	-2.4305094994	-1.6400336294
C	.2256128492	1.6034618368	-2.2648089973
H	-.7351945367	1.3701256648	-2.7391690625
H	.9261311068	1.9591533482	-3.0247860387
C	.0483588278	2.5999719384	-1.1250386936
H	-.7619145921	3.3141347282	-1.2943704005
H	.9664035404	3.1538401098	-.8987105256
O	-1.5757383919	-.8685996383	-.3104816391
O	.5180362155	-2.2386356718	-.0282920395
O	.7590837563	.3913578619	-1.6800153393
O	-.2856075481	1.8420562977	.0710461121
H	.9148567976	-2.4714403341	-.8839951687
H	-.2551259470	.9870006593	2.3864081778
H	2.5676018309	-.8594491851	.0336811674
H	2.6227909544	.9241748373	.2641508931
H	2.7845328324	-.2024224268	1.6293553150

$(gly)_2Re(OH_2)(CH_3)^+$
enthalpy: -653.869432

Re	-.0735346288	.0773182011	.0168592606
O	.0944265408	-1.2237567766	1.7589859640
H	.8617069200	-1.8060598263	1.8697371363
C	-2.2614197466	-1.4242585412	-1.3656569026
C	-1.1105626790	-2.3699675388	-1.6672136162
H	-1.2050958824	-2.8676240858	-2.6353175708
H	-.9959859644	-3.1226734972	-.8844979323
H	-3.1331593118	-1.9436663763	-.9571018001
H	-2.5709864737	-.8458135866	-2.2442555013
C	-.1882880195	2.7772501758	-.6387089382
H	-1.2758081196	2.8698704749	-.7458838597
H	.3017075674	3.5682442688	-1.2115135309
C	.2160771921	2.7703859648	.8337196339
H	-.3783076541	3.4506932595	1.4486269611
H	1.2792986303	3.0000701795	.9651377684
O	-1.7927493027	-.4900512047	-.3857157664
O	.1038824502	-1.5771820406	-1.6190148194
O	.2299755792	1.4990695653	-1.1867227260
O	-.0070243979	1.4165460492	1.3244539853
H	.2850077160	-1.1688945248	-2.4803437038
C	1.9973250012	-.3806351838	-.1759165822
H	2.3693261811	-.0889766178	-1.1589531458
H	2.5070293536	.2304871902	.5796706306
H	2.2076155909	-1.4382590711	.0016141761
H	-.0414530524	-.7365762607	2.5891223265

$(gly)_2Re(OH)(H)(CH_3)^+$ oxidative addition intermediate
enthalpy: -653.807432

Re	-.0486617196	-.0286596415	.0894535669
O	.1935195400	-.7248864115	1.8555032546
C	-2.3147944833	-1.2321300596	-1.4266374048
C	-1.1875955679	-2.0277316881	-2.0484429171
H	-1.3764582393	-2.2631528971	-3.0988992933
H	-.9690239655	-2.9366634567	-1.4796782466
H	-3.1526566394	-1.8618877231	-1.1166092816
H	-2.6695868753	-.4430513267	-2.0987857880
C	-.3804832998	2.6835793618	-.7681548177
H	-1.4740770193	2.7311654544	-.8426802353
H	.0603432315	3.4298525371	-1.4348037499
C	.0770886468	2.8149024700	.6744846010
H	-.5402955088	3.5008119426	1.2613290306
H	1.1269957424	3.1198484136	.7582921255
O	-1.7886636134	-.5874207426	-.2578440331
O	-.0612818654	-1.1089196221	-1.9621601683
O	.0446728916	1.3789056469	-1.1978642653
O	-.0328491004	1.4986430293	1.2605636971
H	.7693787448	-1.5539330903	-2.1897145021
C	2.0562923380	-.1768779695	-.4216658095
H	2.1937298285	.1480057406	-1.4514115590
H	2.4528820011	.5868501307	.2572355130
H	2.5116147157	-1.1389033293	-.1987562187
H	.0736320091	.0016168315	2.4992495479
H	.4231611237	-1.5988721818	.1342484971

