

Iron versus Ruthenium – A Comparison of the Stereoselectivity in the Catalytic Olefin Epoxidation

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Supplementary Material

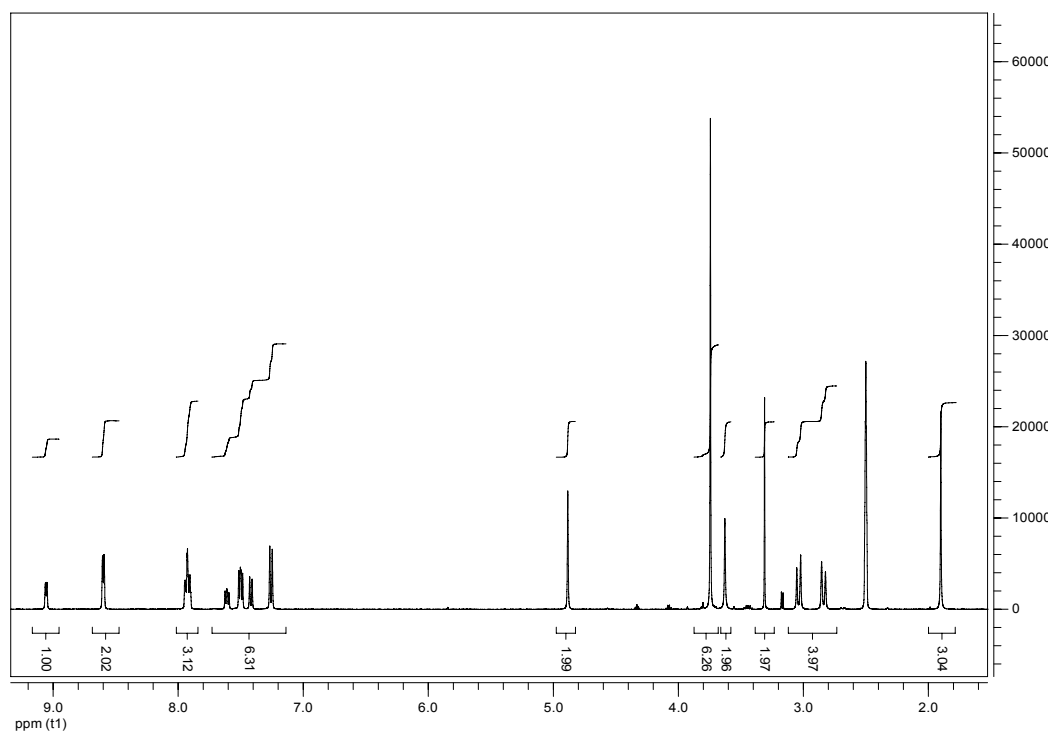


Figure S1 : $^1\text{H-NMR}$ spectrum of $[(\text{L}^1)\text{Ru}(\text{OH}_2)](\text{ClO}_4)_2$ at 400 MHz in DMSO-d_6

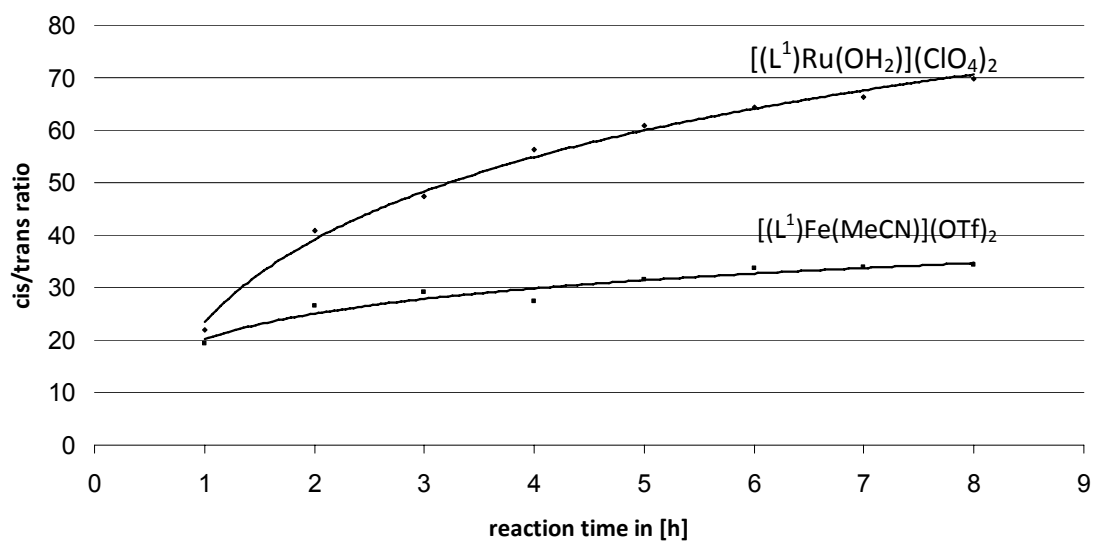


Figure S2. *cis/trans* ratio of the epoxide products vs time for the catalytic reactions with $[(L^1)Ru(OH_2)](ClO_4)_2$ and $[(L^1)Fe(MeCN)](OTf)_2$ and with *cis*- β -methylstyrene as substrate.

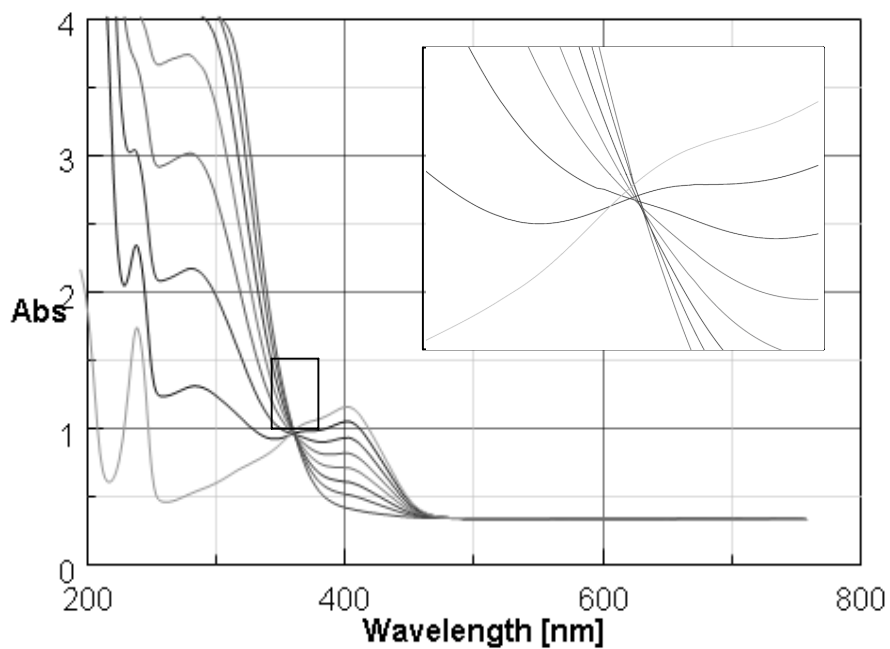
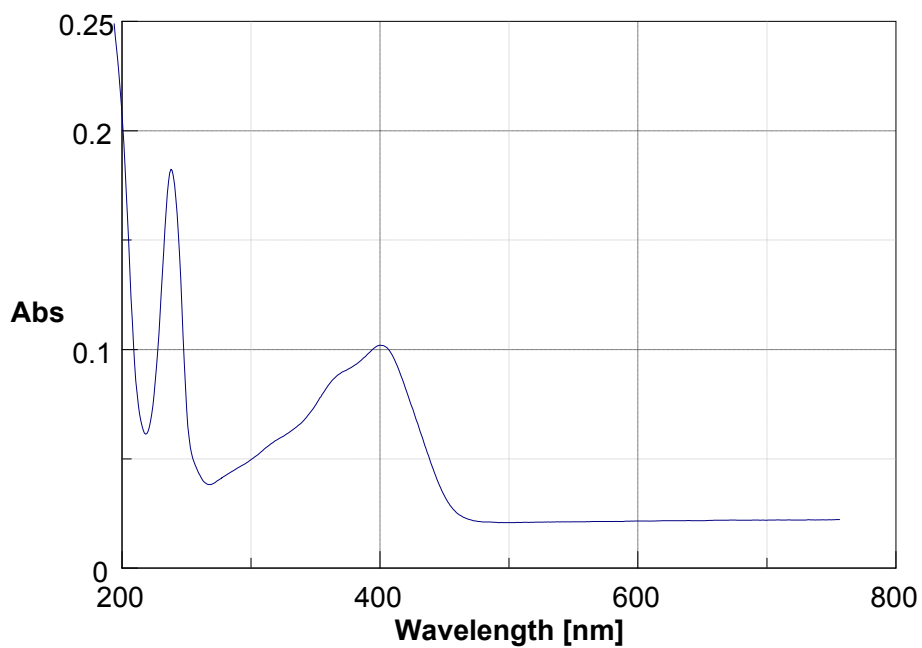


Figure S3. UV/Vis spectra of $[(L^1)Ru(OH_2)](ClO_4)_2$ (top), and after the addition of Ce^{4+} (0.25, 0.5, 0.75, 1.0, 1.25, 1.5, 1.75, 2 equivalents) to a 10^{-4} M aqueous solution of the aqua complex (bottom); the area of the pseudo-isosbestic point is magnified (inset) to show that the oxidation of $[(L^1)Ru(OH_2)]^{2+}$ to $[(L^1)Ru(OH)]^{2+}$ and to $[(L^1)Ru=O]^{2+}$ have nearly coinciding isosbestic points. The end spectrum is rather featureless because $Ru^{IV}=O$ has only low intensity transitions.¹⁻⁵ According to electrochemical measurements the species generated by addition of two equivalents of Ce^{4+} is assumed to be $[(L^1)Ru^{IV}=O]^{2+}$; addition of more oxidant had no effect on the spectrum. Therefore, the existence of a $[(L^1)Ru^V=O]^{3+}$ under these conditions species can be excluded.

Computed coordinates (B3LYP/LACVP) of the corresponding intermediates in Figure 5.

¹cis-alkene (S=1)

Ru	1.0536180713	1.7063257689	-1.1736466572
N	1.4600601531	2.9097213579	0.5334319367
C	1.8252913359	2.4820372584	1.7653640685
C	1.7957681960	3.3354551225	2.8694904844
C	1.3631580329	4.6547204207	2.6981391743
C	0.9750789020	5.0904438238	1.4223017360
C	1.0314458024	4.1987610237	0.3531515302
C	0.7154306062	4.5892962062	-1.0782374546
N	-0.0509970945	3.4290429977	-1.7358155862
C	-1.4765746719	3.4253887160	-1.2225126745
C	-0.0718001742	3.3775866511	-3.2719443524
N	2.8094415432	2.6189259583	-2.3294509705
C	3.1840214209	3.9540121882	-1.7229269244
C	2.0286501381	4.9750710769	-1.8382054423

C	1.6677726088	5.1668660866	-3.3014072948
C	1.2727898781	3.8403018887	-3.9268117193
C	2.4436692541	2.8447342390	-3.7813029292
C	-0.4032071723	1.9570465043	-3.6937741225
C	-1.2187709321	1.6521768924	-4.7814554823
C	-1.4038675219	0.3094672370	-5.1439745334
C	-0.7679598844	-0.6940260351	-4.4054622712
C	0.0323800264	-0.3338037721	-3.3200292915
N	0.2169943750	0.9639743638	-2.9802820280
C	3.9664514752	1.6399978526	-2.2346438179
C	3.7377334249	0.4385368654	-1.3358987496
C	4.7830542548	-0.4584616005	-1.0878572102
C	4.5525438143	-1.5914831618	-0.3028756869
C	3.2721223364	-1.8078426960	0.2252250088
C	2.2677759589	-0.8831076938	-0.0411880520
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H	2.0943176078	2.9660342957	3.8426644706
H	1.3185596055	5.3333885685	3.5420377544
H	0.6264968193	6.1053202781	1.2679209103
H	0.0666698454	5.4733709223	-1.0887952461
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H	-1.9968563033	2.5509098132	-1.6110476517
H	-0.8531447973	4.0619742738	-3.6233733866

H	4.0592052490	4.3568686251	-2.2530413661
H	3.4691083031	3.7933787628	-0.6824690299
H	2.3722624867	5.9298108601	-1.4270730009
O	1.6652659682	6.2482255128	-3.8880678148
H	1.0797714450	3.9915602482	-4.9937783815
H	3.3169237887	3.2486303698	-4.3136881425
H	2.1974280227	1.8805721383	-4.2273638090
H	-1.7102389703	2.4454459371	-5.3333064123
H	-2.0408657393	0.0553148324	-5.9832503420
H	-0.8970044647	-1.7399334891	-4.6545939428
H	0.5232229876	-1.0718978638	-2.7006304247
H	4.1891533902	1.2773553879	-3.2451367049
H	4.8614740012	2.1776659174	-1.9002517433
H	5.7646690648	-0.2712370586	-1.5090429300
H	5.3556194050	-2.2925662188	-0.1072312588
H	3.0554805552	-2.6757379813	0.8357287952
H	1.2607030668	-0.9860239826	0.3429676128
O	-0.2342900019	0.8502682136	-0.2409021893

ts2a

Ru	1.1332551218	1.5985323605	-1.1764207730
N	1.3211907691	2.8423174827	0.5238234550
C	1.7170175459	2.4986597218	1.7747350965
C	1.6063092873	3.3834344632	2.8494247356
C	1.0585249299	4.6523523621	2.6323643072

C	0.6531496911	5.0090190298	1.3376122348
C	0.8020786642	4.0919103380	0.2982319197
C	0.5252867279	4.4373527068	-1.1544415603
N	-0.0879488738	3.2130805725	-1.8401111914
C	-1.5403433785	3.1117568862	-1.4453384649
C	0.0035158343	3.1261099715	-3.3721309962
N	2.8585376118	2.6535051292	-2.2102584341
C	3.0736139335	4.0292556625	-1.6227359589
C	1.8424546346	4.9363062153	-1.8379957279
C	1.5627245336	5.0658716728	-3.3251591953
C	1.3414168205	3.6974444057	-3.9440275204
C	2.5789965556	2.8143634234	-3.6895419965
C	-0.1756338651	1.6729375613	-3.7800162680
C	-0.8846322892	1.2842419391	-4.9151613642
C	-0.9358697616	-0.0749722135	-5.2578808577
C	-0.2823493947	-1.0087146623	-4.4475536445
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N	0.4670220299	0.7497954253	-2.9974045843
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H	-1.9455945151	2.1625521160	-1.7909786954
H	-0.8077090627	3.7305837735	-3.7962819116
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H	-1.1795295982	-0.4666278525	2.9600220075
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cis-rad

Ru	1.1144892918	1.6583753095	-1.0534887757
N	1.3167256357	2.9880175236	0.5772241305