Trans protonated

$(gly)_2Re(OH)(OH_2)^+$
enthalpy: -689.832839

Re	-0.8358705484	-0.0605429279	0.0677173297
O	-0.4012251628	-2.0070448276	-0.8933918401
H	-0.2011440467	-1.8434557075	-1.8313387692
O	0.7662254918	-0.5322727016	0.9761126724
H	1.2977423459	-1.2195667584	0.5361043834
H	-1.1866335877	-2.5787128089	-0.8263294849
C	-2.5500711952	0.3490862591	2.4780643404
C	-2.8845199529	-1.0328202531	1.9416112447
H	-3.9616377215	-1.1578908680	1.7928663847
H	-2.5273986818	-1.8311173385	2.6037856710
H	-2.6390897628	0.4374111135	3.5626019403
H	-3.1294146189	1.1346258584	1.9931430061
C	-1.2223704345	2.4487161407	-1.3004152246
H	-0.4004551166	3.0601011915	-0.9126527110
H	-2.0503620722	3.0920758638	-1.6104698277
C	-0.7552494023	1.4829805502	-2.3848760910
H	-0.0010135819	1.9124793831	-3.0501912318
H	-1.5939259798	1.0966342391	-2.9761215359
O	-1.1671661529	0.6247932038	2.0797481398
O	-2.2253234765	-1.2136474292	0.6701068500
O	-1.6913336786	1.5773751669	-0.2618780519
O	-0.1535989745	0.4128312453	-1.6468673747
H	-0.4991994132	0.2377270883	2.6742541080

$(gly)_2Re(OH)(H)(CH_3)^{+‡}$ metathesis transition state
enthalpy: -653.810040

Re	-0.0396055020	-0.1925684485	0.0493872069
O	0.2396770883	0.6179666156	2.2044004866
O	1.7923857161	-0.0511046341	0.2767613734
O	-0.3855392518	-1.9616675543	0.5434778844
O	-0.0612160945	-0.8315613359	-1.7047446903
O	-1.7250760574	0.5538472863	0.1959931008
C	0.6708814924	2.5950127197	-1.3376680808
H	0.3026728347	2.3120531557	-0.3275929469
H	-2.1695456953	0.8730504865	0.9953069390
C	1.5773279155	0.2182791129	2.6266437732
C	2.4949152305	0.4463845550	1.4273214932
H	3.4338890274	-0.1059217730	1.5112274016
H	2.7168786914	1.5068391359	1.2565919379
H	1.8708409631	0.7835406971	3.5148977537
H	1.4895630705	-0.8405865342	2.8718978756
C	-0.7349697707	-2.8432456741	-0.5741252975
H	-1.8274753005	-2.8509552255	-0.6355444793
H	-0.3799443497	-3.8387414403	-0.3036029932
C	-0.1040958617	-2.2853427183	-1.8346931593
H	-0.6738974869	-2.5048585274	-2.7411976274
H	0.9301248279	-2.6231116879	-1.9643617767
H	1.7602240032	2.5954827490	-1.3316317866
H	0.2966283391	1.9172360365	-2.1032676456
H	0.2723749351	3.5946430298	-1.5270263907
H	0.1477596946	1.5781701364	2.3147659158

$(gly)_2Re(OH_2)(CH_3)^+$
enthalpy: -653.857007

Re	-0.8472102652	-0.0789432520	0.0704274609
O	1.0302804412	-1.0444456594	0.6734819992
H	1.4212007833	-1.5696280896	-0.0463792425
C	-2.5698662290	0.6186091142	2.4564139725
C	-2.9226166151	-0.8111228161	2.0630876764
H	-3.9928687818	-0.9161657746	1.8557557096
H	-2.6547621563	-1.5380998208	2.8411201336
H	-2.7096087854	0.8327575655	3.5182321806
H	-3.0945890985	1.3559824942	1.8504493922
C	-1.7221174696	1.8956009898	-1.7728135635
H	-2.1672185682	2.8925916336	-1.8336778420
H	-2.1889772085	1.2332569433	-2.5104350645
C	-0.1947062652	1.9111750849	-1.9327972048
H	0.2669985621	2.7860321588	-1.4603094408
H	0.1288519355	1.8459882581	-2.9749736349
O	-1.1583034052	0.8022211790	2.1057212418
O	-2.1851855477	-1.1576787439	0.8902881802
O	-1.9229127370	1.3840086891	-0.4532807529
O	0.2403705057	0.7442980808	-1.2223908921
H	-0.5972331795	0.4404422101	2.8089590530
H	1.7344238535	-0.4843155726	1.0339750382
C	-0.8838476770	-1.8015382603	-1.1897311967
H	-1.8690501276	-1.9088599603	-1.6453685500
H	-0.1130852239	-1.7005175450	-1.9585518555
H	-0.6958502074	-2.6836613878	-0.5693156733