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C	0.8173871298	4.2343123250	0.2906883894
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C	-3.1901136748	-0.3876402320	-0.0490403364
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C	-5.3153084233	-1.3533229571	-0.8260991433
C	-4.6317582524	-2.4618549019	-1.3560496238
C	-3.2326500173	-2.5337418922	-1.2406256350
C	-2.5183878551	-1.5208293027	-0.6081703228
H	-5.1519112469	0.5069455686	0.2339702605
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H	-5.1815756468	-3.2590412350	-1.8439100428
H	-2.7062977527	-3.3949424156	-1.6409774397
H	-1.4402754372	-1.5822449799	-0.5318681195
H	-1.2926353273	-0.0766010211	3.0198997964
H	-0.8824047677	-1.2757595213	1.7866974115
H	0.3654899870	-0.1530975482	2.3910488647

ts3a

Ru	1.0366676361	1.8407054999	-1.2656731968
N	1.2849986844	2.9519015093	0.5252360573
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C	1.5570019029	3.3227088894	2.8899241321
C	1.2435324250	4.6763734503	2.7268304585
C	0.9649341480	5.1594598570	1.4409254715
C	1.0032963127	4.2858996650	0.3533256331
C	0.8606419548	4.7848393773	-1.0785562103
N	0.1896940138	3.6981873275	-1.9191395400
C	-1.2971662502	3.7260054131	-1.6551882527
C	0.4277357655	3.7093045426	-3.4335037476
N	3.1754822491	2.9592611605	-2.0464269412
C	3.4128056455	4.2714185341	-1.3718805469
C	2.2512399474	5.2522526768	-1.6321836830
C	2.1363541152	5.4666833460	-3.1297143092
C	1.8746940559	4.1491475653	-3.8381828675
C	3.0099456022	3.1448276914	-3.5190114397
C	0.0974802988	2.3373871682	-3.9935381270
C	-0.4692121877	2.1653779095	-5.2563631697
C	-0.6752854678	0.8684629270	-5.7462780038
C	-0.3195687937	-0.2233171180	-4.9476284241
C	0.2294692293	0.0078728104	-3.6850968609
N	0.4471730660	1.2619038838	-3.2188918606
C	4.2441359044	1.9803785435	-1.6935841916

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C	4.7123754743	-0.5011899530	-1.7152281795
C	4.3359581256	-1.8173271435	-1.4346471067
C	3.0311234442	-2.0681906143	-0.9917262355
C	2.1455980247	-1.0015552398	-0.8651770118
N	2.5189912779	0.2810220603	-1.1375433829
H	1.7882926966	1.4336462459	1.8458229370
H	1.7918459860	2.9161020363	3.8660589142
H	1.2197159082	5.3451499942	3.5792823928
H	0.7272951886	6.2062164327	1.2863378167
H	0.2107391425	5.6697267032	-1.0911968122
H	-1.7292615046	4.6582447343	-2.0398002216
H	-1.4722166541	3.6623373732	-0.5809151789
H	-1.7678261724	2.8728207848	-2.1421176471
H	-0.2518464906	4.4505027972	-3.8759941826
H	4.3463401627	4.7317995887	-1.7351551070
H	3.5292534539	4.0938607671	-0.3010452165
H	2.4860699453	6.2077773931	-1.1528383304
O	2.2204075906	6.5604193323	-3.6906195631
H	1.8636483583	4.3240801143	-4.9187280801
H	3.9425500531	3.5317986593	-3.9626554154
H	2.8070096477	2.1721296938	-3.9730314257
H	-0.7468640882	3.0296261541	-5.8495472750
H	-1.1101935048	0.7180355059	-6.7275804364
H	-0.4685622852	-1.2395997969	-5.2912306636

H	0.4968956165	-0.8036653782	-3.0238174621
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H	5.7168910206	-0.2765886290	-2.0560265365
H	5.0445107302	-2.6280466602	-1.5589574435
H	2.7012440899	-3.0731476135	-0.7583258716
H	1.1157479848	-1.1329502415	-0.5579674993
O	-0.6730357694	0.5997165485	-0.5792417493
C	-1.6175589627	0.4952343936	0.5758815244
C	-2.2707546743	-0.3652238048	-0.4380936255
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C	-2.9436082753	-2.2668143012	-1.8044602440
C	-3.0369365166	-3.6287742182	-2.0788546508
C	-2.4452462103	-4.5571208961	-1.2102387347
C	-1.7663352594	-4.1119465222	-0.0652300555
C	-1.6722752878	-2.7502710446	0.2169298491
H	-3.4159154780	-1.5500018896	-2.4699863809
H	-3.5758888640	-3.9706529939	-2.9553344390
H	-2.5229703186	-5.6190908754	-1.4156431037
H	-1.3262341207	-4.8328638239	0.6150129277
H	-1.1689881297	-2.4383883572	1.1206960193
H	-1.8272341205	-0.4616634666	2.5023283200

H -0.2470166715 -0.7333771317 1.7353747884

H -0.6327467220 0.8350244490 2.4575006230

cis-epoxide

Ru 1.1816383266 1.9491121608 -1.5774375510

N 1.1242847099 2.7338281642 0.4145315877

C 1.1284382312 2.0457861900 1.5831125105

C 1.0312513771 2.6982676924 2.8132517543

C 0.9134777053 4.0929736403 2.8343383714

C 0.8904723245 4.8005940802 1.6232034541

C 0.9976399821 4.0990407653 0.4230269743

C 1.0199651539 4.7847489022 -0.9356746870

N 0.3059324041 3.8698716337 -1.9288764473

C -1.1787172903 3.9452969968 -1.6801166150

C 0.5743781430 4.0970370020 -3.4142836787

N 3.2663642066 2.9103220291 -2.1437267374

C 3.5497269998 4.0717522057 -1.2406004230

C 2.4762418221 5.1764942506 -1.3689390916

C 2.4210406694 5.6348482083 -2.8156268252

C 2.0655812644 4.4732908156 -3.7296261277

C 3.1258898488 3.3531360444 -3.5692290271

C 0.1379332910 2.8494289647 -4.1666602235

C -0.4196972090 2.8920244192 -5.4441891519

C -0.7443119987 1.6906254785 -6.0905431258

C -0.5076133075 0.4742263367 -5.4385894456

C	0.0462163997	0.4903011053	-4.1583404343
N	0.3677289661	1.6533576413	-3.5369593738
C	4.2675905245	1.8064843569	-1.9660377567
C	3.6944377497	0.3979225729	-1.8543503398
C	4.5389671027	-0.7032353427	-2.0387871788
C	4.0578471283	-1.9960343376	-1.8126318553
C	2.7295162068	-2.1651449298	-1.4000976696
C	1.9235676251	-1.0408415725	-1.2491804303
N	2.3916763233	0.2181898864	-1.4801871385
H	1.1953642645	0.9700162582	1.5007214071
H	1.0435041849	2.1245841770	3.7317382548
H	0.8303187303	4.6238807111	3.7757731602
H	0.7819124578	5.8794079957	1.6175024261
H	0.4590031065	5.7271114614	-0.8708709208
H	-1.5538444087	4.9542605327	-1.8941645532
H	-1.3812975003	3.6943646236	-0.6393367219
H	-1.6886456683	3.2251813283	-2.3195539137
H	-0.0310964835	4.9495552029	-3.7525907753
H	4.5293070990	4.5142929675	-1.4823486317
H	3.5988102119	3.7028387057	-0.2132475868
H	2.7802440706	6.0206922962	-0.7416728343
O	2.6068217587	6.7925243556	-3.1925665895
H	2.0938397138	4.8193191687	-4.7679498539
H	4.0887006298	3.7427300649	-3.9375147130
H	2.8699366854	2.4831677160	-4.1799555572

H	-0.6039657945	3.8449682556	-5.9274235736
H	-1.1796378518	1.7071324725	-7.0831496705
H	-0.7494864993	-0.4696250352	-5.9114588809
H	0.2460140177	-0.4190153183	-3.6074164418
H	5.0087991422	1.8347118674	-2.7756830435
H	4.8208635021	2.0100518494	-1.0404817866
H	5.5665150864	-0.5462485864	-2.3478769521
H	4.7076850427	-2.8524206980	-1.9512592769
H	2.3207519866	-3.1481198483	-1.2006793842
H	0.8919334664	-1.1066090523	-0.9324696306
O	-0.9184542835	0.3038901612	-0.3775394579
C	-2.3470308280	0.4273354711	0.1351097556
C	-2.0004086264	-0.6846037079	-0.7948769508
C	-2.5832597108	0.2677365478	1.6083662344
C	-1.8237369220	-2.1134474142	-0.4174439309
H	-2.3100644167	-0.5359757671	-1.8279448429
H	-2.8537140603	1.2773206104	-0.3202057951
C	-2.5774382070	-3.0782670535	-1.1118985462
C	-2.4704255452	-4.4332240889	-0.7851285103
C	-1.5953819996	-4.8441234013	0.2283247005
C	-0.8285429248	-3.8932645957	0.9131802251
C	-0.9416829752	-2.5352234878	0.5952058534
H	-3.2573815323	-2.7676085828	-1.9006396835
H	-3.0655420575	-5.1654556951	-1.3197715538
H	-1.5125936739	-5.8953300493	0.4816199043

H -0.1506658309 -4.2081936542 1.6997387165
H -0.3429105874 -1.8024939918 1.1251870447
H -3.6624602310 0.2242460468 1.7974660436
H -2.1375194393 -0.6454404769 2.0051995583
H -2.1870819214 1.1262911110 2.1621979322

ts4

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N 1.4670845796 3.1163579405 0.6135460589
C 1.8777715576 2.7646671079 1.8572325983
C 1.9431564847 3.6891522407 2.9021426080
C 1.5635849676 5.0133121083 2.6623158978
C 1.1697790289 5.3857046101 1.3684057773
C 1.1460033604 4.4266551325 0.3570755795
C 0.9485407978 4.7899122575 -1.1046607327
N 0.1797669701 3.6618422410 -1.7942410454
C -1.2855632190 3.8400701898 -1.4744951714
C 0.3362191545 3.5253616007 -3.3206400730
N 3.0124108671 2.6644233359 -1.9620807899
C 3.4154462514 4.0276479109 -1.4422594438
C 2.3434956876 5.0889319919 -1.7506132181
C 2.1729245397 5.1871807588 -3.2549772428
C 1.7823530512 3.8371646360 -3.8293826010
C 2.8473686236 2.7777532713 -3.4621425536
C -0.0555500920 2.1205057864 -3.7363071246

C	-0.7352972978	1.8426719246	-4.9212068104
C	-0.9601265930	0.5062703703	-5.2830337628
C	-0.5103996427	-0.5140947497	-4.4389625222
C	0.1530492804	-0.1765538361	-3.2575819440
N	0.3918340516	1.1133906961	-2.9235499918
C	4.1061982931	1.6745523195	-1.6050339953
C	3.6138213166	0.2967540519	-1.2351790653
C	4.4629704003	-0.8121376022	-1.2842116104
C	4.0127452185	-2.0473107044	-0.8052071357
C	2.7129924928	-2.1447049808	-0.2934668512
C	1.8983612431	-1.0141972697	-0.2907801318
N	2.3444889922	0.1860643357	-0.7520403381
H	2.1602564903	1.7302428643	1.9939688391
H	2.2799257718	3.3707340257	3.8810420005
H	1.5856648985	5.7474617347	3.4592777077
H	0.8972575323	6.4120427976	1.1490132592
H	0.3559027190	5.7088321617	-1.1859976594
H	-1.6523126961	4.7702732159	-1.9253673328
H	-1.4111759702	3.8915531328	-0.3932983037
H	-1.8595941816	2.9988010701	-1.8542546818
H	-0.3330915297	4.2530750176	-3.7955447546
H	4.3629352430	4.3247568527	-1.9147064092
H	3.5908735799	3.9501204064	-0.3696464037
H	2.6853802197	6.0541832840	-1.3640240251
O	2.2998567178	6.2210032166	-3.9108036345

H	1.7330670574	3.9124273986	-4.9204384523
H	3.8080588610	3.0782473905	-3.9047082858
H	2.5880888798	1.7959358232	-3.8592223402
H	-1.0860526501	2.6528797642	-5.5506660324
H	-1.4852708637	0.2708069897	-6.2015047081
H	-0.6808602452	-1.5557513170	-4.6808229166
H	0.4888087165	-0.9281771179	-2.5583868725
H	4.8331951603	1.6182237601	-2.4239223246
H	4.6407818987	2.0852826639	-0.7401154877
H	5.4649656343	-0.7076662259	-1.6848712071
H	4.6625685511	-2.9142661599	-0.8334137384
H	2.3296035590	-3.0833361092	0.0875872245
H	0.8718977898	-1.0238265501	0.0498777295
O	-0.4062167468	0.8378699341	-0.2904476084
C	-1.3703135674	1.0585704065	0.8196559079
C	-2.6695437519	0.3283331857	0.5963433111
C	-0.7545657902	0.5620518775	2.1408529294
C	-3.5383820804	0.3019713533	-0.5276827399
H	-3.0550004366	-0.1478652471	1.4955309250
H	-1.5372455992	2.1467256994	0.8844084171
C	-4.8689614868	-0.1913131815	-0.3385069150
C	-5.7902644447	-0.2076612025	-1.3784319581
C	-5.4267326875	0.2535064640	-2.6550008573
C	-4.1168062689	0.7083809431	-2.8779911281
C	-3.1860129883	0.7293968616	-1.8422821464

H	-5.1606885109	-0.5414722716	0.6468553290
H	-6.7955335594	-0.5740901185	-1.2016248807
H	-6.1489330474	0.2462908495	-3.4638128975
H	-3.8293078542	1.0388156834	-3.8715510267
H	-2.1621299294	1.0215135875	-2.0318457155
H	-1.4552324117	0.7480880415	2.9614245077
H	-0.5727984256	-0.5162328776	2.0927709844
H	0.1781932014	1.0695868091	2.3766865795

trans-rad

Ru	0.6502221227	1.9438641568	-1.4509275822
N	1.3444014103	2.5397969249	0.4712873003
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C	1.9129181554	2.3473147357	2.8012179314
C	1.9503356262	3.7400116070	2.9210459678
C	1.7026112357	4.5277310199	1.7873872283
C	1.4195174184	3.9060989595	0.5721184755
C	1.3506595221	4.6694740542	-0.7379882111
N	0.2871270603	4.0320707397	-1.6370994748
C	-1.0775032333	4.4606526165	-1.1503080264
C	0.3748685300	4.2968345356	-3.1470779654
N	2.6672005497	2.3594999185	-2.3581954988
C	3.4629797417	3.3096573152	-1.4896333003
C	2.7753115640	4.6901344416	-1.3882759160
C	2.6319265875	5.2900448572	-2.7761647734

C	1.8442085230	4.3559898697	-3.6760142604
C	2.5475277244	2.9870591720	-3.7333962855
C	-0.4040590762	3.2076409850	-3.8642426905
C	-1.1783605878	3.4454890316	-4.9977711528
C	-1.8091099947	2.3651522639	-5.6338592232
C	-1.6599959481	1.0797323961	-5.1051785848
C	-0.8829563372	0.9023771959	-3.9573991312
N	-0.2505020523	1.9408704150	-3.3656963139
C	3.3878258233	1.0287585836	-2.4935145044
C	2.7637619134	-0.1190259188	-1.7353722362
C	3.4675953026	-1.3130714577	-1.5509822121
C	2.8247637250	-2.4116770956	-0.9729012029
C	1.4820196360	-2.2891435842	-0.5938824924
C	0.8325511346	-1.0712865267	-0.7792502369
N	1.4676600422	0.0003227769	-1.3329420863
H	1.5332694783	0.7094641220	1.4321136420
H	2.1145971625	1.7066766234	3.6509155628
H	2.1744658196	4.2072019539	3.8729099924
H	1.7423219753	5.6096614661	1.8478642959
H	1.0665728591	5.7124628146	-0.5520700667
H	-1.2031516218	5.5392478910	-1.3021048386
H	-1.1701063946	4.2263569427	-0.0907802168
H	-1.8403835752	3.9107700439	-1.6984114789
H	-0.0797749929	5.2741676718	-3.3502444719
H	4.4597794118	3.4475172074	-1.9330666281