Cis cross protonated

$(gly)_2Re(OH)(OH_2)^{2+}$
enthalpy: -690.229361

Re	-0.7777898347	-0.2221363076	0.0842078016
O	-0.5833176861	-1.6533760613	-1.6588706343
H	0.0342454080	-1.4091587149	-2.3703117219
O	0.3179389447	-1.4533154809	0.8542247699
H	0.7674217850	-2.1754831297	0.3702154625
H	-1.2713759116	-2.2171834294	-2.0447564836
C	-1.9871902802	1.0308521482	2.3484502435
C	-2.6608209476	-0.3264920996	2.4143987603
H	-3.7261676684	-0.2752749707	2.6442021257
H	-2.1422012049	-1.0261218153	3.0738338796
H	-1.6989429198	1.3838224703	3.3422020951
H	-2.6222069477	1.7812718114	1.8653410625
C	-1.8874131796	2.1872380541	-1.6644839297
H	-2.3999351907	3.1387196326	-1.5044527179
H	-2.0629458635	1.8182869831	-2.6780251666
C	-0.4038007116	2.2660670387	-1.3303475378
H	-0.2063945156	2.7916460125	-0.3904512380
H	0.1944194429	2.6848568704	-2.1423807704
O	-0.7694869280	0.9062330744	1.5710952374
O	-2.5290955575	-0.8649173028	1.0099832547
O	-2.3927352373	1.1952375179	-0.6988754931
O	-0.0190272126	0.8725684066	-1.1695287703
H	-2.9078017988	-1.7569421723	0.9245052445
H	-3.2950305437	0.9083002212	-0.9119756233

$(gly)_2Re(OH)(H)(CH_3)^{2+‡}$ metathesis transition state
enthalpy: -654.208139

Re	-0.0020053533	-0.0085744130	0.0186304988
O	0.4210477634	-0.4117364048	1.8497878694
H	1.5920179541	0.0814818602	1.4633606544
C	2.1149532754	0.6561047682	0.4003002420
H	-0.0927473597	-1.0523768750	2.3839444082
C	-1.2321129580	-2.4297774901	-0.9724127780
C	0.1952981706	-2.7640025548	-1.3485893733
H	0.3214737512	-3.1150255821	-2.3740234755
H	0.6911412118	-3.4230448928	-0.6329339189
H	-1.7755760913	-3.3169468838	-0.6355468561
H	-1.7713086690	-1.9558286271	-1.7976720417
C	-1.2842686539	1.9209450931	-2.1615334820
H	-2.0443054542	1.9737846776	-2.9459679419
H	-0.4719939727	2.6247467834	-2.3632382708
C	-1.8902027272	2.1309008523	-0.7845620920
H	-2.8364401720	1.6065203573	-0.6305807056
H	-1.9797916109	3.1816308582	-0.5012901338
O	-1.1436416343	-1.5205493862	0.1448501544
O	0.8678133527	-1.4187178394	-1.2416446170
O	-0.7457799585	0.5609567935	-2.0933383129
O	-0.9165471387	1.5209107697	0.1265656561
H	1.8103168590	-1.4336501175	-1.4793090280
H	-0.2055351689	0.3659651052	-2.8753101340
H	2.6277797575	0.7385822659	1.4091620077
H	2.8741326118	0.1685311386	-0.2088131181
H	1.9937785905	1.7169839268	0.1580783940