H	3.5950116341	2.8548139333	-0.5078360187
H	3.4042862660	5.3454608966	-0.7774476313
O	3.0590278029	6.3954341874	-3.1094438679
H	1.8126770699	4.7728887865	-4.6877658728
H	3.5555470623	3.1199827513	-4.1520280099
H	2.0039234813	2.2960637769	-4.3775100030
H	-1.2952119626	4.4545541337	-5.3771129593
H	-2.4134422777	2.5318024605	-6.5180342719
H	-2.1463250887	0.2260946523	-5.5602038831
H	-0.7676593426	-0.0640597946	-3.4880324744
H	3.3919626251	0.7639630442	-3.5576958907
H	4.4372031522	1.1526249646	-2.2020860898
H	4.5017170419	-1.3839584255	-1.8694346018
H	3.3576870054	-3.3445408705	-0.8300786161
H	0.9446241284	-3.1231020240	-0.1595249527
H	-0.2041444869	-0.9202730668	-0.5101747883
O	-1.1862223758	1.4382734077	-0.9572690387
C	-2.1542092567	1.1272191447	0.1468373292
C	-2.6283259573	-0.2857680075	-0.0149595547
C	-1.6525572887	1.4118598910	1.5592943776
H	-2.3317770516	-0.9897882054	0.7613240651
C	-3.4848768697	-0.7570451850	-1.0448862775
H	-2.9762992970	1.8204824833	-0.0879242358
H	-2.4861715828	1.3100397533	2.2630469461
H	-0.8783960372	0.7001515042	1.8623857737

H	-1.2588022835	2.4272883071	1.6543582520
C	-3.9001529320	-2.1261255863	-1.0427402032
C	-4.7578209721	-2.6197790596	-2.0182424393
C	-5.2388724105	-1.7732305281	-3.0327346829
C	-4.8448840890	-0.4234309728	-3.0589823500
C	-3.9818216465	0.0809214179	-2.0916685709
H	-3.5467917100	-2.7800479797	-0.2505991002
H	-5.0659349773	-3.6593257708	-1.9912076341
H	-5.9188812501	-2.1573209174	-3.7851415281
H	-5.2306646420	0.2331783054	-3.8325294792
H	-3.6875991803	1.1240017464	-2.1241771379

ts3b

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C	1.0259055791	2.2370975619	1.6431738726
C	0.9030981729	3.0554945496	2.7665873583
C	0.6589110004	4.4213521789	2.5876495096
C	0.5640458632	4.9285944220	1.2848253729
C	0.7114503003	4.0676613744	0.1960457685
C	0.7527494035	4.5918380090	-1.2329206932
N	0.1511154247	3.5403642358	-2.1637042967
C	-1.3545618443	3.6120770579	-2.0676560910
C	0.5591685033	3.5692738893	-3.6392065079

N	3.1085257084	2.7174684533	-1.9630115323
C	3.3048954786	4.0112356398	-1.2428775308
C	2.2085036620	5.0289614296	-1.6155478813
C	2.2708721131	5.2685099484	-3.1124766271
C	2.0551848659	3.9697631650	-3.8694406485
C	3.1171618098	2.9268690420	-3.4410305184
C	0.2518450797	2.2197398994	-4.2612299254
C	-0.1664136613	2.0891897416	-5.5852861531
C	-0.3571221357	0.8093770195	-6.1235036923
C	-0.1345517176	-0.3075971334	-5.3115852976
C	0.2691330947	-0.1169542445	-3.9890564370
N	0.4710380957	1.1200623797	-3.4726857848
C	4.1008047808	1.7037564500	-1.5055120978
C	3.6013756486	0.2740848034	-1.4601635732
C	4.5092756138	-0.7876290540	-1.5580263401
C	4.0716822516	-2.1006609787	-1.3670222390
C	2.7182900420	-2.3282880116	-1.0868020414
C	1.8515893293	-1.2409140233	-1.0280708365
N	2.2830182101	0.0392216236	-1.2104537805
H	1.2109658246	1.1750540838	1.7302006777
H	0.9948491769	2.6275358582	3.7573481584
H	0.5474132804	5.0802305135	3.4408947798
H	0.3821273483	5.9846998013	1.1181091692
H	0.1326782439	5.4950884443	-1.3029567475
H	-1.7102041678	4.5600448084	-2.4906185749

H	-1.6491722568	3.5481883173	-1.0204550457
H	-1.7980380875	2.7750917181	-2.6042784867
H	-0.0427990236	4.3396393857	-4.1406634776
H	4.2865508929	4.4485182486	-1.4893283218
H	3.2932909051	3.8145109123	-0.1690448260
H	2.4122004027	5.9703077657	-1.0956490011
O	2.4474474001	6.3677523739	-3.6405087332
H	2.1724675180	4.1606745595	-4.9408923352
H	4.1051437709	3.2901420647	-3.7704914902
H	2.9380413606	1.9669317745	-3.9311579335
H	-0.3416123177	2.9731958844	-6.1885030501
H	-0.6770988135	0.6911157052	-7.1522194700
H	-0.2737875921	-1.3120634407	-5.6922873144
H	0.4368062128	-0.9490871226	-3.3205593922
H	5.0167848963	1.7538118953	-2.1120562240
H	4.3936738210	1.9770543428	-0.4838551017
H	5.5516785543	-0.5805512824	-1.7727870446
H	4.7699127513	-2.9267833117	-1.4351247438
H	2.3398374461	-3.3301603853	-0.9245013593
H	0.7919481049	-1.3532532503	-0.8413519709
O	-0.9951754607	0.4704565561	-0.9969454122
C	-1.8774182042	0.1885707004	0.1754731289
C	-2.6914202545	-0.3107007190	-0.9463335013
C	-1.3515687563	-0.8071754658	1.1861739332
H	-2.4737701938	-1.3268141939	-1.2597410384

C	-3.7865383595	0.3583615338	-1.6016177460
H	-2.2226929161	1.1127102057	0.6421988873
H	-2.1295551970	-1.0442427383	1.9212410927
H	-1.0493957570	-1.7421604962	0.7029538083
H	-0.4926453143	-0.4025165175	1.7302087598
C	-4.3721960644	-0.2563888262	-2.7384504652
C	-5.4742302124	0.3161513883	-3.3703058822
C	-6.0142963602	1.5157520811	-2.8828955294
C	-5.4478539470	2.1398656678	-1.7591940614
C	-4.3462771867	1.5713446039	-1.1231533645
H	-3.9634005636	-1.1933334739	-3.1054700690
H	-5.9212647858	-0.1705539579	-4.2299380346
H	-6.8789410989	1.9565521707	-3.3670856901
H	-5.8820337519	3.0564844731	-1.3747215896
H	-3.9390687680	2.0486767843	-0.2383277292

trans-epoxide

Ru	0.8706145048	1.6786702187	-1.7480314883
N	0.6694732270	2.7989104733	0.0530384991
C	0.5211512135	2.3430584494	1.3225334617
C	0.2308319894	3.1976215537	2.3865965559
C	0.0764242967	4.5656918820	2.1377864486
C	0.2239616137	5.0389070239	0.8270747963

C	0.5255178441	4.1403254397	-0.1961719803
C	0.7815141879	4.5927501386	-1.6220991249
N	0.2297518616	3.5327807717	-2.5820391132
C	-1.2797008070	3.6291246116	-2.5973238023
C	0.7377579907	3.5447415340	-4.0275902517
N	3.1561035889	2.6016177069	-2.3259806775
C	3.3068986408	3.8127092326	-1.4645194447
C	2.2952525668	4.9190085422	-1.8544996041
C	2.4357437621	5.2509283228	-3.3306161687
C	2.2266262685	4.0098971060	-4.1783360874
C	3.2767133557	2.9567830283	-3.7717149093
C	0.5374163295	2.1580102733	-4.6222459749
C	0.2657773385	1.9645837780	-5.9768968491
C	0.1819475366	0.6603508089	-6.4845212203
C	0.3628813031	-0.4209520886	-5.6152178466
C	0.6166492165	-0.1715923323	-4.2653379992
N	0.7108126671	1.0906330139	-3.7763396514
C	4.0939985447	1.5018553603	-1.9651418707
C	3.5865302943	0.5257272246	-0.9227840878
C	4.4985024172	-0.1989889961	-0.1461724131
C	4.0453560559	-1.2136310310	0.7010938760
C	2.6727059986	-1.4840853990	0.7565139525
C	1.8052446017	-0.7145132594	-0.0142643893
N	2.2487518613	0.2772426023	-0.8372327319
H	0.6393534512	1.2779588788	1.4662348828

H	0.1240762613	2.7951024428	3.3865126353
H	-0.1579221610	5.2514166769	2.9436909895
H	0.1036520813	6.0933852664	0.6048201561
H	0.2356564841	5.5280943555	-1.8051392956
H	-1.5856926865	4.6040882795	-2.9973337082
H	-1.6714942231	3.5093279552	-1.5875152884
H	-1.6879452030	2.8371113621	-3.2240284357
H	0.1317072619	4.2690736001	-4.5873512270
H	4.3227803053	4.2292340296	-1.5679451760
H	3.1765303037	3.5169467800	-0.4207986743
H	2.5213934895	5.8146308818	-1.2669953649
O	2.6565892893	6.3777084381	-3.7770431643
H	2.3797872717	4.2685778673	-5.2308177444
H	4.2794469483	3.3598246983	-3.9897297921
H	3.1521130662	2.0472273525	-4.3627907510
H	0.1221582540	2.8191161490	-6.6290037459
H	-0.0240131635	0.4958229591	-7.5358397030
H	0.3070028410	-1.4416139151	-5.9735573630
H	0.7428284865	-0.9696072607	-3.5468128756
H	4.2851559080	0.9268244819	-2.8801859814
H	5.0655875123	1.9071578244	-1.6473423053
H	5.5566605205	0.0263487127	-0.2171633657
H	4.7470823279	-1.7816585434	1.3007596918
H	2.2802662749	-2.2701148570	1.3900322615
H	0.7347368488	-0.8698308170	-0.0021273181

O -1.0723912812 -0.0497303520 -1.3472386902
C -2.0164051661 -1.1391203308 -0.8324983793
C -2.5542502301 -0.1210355985 -1.7632665264
C -1.7127982235 -2.5434970126 -1.2694996060
H -2.6526196644 -0.4331137345 -2.8005452042
C -3.4438560750 0.9941822928 -1.3617589814
H -2.2486685047 -1.0034488416 0.2216242809
H -2.5840759678 -3.1841501185 -1.0885368665
H -1.4757408173 -2.5849667675 -2.3368430002
H -0.8728484536 -2.9675708581 -0.7086818337
C -4.4015260709 1.4565671438 -2.2830849998
C -5.2894043916 2.4808621549 -1.9355598232
C -5.2227321957 3.0623518371 -0.6641801020
C -4.2651191357 2.6143334869 0.2582616173
C -3.3810626224 1.5875891831 -0.0860719826
H -4.4693189836 0.9972713881 -3.2655106866
H -6.0345278861 2.8148694979 -2.6493151834
H -5.9168587317 3.8487895366 -0.3889376159
H -4.2225165268 3.0542827820 1.2491139260
H -2.6475383311 1.2452221538 0.6368573320

ts2b

Ru 0.5149908904 2.0278504914 -1.5384612976
N 1.1426197819 2.4371795590 0.4389381661
C 1.2075378067 1.5926307271 1.4966938197

C	1.5071191885	2.0458686573	2.7831530962
C	1.7194171557	3.4126676723	2.9903835896
C	1.6485204997	4.2874946733	1.8962745202
C	1.3714006668	3.7764127603	0.6291132030
C	1.4508125403	4.6227745553	-0.6304979410
N	0.3751006172	4.1542705371	-1.6167916296
C	-0.9586364253	4.7120107812	-1.1841077276
C	0.5738534213	4.4852630700	-3.1038308908
N	2.6476570836	2.2986906095	-2.3379123942
C	3.4681147700	3.1187794511	-1.3702297300
C	2.9016506260	4.5477492407	-1.2151788048
C	2.8875770398	5.2335504050	-2.5701312922
C	2.0668870516	4.4297300729	-3.5614215423
C	2.6483003843	3.0072730293	-3.6735647826
C	-0.2719136576	3.5246999443	-3.9219801972
C	-0.9504897507	3.9064202175	-5.0780541770
C	-1.6533621752	2.9379241248	-5.8099154258
C	-1.6673494537	1.6158301315	-5.3545004847
C	-0.9813347707	1.2935342967	-4.1810164178
N	-0.2828156837	2.2248657756	-3.4918473167
C	3.2511779070	0.9181879371	-2.5042699090
C	2.4217832477	-0.2252175408	-1.9619802028
C	2.9568787982	-1.5176608631	-1.9282484147
C	2.1545324557	-2.5904896783	-1.5323458472
C	0.8217508231	-2.3437129972	-1.1793816215

C	0.3435339613	-1.0376003231	-1.2118392506
N	1.1338399807	0.0080453803	-1.5874298081
H	1.0129460537	0.5490926649	1.2892428825
H	1.5635384286	1.3403695514	3.6031747503
H	1.9389925406	3.7937048717	3.9809598599
H	1.8157131237	5.3506520909	2.0287967031
H	1.2596167339	5.6749222095	-0.3854789794
H	-0.9680441122	5.8007775782	-1.3151986694
H	-1.1232631752	4.4702471205	-0.1367510427
H	-1.7486796220	4.2532705773	-1.7765523268
H	0.2293668637	5.5132992028	-3.2712042152
H	4.5007972807	3.1917404006	-1.7428875407
H	3.4962627481	2.5972650928	-0.4128478326
H	3.5553882558	5.1066319977	-0.5379951981
O	3.4347954571	6.3082871798	-2.8182080597
H	2.1251438627	4.9069099676	-4.5449913769
H	3.6807332698	3.0748885250	-4.0473202541
H	2.0741339863	2.4063720549	-4.3794599573
H	-0.9388010792	4.9414881169	-5.4008532667
H	-2.1857155680	3.2168351306	-6.7118728793
H	-2.2062985244	0.8454820337	-5.8921102551
H	-0.9878260847	0.2943994340	-3.7683839825
H	3.4047739670	0.7443012259	-3.5761607061
H	4.2478814839	0.9027663892	-2.0475987523
H	3.9881977955	-1.6798125206	-2.2218555070

H	2.5579312840	-3.5960263879	-1.5082951502
H	0.1585036406	-3.1475502968	-0.8848198466
H	-0.6742527739	-0.7856816989	-0.9533224384
O	-1.3094149887	1.6346238576	-1.1046355500
C	-2.5727248681	1.3739444498	0.3322868260
C	-2.6530727292	-0.0299333949	0.4907668687
C	-2.2049834891	2.2135809757	1.5308443515
H	-2.1720569867	-0.4582506803	1.3697733687
C	-3.3129979943	-0.9530747217	-0.3894329077
H	-3.2988939796	1.8345665915	-0.3310419703
H	-3.1113116456	2.4087385617	2.1206259941
H	-1.4910907700	1.7058707611	2.1849080127
H	-1.7957474865	3.1853332886	1.2495755069
C	-3.3825735988	-2.3281303500	-0.0225538066
C	-4.0359786405	-3.2545024511	-0.8303266110
C	-4.6341775869	-2.8413869646	-2.0321140320
C	-4.5688080400	-1.4912940147	-2.4189295983
C	-3.9193761150	-0.5578796345	-1.6164713166
H	-2.9409261381	-2.6455534675	0.9178858882
H	-4.0949147897	-4.2935912510	-0.5255382094
H	-5.1530070799	-3.5608720834	-2.6559733133
H	-5.0405688975	-1.1739739329	-3.3428039583
H	-3.8748954254	0.4795398479	-1.9271074630

Computed coordinates (B3LYP/LACVP) of the corresponding intermediates in Figure 7.