$(gly)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -654.271498

Re	-0.8675490085	-0.0236852116	0.1117051511
O	0.7052300923	-1.2416085585	0.6543835262
H	1.6058522271	-0.8930314680	0.5011184084
C	-2.2929844355	0.4512279417	2.7207087903
C	-2.6723272427	-1.0112585724	2.5853565797
H	-3.6908540586	-1.1944825123	2.9379370518
H	-1.9699994330	-1.6689286612	3.1068867606
H	-1.8563528161	0.7073538439	3.6889444146
H	-3.1151459243	1.1370630088	2.4931208066
C	-1.2724365769	1.9963624279	-2.0867126831
H	-1.7916399795	2.9539494100	-2.1561766295
H	-1.3151551198	1.4558033668	-3.0347302534
C	0.1316769476	2.1128326448	-1.5205506396
H	0.2209103815	2.9190705065	-0.7867315052
H	0.8645739438	2.2690555929	-2.3164479249
O	-1.2726601090	0.7159896575	1.7132667377
O	-2.5947890674	-1.2400829781	1.1498244282
O	-2.0211448657	1.1540121655	-1.0873799629
O	0.4675626386	0.8682632568	-0.8432512252
H	-2.8269392352	-2.1529966759	0.9218291092
H	-2.8726471979	0.8459116521	-1.4464505432
H	0.7255580682	-2.2135647554	0.6989993272
C	-1.4112772070	-1.5551315319	-1.2649961261
H	-0.7868637567	-1.3856354000	-2.1506670959
H	-1.1807915451	-2.5502107882	-0.8734584602
H	-2.4640135446	-1.5152937781	-1.5548045486

$(gly)_2Re(OH)(H)(CH_3)^{2+}$ oxidative addition intermediate
enthalpy: -654.211846

Re	-0.0224882097	0.0658289249	-0.0415121281
O	-0.0213718187	-0.2262196325	1.7910357729
O	2.0676166465	0.0497006349	0.6450553053
O	0.4528262568	-2.1735993412	0.0410831752
O	-1.3138958225	-0.7471333908	-1.0533178830
O	-1.2045878040	1.4778866573	0.2082681744
C	1.1863645297	-0.1491027095	-1.9022483487
H	0.6728523809	1.3860611972	-0.6766410569
H	-1.1945732170	2.3397100118	-0.2495769832
C	1.0723741673	-0.6713256821	2.6184370940
C	2.2664700218	0.1091913211	2.1194547294
H	3.2260749900	-0.3625135379	2.3424940583
H	2.2514125333	1.1571573322	2.4275305079
H	0.8034388402	-0.4256539611	3.6502479598
H	1.1868571178	-1.7526524847	2.5034322034
C	-0.7830352123	-2.9220884180	-0.2293650910
H	-1.3418206465	-2.9186014470	0.7080553508
H	-0.5395017685	-3.9488490588	-0.5117832860
C	-1.5129688261	-2.1599227578	-1.3288989333
H	-2.5930791601	-2.3355943365	-1.3180825155
H	-1.1238913492	-2.3375110269	-2.3370753634
H	1.3350161035	-1.2116097188	-2.0864595694
H	0.5275261732	0.2898266407	-2.6549809239
H	2.1370887326	0.3807573982	-1.8895789734
H	1.2126115640	-2.5422790941	-0.4390872460
H	2.7349202784	0.5757950214	0.1726406792

Trans diprotonated

$(gly)_2Re(OH)(OH_2)^{2+}$
enthalpy: -690.233705

Re	-0.8685463755	-0.2074855427	0.0037963684
O	-0.8729948161	-1.4746669221	-1.6372220556
H	-0.2583598567	-1.2371938292	-2.3605672087
O	0.4706534576	-1.1285666641	0.8509931407
H	1.4354698980	-1.1983788111	0.9545421685
H	-1.3887222420	-2.2733310917	-1.8349644315
C	-2.1378738157	0.9453376618	2.5387015402
C	-2.6027197203	-0.4937014240	2.5939208190
H	-3.6598331080	-0.5535328663	2.8641528244
H	-2.0014120997	-1.1174948361	3.2613044543
H	-1.9758946335	1.3623820721	3.5345834800
H	-2.8266020575	1.5785192335	1.9790534956
C	-1.5725851557	2.1680083705	-1.4699316635
H	-1.9535578316	3.1213298746	-1.0952216073
H	-1.9946986588	1.9571230466	-2.4580155016
C	-0.0181361534	2.0736038910	-1.4114714882
H	0.3582306011	2.6102521184	-0.5334813428
H	0.4536104321	2.4547057581	-2.3212950552
O	-0.8667898802	1.0057286567	1.7857840340
O	-2.4339799491	-1.0163207765	1.2195578300
O	-2.0011604712	1.1001472007	-0.5962954083
O	0.2230937175	0.6775748410	-1.3015021827
H	-0.0894453197	0.9635906114	2.3680477896
H	-2.8568229699	-1.8833241366	1.1102565231