²cis-alkene (S=1)

Fe	1.0562896725	1.7572662009	-1.2011926946
N	1.4894754382	2.8434608356	0.4361429402
C	1.8974030163	2.3608848704	1.6337954496
C	1.9155352563	3.1661141293	2.7731219716
C	1.4841026677	4.4938827673	2.6775157193
C	1.0519746641	4.9859984440	1.4381329256
C	1.0650126940	4.1374014023	0.3334582346
C	0.7095988343	4.5634680681	-1.0707949042
N	-0.0136259097	3.3840483276	-1.7205118978
C	-1.4305466974	3.3336716432	-1.1831842036
C	-0.0740058101	3.3575200223	-3.2474330900
N	2.7500891442	2.6400702881	-2.3184909947
C	3.1512381140	3.9780135267	-1.7333631715
C	1.9977645212	4.9963326855	-1.8397318289
C	1.6204028184	5.1899351052	-3.2988999583
C	1.2401950292	3.8592925035	-3.9256138850
C	2.4145263168	2.8735207928	-3.7771587635
C	-0.3498222452	1.9261941181	-3.6473790534
C	-1.1354199686	1.5524990860	-4.7354088710
C	-1.2479968435	0.1924554787	-5.0567684305
C	-0.5709728377	-0.7535738300	-4.2787583974
C	0.1935178193	-0.3207552338	-3.1947462249
N	0.3074899554	0.9946518740	-2.8954806759
C	3.9040343806	1.6646103376	-2.2219807522

C	3.6317527240	0.4837756943	-1.3244474479
C	4.6355628775	-0.4486754246	-1.0378251110
C	4.3360223797	-1.5640506367	-0.2524434881
C	3.0306093652	-1.7259900413	0.2335115286
C	2.0726021242	-0.7650542722	-0.0708700697
N	2.3744999953	0.3233711663	-0.8373097980
H	2.1915881933	1.3220346862	1.6679534644
H	2.2483973624	2.7533776439	3.7172364699
H	1.4746031804	5.1341250574	3.5519843891
H	0.7034750151	6.0075995469	1.3371824311
H	0.0283214116	5.4225225299	-1.0540199858
H	-1.9668592335	4.2390750223	-1.4893946952
H	-1.4047604118	3.2624651159	-0.0975327566
H	-1.9341950547	2.4506320880	-1.5719797387
H	-0.8889944600	4.0142711690	-3.5740616274
H	4.0198109857	4.3635578339	-2.2861542272
H	3.4560548877	3.8287910805	-0.6974209356
H	2.3297320671	5.9527842918	-1.4237425141
O	1.5959157546	6.2735549585	-3.8808375360
H	1.0328640556	4.0082223286	-4.9900218078
H	3.2973800928	3.2860230796	-4.2860199468
H	2.1836320159	1.9134540169	-4.2387946752
H	-1.6570896240	2.3049461030	-5.3159518997
H	-1.8607975624	-0.1208133879	-5.8940815103
H	-0.6437906346	-1.8117453236	-4.4966341424

H	0.7077982404	-1.0150426596	-2.5458299833
H	4.1330008676	1.2952752157	-3.2288085789
H	4.8015717659	2.1937794490	-1.8809999102
H	5.6354220351	-0.3011578540	-1.4305365177
H	5.1039076028	-2.2941387496	-0.0242225585
H	2.7598038635	-2.5802370303	0.8415650017
H	1.0509799164	-0.8237955491	0.2815341696
O	-0.1348420032	0.9914136349	-0.3550351068

²cis-alkene (S=2)

Fe	1.1112089014	1.6013393501	-1.2451435543
N	1.4067178233	2.8621209920	0.5178209083
C	1.7085075235	2.4014252047	1.7555735195
C	1.6471459549	3.2309997436	2.8759256505
C	1.2471372101	4.5629786705	2.7132275992
C	0.9214523301	5.0296300110	1.4325499698
C	1.0100706735	4.1508604498	0.3531712220
C	0.7390729963	4.5487163900	-1.0808241897
N	-0.0087664545	3.4097932138	-1.7454311826
C	-1.4083387201	3.3330774883	-1.1828231323
C	-0.0803160760	3.4329911485	-3.2594791397
N	2.7472578524	2.5124650870	-2.3765545291
C	3.1714377423	3.8118268391	-1.7152568831
C	2.0761160154	4.8977720215	-1.8090390935
C	1.7312110081	5.1535500246	-3.2662756298

C	1.2635840054	3.8683928419	-3.9264770855
C	2.3829020438	2.8168076369	-3.8186243602
C	-0.4753423793	2.0434720493	-3.7226965072
C	-1.3325486688	1.7973811809	-4.7947420689
C	-1.5889527610	0.4704226765	-5.1677372038
C	-0.9867366737	-0.5734904385	-4.4545365926
C	-0.1458134788	-0.2636435598	-3.3852483312
N	0.1114806186	1.0220716243	-3.0439077398
C	3.9037227223	1.5283257481	-2.3833574060
C	3.8113519452	0.4828953358	-1.3045446819
C	4.9118274146	-0.2830777187	-0.9123632344
C	4.7244005115	-1.3343990044	-0.0076779247
C	3.4385568558	-1.5988069664	0.4862682517
C	2.3813820539	-0.7909698926	0.0792880188
N	2.5735493032	0.2346544467	-0.7974074518
H	1.9892057947	1.3602733670	1.8354045456
H	1.8958605111	2.8376851377	3.8538212667
H	1.1788058068	5.2250742556	3.5687897915
H	0.5954320958	6.0524828013	1.2800540307
H	0.1103552677	5.4491079881	-1.1040871384
H	-1.9631092330	4.2452689027	-1.4350790637
H	-1.3623185796	3.2174946511	-0.1012374345
H	-1.9203055738	2.4649695004	-1.5952005735
H	-0.8472602291	4.1566088004	-3.5661693585
H	4.0699667603	4.1838057758	-2.2281086979

H	3.4399588236	3.6010037560	-0.6795848154
H	2.4677492942	5.8185907229	-1.3650985043
O	1.7866845846	6.2503455025	-3.8209799570
H	1.0670132483	4.0584617355	-4.9863774578
H	3.2779369156	3.1976662269	-4.3311264431
H	2.0935413908	1.8830108299	-4.3012431035
H	-1.8003625340	2.6220270472	-5.3208842687
H	-2.2580308626	0.2566521464	-5.9933461095
H	-1.1751269024	-1.6084340594	-4.7115770338
H	0.3189319774	-1.0324120961	-2.7817291916
H	3.8952627809	1.0164790199	-3.3531907325
H	4.8539267620	2.0716901527	-2.3245907903
H	5.8948972582	-0.0690866849	-1.3159922449
H	5.5673499819	-1.9410534186	0.3033633123
H	3.2604409649	-2.4131060540	1.1775999044
H	1.3668134372	-0.9291037914	0.4312800940
O	-0.0233601075	0.7646512647	-0.3957783842

ts2a

Fe	0.6924356171	1.9513079528	-1.3009740944
N	1.2675453635	2.7190248821	0.4575224179
C	1.4084355394	2.0596688355	1.6325327669
C	1.6094595396	2.7384235664	2.8354814370
C	1.6273309200	4.1381184278	2.8306239387
C	1.4539565666	4.8204986326	1.6184848889