$(gly)_2Re(OH)(H)(CH_3)^{2+‡}$ metathesis transition state
enthalpy: -654.192929

Re	0.0235900821	-0.0052511429	0.0168359826
O	-0.1154750843	-0.1164392608	1.9922271952
H	1.1806520403	-0.1198241768	1.7405778846
C	2.1564820277	-0.0519986509	0.8836411670
C	-1.8874315712	-2.2025295251	-0.9506695342
C	-0.5926626095	-2.9803000305	-0.9017063153
H	-0.3833973947	-3.4795763039	-1.8499106349
H	-0.5470339161	-3.6853840004	-0.0688270483
H	-2.7469267376	-2.8366855314	-0.7219187499
H	-2.0284466802	-1.6658772029	-1.8901814867
C	-0.4302018339	1.7644721628	-2.2476398351
H	-1.3107833099	2.0059195936	-2.8472564575
H	0.4668930041	1.7542384213	-2.8739757837
C	-0.2760800524	2.6795385795	-1.0144013566
H	-1.2293847257	3.0626169958	-0.6356341449
H	0.4252940727	3.5023750191	-1.1735849283
O	-1.7438325382	-1.2054891225	0.1343085982
O	0.4545711239	-1.9552665643	-0.6615239582
O	-0.5926605719	0.4514701012	-1.6777525057
O	0.2699162257	1.8107638708	-0.0008718436
H	-2.5852375661	-0.7542505667	0.3274012660
H	1.3534959049	-2.2927389401	-0.8109545414
H	2.5545395990	0.7922262797	0.3209973916
H	2.4664844845	0.2154557397	1.9284064081
H	2.6546325205	-0.9921610216	0.6524004169
H	-0.7617741370	-0.6446015804	2.4920383547

$(gly)_2Re(OH_2)(CH_3)^{2+}$
enthalpy: -654.266986

Re	-0.8021569392	-0.0669630438	0.0513623205
O	1.0652030732	-0.9702419576	0.6832013408
H	1.6071247737	-1.4169183945	0.0071509390
C	-2.5513917930	0.5823361614	2.4806792234
C	-3.0798414258	-0.8080069207	2.1925608011
H	-4.1645504892	-0.8089073306	2.0612386094
H	-2.7845963132	-1.5517339608	2.9376174466
H	-2.6004822438	0.8478021113	3.5383119573
H	-3.0268767535	1.3505871068	1.8719048797
C	-1.7868455299	1.8911231418	-1.7469444678
H	-2.2955964295	2.8579151421	-1.7725205549
H	-2.1671602979	1.2275781567	-2.5294187567
C	-0.2488403904	2.0278533998	-1.8304488887
H	0.1371599756	2.8813038144	-1.2648154026
H	0.1324121373	2.0385254838	-2.8542291857
O	-1.1362684305	0.5793128285	2.0486495726
O	-2.4379606011	-1.1794225585	0.9170617075
O	-1.9721522126	1.3037824418	-0.4527922085
O	0.2108075113	0.8175320787	-1.1838811761
H	-0.5267899725	0.4188760571	2.7876579050
H	-2.8347840349	-1.9657822309	0.5073957005
C	-0.8582039865	-1.8380651809	-1.1087917150
H	-1.8394181470	-1.9901790672	-1.5679255091
H	-0.1008999676	-1.7479244029	-1.8927247205
H	-0.6123450349	-2.6889017413	-0.4610987031
H	1.6772574107	-0.6035115893	1.3431428054

$(gly)_2Re(OH)(H)(CH_3)^{2+}$ oxidative addition intermediate
enthalpy: -654.192929

Re	-0.5703566615	-0.2158868976	0.1536495666
O	1.1447337776	-0.0506231349	0.8737005783
H	-0.3404981428	-1.5927601932	1.0337611162
C	-0.6203120376	-1.9529938690	-1.1492817091
C	-2.5232435940	0.2984796091	2.6469103461
C	-2.8501203697	-1.1208056313	2.2579299822
H	-3.9192006166	-1.3320744993	2.3533025010
H	-2.2610084728	-1.8610830730	2.8072758678
H	-2.5084017803	0.4505301988	3.7277552971
H	-3.1794424948	1.0249144811	2.1664537787
C	-1.6906899589	1.8160210655	-1.5074677825
H	-1.4511397493	2.7150864780	-0.9279180346
H	-2.5834531059	1.9989774152	-2.1113939518
C	-0.4670899267	1.3090103392	-2.2831345534
H	0.2027425159	2.1052653451	-2.6244382110
H	-0.7132643659	0.6665323351	-3.1372068820
O	-1.1697858654	0.5595266969	2.1088956318
O	-2.5046083558	-1.1737901575	0.8313256043
O	-2.0024327153	0.7380518416	-0.5868443657
O	0.2802957437	0.5117201641	-1.3355779711
H	-0.4897165114	0.6441675371	2.7986139283
H	-2.7337232203	-2.0330622920	0.4390413288
H	-1.1430963680	-1.6604236186	-2.0606454714
H	0.4382762474	-2.1432745421	-1.3478989615
H	-1.0766557471	-2.8117701573	-0.6612059103
H	1.5921874812	-0.6630313151	1.4866704301

Species without water (2)

$(acac)(cat)Re(OH)^-$ *cis*
enthalpy: -803.060835

Re	-.8326092935	.0205083534	.1519954498
C	-1.7954502329	2.5173438114	-1.1449834546
H	-2.6432079670	3.1234780181	-1.4829267999
C	.6695376764	2.2917525093	-1.0498842091
C	-.5015121776	2.9883929496	-1.3711712365
H	1.6384348165	2.7418702860	-1.2922331781
H	-.3963027963	3.9577025750	-1.8514648418
O	-2.1267409350	1.3887683906	-.6003426546
O	.7306587100	1.1351265929	-.4731522403
O	.1171146112	-1.6199038695	-.2315573045
H	-.4462124053	-2.3776290504	-.0108395563
O	-1.1873625389	1.0176412664	1.8847813372
O	-2.3482513125	-1.1196136338	.9000130050
C	-2.3121721963	.6086443047	2.4968886964
C	-2.8586097068	1.2471206286	3.6120626358
C	-2.9273819111	-.5664530581	1.9795562955
C	-4.0093440829	.7254522952	4.2225027720
H	-2.3747165356	2.1444123227	3.9906287312
C	-4.0678785076	-1.0796377763	2.6012296431
C	-4.6090275130	-.4306706810	3.7216496981
H	-4.4336187585	1.2294235956	5.0891430266
H	-4.5234981825	-1.9800669086	2.1954463231
H	-5.5019956083	-.8324489337	4.1971840760

(acac)(cat)Re(OH)$^-$ *trans*
enthalpy: -803.060554

Re	-1.2506551460	.3817612453	-.1563167670
C	-.9999174944	3.2374833173	.6355837415
H	-1.4076955861	4.0882967648	1.1928088273
C	.7572045083	2.4442654391	-.9192867594
C	.1620549603	3.4232200778	-.1143924647
H	1.6601904692	2.6984858727	-1.4851113503
H	.6276135350	4.4048177228	-.0844296065
O	-1.7027095587	2.1520175859	.7250454591
O	.3398371394	1.2291646448	-1.0679168945
O	-1.5988366923	-.7460759238	-1.6877817081
H	-2.3732228278	-1.3021952826	-1.5107937310
O	-.3517975568	.0186540677	1.6286641770
O	-2.7705282155	-.5765742448	.8045930612
C	-1.2134564377	-.4209756642	2.5621287263
C	-2.5177051171	-.7702109519	2.1105196740
C	-.8758533845	-.5851492041	3.9072329692
C	-3.4467273545	-1.2879928619	3.0157297400
C	-1.8211792972	-1.0988921267	4.8078975196
H	.1250920511	-.3113945927	4.2324677887
C	-3.0971546377	-1.4493039606	4.3651753238
H	-4.4374101853	-1.5530853046	2.6534006386
H	-1.5541004490	-1.2212552486	5.8560965563
H	-3.8281942862	-1.8472931713	5.0666738897

(acac)(gly)Re(OH)$^-$ *cis*
enthalpy: -650.627612

Re	-.8828396543	.1395200535	.2583310261
C	-1.5474573130	2.1669331427	-1.7196590452
H	-2.3149871733	2.6161299457	-2.3566734256
C	.8237161150	2.2284411192	-.9761944334
C	-.2603671897	2.6831982733	-1.7456041183
H	1.7933095688	2.7305201719	-1.0710606045
H	-.0821527802	3.5231111461	-2.4148871877
O	-2.0005200486	1.1505664410	-.9998625136
O	.7745521023	1.2544296924	-.1227600727
O	-.2570704908	-1.5413838469	-.4040212005
H	-1.0569197937	-2.1045181416	-.3468709753
C	-2.2667230727	.1175048132	2.7459761753
C	-2.6338445473	-1.2116264219	2.0809792543
H	-3.6395857862	-1.5386137518	2.4167419394
H	-1.9146888000	-1.9785020306	2.4554127434
H	-2.0712977569	.0200778456	3.8269231251
H	-3.0809451246	.8465841681	2.6031680141
O	-2.5805895234	-1.0379439071	.7040357141
O	-1.0794145985	.6075038763	2.1092329000

(acac)(gly)Re(OH)$^-$ *trans*
enthalpy: -650.627612

Re	-1.2853582320	.4173729968	-.0977110864
C	-.8944267556	3.3425955385	.3111072782
H	-1.2411195309	4.2796009998	.7621189483
C	.7394704375	2.2982392055	-1.2437450763
C	.2230866686	3.3814595694	-.5265163230
H	1.6105868744	2.4547603368	-1.8898572365
H	.7151438035	4.3436132187	-.6525705615
O	-1.6300675970	2.3048479227	.5929993693
O	.2804582905	1.0777788069	-1.2184248616
O	-1.5504303775	-.8960599020	-1.5186541488
H	-.8138375510	-.8098651781	-2.1441483515
C	-1.2076901529	.1438872129	2.7151459183
C	-2.4092671299	-.7104656420	2.2972418921
H	-3.2532159014	-.5873153081	3.0016835996
H	-2.1166543828	-1.7798880884	2.3238505991
H	-.6927019102	-.2671847704	3.6014702349
H	-1.5565467368	1.1627482731	2.9607808607
O	-2.7895456345	-.3227230776	1.0012721656
O	-.3133289740	.1739698563	1.6233389766

(acac)(cat)Re(OH)$^+$ *cis*
enthalpy: -802.726780

Re	-.8607449999	.1058553598	.2404107525
C	-1.5276919242	2.1825154569	-1.8075790926
H	-2.3627448850	2.5946462128	-2.3727984333
C	.8283065054	2.1579905052	-1.2185531192
C	-.2514835539	2.6764710267	-1.9538966341
H	1.8400794669	2.5423927342	-1.3589560756
H	-.0787673238	3.4914132491	-2.6466812018
O	-1.8862312706	1.2070676972	-.9969592360
O	.7038985487	1.2309977979	-.3447025421
O	.1729786912	-1.4167471462	.4039104175
H	1.0497167679	-1.4987694677	-.0117689286
O	-1.1733347158	.8154676703	1.9767984555
O	-2.5172010905	-.8040120177	.6704767038
C	-2.3116681752	.3968105050	2.6148559526
C	-2.7188662571	.8336987894	3.8651386285
C	-3.0651865446	-.5212040604	1.8599181169
C	-3.9244147379	.3098856196	4.3465420233
H	-2.1298237160	1.5464275472	4.4313303742
C	-4.2769295563	-1.0339140966	2.3390095008
C	-4.6882891670	-.6076479141	3.5976326559
H	-4.2816318084	.6226536114	5.3224796300
H	-4.8481211427	-1.7394703220	1.7458472810
H	-5.6163482491	-.9858453613	4.0131333105

(acac)(cat)Re(OH)$^{+}$ *trans*
enthalpy: -802.724492

Re	-1.2233640551	.4139243423	-.0734105924
C	-1.3008689890	3.3852535572	.1147968842
H	-1.9161813599	4.2148202411	.4608982616
C	.6985867411	2.5469445259	-.9763051514
C	-.0937893223	3.6065100907	-.5134308620
H	1.6446461084	2.7205776451	-1.4899518232
H	.2472611316	4.6252799358	-.6530340354
O	-1.8349356968	2.2108231045	.3778516093
O	.3698344205	1.3159267620	-.8229573351
O	-1.5112306720	-.7408181697	-1.4755675150
H	-2.2011054667	-1.4253350374	-1.5335994288
O	-.4414330628	-.3105919503	1.5200893788
O	-2.8272395178	-.1893087659	.8746189454
C	-1.2906622263	-.7425261086	2.4855527207
C	-2.6510938557	-.6508791769	2.1110368838
C	-.8994337545	-1.2367079237	3.7254936381
C	-3.6743546838	-1.0332019502	2.9925065077
C	-1.9213794824	-1.6171805632	4.5934493946
H	.1482914094	-1.3047484523	3.9959625415
C	-3.2866159847	-1.5180921825	4.2321723057
H	-4.7140161717	-.9506501081	2.6955065651
H	-1.6644710018	-1.9967050699	5.5773337554
H	-4.0428174531	-1.8300366774	4.9449878583

(acac)(gly)Re(OH)$^{+}$*cis*
enthalpy: -650.310447

Re	-.8820394505	.0266220611	.2434026592
C	-1.4169881578	2.0088319374	-1.9000958604
H	-2.1017412659	2.2826697477	-2.7051441054
C	.6400295875	2.4659982251	-.6638153240
C	-.2752316217	2.7557376594	-1.6855963357
H	1.5265801871	3.0954999464	-.5443552112
H	-.0843894049	3.6056443683	-2.3299282206
O	-1.8303092883	.9650848432	-1.2304366409
O	.5481771733	1.5116796084	.1831459137
O	.1238315718	-1.3636842531	-.3362654468
H	.6030060136	-2.0971118894	.0846382132
C	-2.1690231229	.2318776403	2.7851828991
C	-2.8995630962	-.8511533193	2.0012483221
H	-3.9807607748	-.8317820165	2.1562164544
H	-2.5133904400	-1.8506581593	2.2317883143
H	-1.8425639978	-.0830508437	3.7792576597
H	-2.7449822684	1.1587086061	2.8638692545
O	-2.6356448293	-.5532990091	.6131479238
O	-.9689159694	.5427281069	2.0186273772

(acac)(gly)Re(OH)$^{+}$ *trans*

enthalpy: -650.310445

Re	-1.3183215507	.4647415254	-.0214979196
C	-.9976851033	3.3949279629	-.3687987501
H	-1.5147458185	4.3554555776	-.3252575660
C	1.0498317525	2.1452594001	-.8332024308
C	.3248680699	3.3433981352	-.7628413505
H	2.0950756766	2.1697345123	-1.1547747667
H	.8240448085	4.2693235032	-1.0225147148
O	-1.7656571350	2.4012092468	-.0055998508
O	.6090557675	.9790539080	-.5472845177
O	-1.8144033595	-.3664421799	-1.5526274993
H	-1.8661253671	-1.2882007835	-1.8565073855
C	-1.1769818062	-.7186802648	2.5744430128
C	-2.6518460861	-.6330922446	2.2028132798
H	-3.2884558793	-.3647338515	3.0490270707
H	-3.0126700685	-1.5652946791	1.7531908507
H	-.8553343046	-1.7139742652	2.8903910249
H	-.8875010346	.0183570617	3.3293366465
O	-2.7321290506	.4240871948	1.2225490733
O	-.4373363168	-.3946519986	1.3606033248