C	1.2726152083	4.0869165018	0.4460789025
C	1.2569068496	4.7123234009	-0.9361572312
N	0.3073124637	3.8893884024	-1.7974642204
C	-1.1025070188	4.3280715135	-1.4877148528
C	0.4853778572	3.9585881675	-3.3125105356
N	2.7703727758	2.3176117593	-2.0921173632
C	3.4769398335	3.4400866158	-1.3655033042
C	2.7116987473	4.7665890072	-1.5031336642
C	2.6415482826	5.1290281029	-2.9764744232
C	1.9764014126	4.0122100137	-3.7649994719
C	2.7357454921	2.6846862975	-3.5556082734
C	-0.2004411194	2.7419784400	-3.8856027799
C	-0.8901023236	2.7398110997	-5.0971661692
C	-1.4009573644	1.5294366896	-5.5837661085
C	-1.2281239582	0.3648714157	-4.8280142992
C	-0.5448047202	0.4381914731	-3.6132538992
N	-0.0305714197	1.6033174675	-3.1571410394
C	3.5443933714	1.0417536519	-1.8765900086
C	2.6914751439	-0.1406578366	-1.4990098226
C	3.2124459794	-1.4386862208	-1.5523212952
C	2.4311612974	-2.5129370831	-1.1221683296
C	1.1318713102	-2.2621490384	-0.6610120135
C	0.6612980740	-0.9524731784	-0.6420188579
N	1.4257007536	0.0946523561	-1.0643379685
H	1.3972191869	0.9794211117	1.5823266602

H	1.7522671000	2.1806628134	3.7528187597
H	1.7814206438	4.6900764467	3.7506623805
H	1.4632256288	5.9042574893	1.5873449321
H	0.8894126986	5.7444640148	-0.8867918723
H	-1.2460483966	5.3602671258	-1.8301462867
H	-1.2645994201	4.2741871076	-0.4161503183
H	-1.8044428414	3.6558422454	-1.9748945212
H	0.0027760697	4.8738546644	-3.6775705221
H	4.4863027237	3.5641572828	-1.7851992158
H	3.5863620388	3.1610152572	-0.3175215121
H	3.2541366051	5.5493874731	-0.9636122546
O	3.0441282624	6.1870254922	-3.4605679825
H	1.9933001543	4.2673567527	-4.8292099125
H	3.7649461449	2.8032497868	-3.9260328424
H	2.2680566137	1.8720797643	-4.1122731479
H	-1.0271728984	3.6630520770	-5.6488657661
H	-1.9353780842	1.5016622808	-6.5263357898
H	-1.6247288994	-0.5841984384	-5.1664022566
H	-0.4122555429	-0.4304174321	-2.9860226240
H	4.1376991934	0.8103522622	-2.7699381424
H	4.2671959489	1.2122867594	-1.0694638785
H	4.2230381122	-1.5974782373	-1.9117570329
H	2.8218063495	-3.5234321173	-1.1552526776
H	0.4930261966	-3.0691346190	-0.3239256842
H	-0.3450312722	-0.7012838533	-0.3450555519

O	-0.9772716196	1.5663134583	-0.7675101022
C	-1.7789779568	1.2205343935	0.7663256501
C	-2.6752990079	0.1250760707	0.4512527655
H	-0.9353909643	0.8799754552	1.3655104461
H	-2.3065972715	-0.8677129376	0.7061542604
C	-3.9670911087	0.1425218422	-0.1606193997
C	-2.3103356062	2.5422091580	1.2868567400
H	-2.8750838947	2.3571793443	2.2095590101
H	-1.4899985032	3.2199364689	1.5392809139
H	-2.9828737078	3.0426054650	0.5928196380
C	-4.7339825503	-1.0631817491	-0.1330415071
C	-5.9900396551	-1.1345480427	-0.7231513551
C	-6.5225592618	-0.0138726855	-1.3809739006
C	-5.7788861547	1.1764688720	-1.4474959513
C	-4.5274106339	1.2602023065	-0.8465422147
H	-4.3316616129	-1.9293867527	0.3840575445
H	-6.5602782035	-2.0555174881	-0.6742916497
H	-7.5013214663	-0.0699954531	-1.8446029775
H	-6.1807006519	2.0345500124	-1.9757817154
H	-3.9591748498	2.1759830158	-0.9362535202

cis-rad_{triplet}

Fe	0.6602186153	2.0176424688	-1.2939358990
N	1.2852509365	2.7733187243	0.4535915120
C	1.4708657866	2.1176807328	1.6248832731

C	1.7226763876	2.8007790267	2.8157088174
C	1.7704568469	4.1994487110	2.7993452897
C	1.5959182249	4.8760048157	1.5838659424
C	1.3657995616	4.1392418045	0.4224146920
C	1.3420193116	4.7576504489	-0.9624011373
N	0.3457770703	3.9683496790	-1.8024930573
C	-1.0390207388	4.4776058256	-1.4765103740
C	0.5058851958	4.0113000540	-3.3213677130
N	2.7096340789	2.2906419790	-2.0759500648
C	3.4871836161	3.3971286041	-1.3902230134
C	2.7865705456	4.7539868398	-1.5574492929
C	2.7117520149	5.0838524672	-3.0384556455
C	1.9911376116	3.9788248614	-3.7915307178
C	2.6813709854	2.6215017017	-3.5514750130
C	-0.2488709627	2.8262850746	-3.8712470854
C	-0.9640776016	2.8491149687	-5.0670612056
C	-1.5767346583	1.6704673956	-5.5132594618
C	-1.4625319047	0.5101512428	-4.7409319711
C	-0.7406796606	0.5557220679	-3.5472504845
N	-0.1296806206	1.6886566357	-3.1290328175
C	3.4442186725	0.9917063926	-1.8356942503
C	2.5431219671	-0.1613508797	-1.4925644974
C	3.0164516084	-1.4761981158	-1.5518132076
C	2.1908600440	-2.5253647403	-1.1419291707
C	0.8983761842	-2.2292622686	-0.6918607835

C	0.4714225359	-0.9039496173	-0.6735972568
N	1.2841323022	0.1213939125	-1.0602559073
H	1.4169196611	1.0382920043	1.5889951789
H	1.8708940376	2.2464852325	3.7342461070
H	1.9474540789	4.7553032440	3.7129133658
H	1.6437431920	5.9583619465	1.5411608067
H	1.0090943298	5.8009696477	-0.9097778395
H	-1.1368370289	5.5077841926	-1.8391387938
H	-1.1925364639	4.4475958788	-0.4018147337
H	-1.7808757717	3.8367063879	-1.9446753980
H	0.0678257693	4.9467416412	-3.6906863386
H	4.4933418448	3.4483625362	-1.8307090710
H	3.6013779768	3.1418639956	-0.3372756596
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H	2.0092328206	4.2021342126	-4.8629040540
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H	4.0626832489	0.7477407200	-2.7078281234
H	4.1385726170	1.1459516938	-1.0011391322
H	4.0205611742	-1.6697769466	-1.9123577712

H	2.5446720859	-3.5491883684	-1.1798347432
H	0.2226862751	-3.0127202924	-0.3715904626
H	-0.5353850212	-0.6405028565	-0.3792259141
O	-1.0440327963	1.7864891445	-0.7097191396
C	-1.6158300575	1.3611654962	0.5850723015
C	-2.5647522860	0.2057146784	0.3926428220
H	-0.8043362809	1.0150578344	1.2388115507
H	-2.4822539874	-0.5823825753	1.1402872680
C	-3.6490319448	0.1087179279	-0.5205097764
C	-2.2883446833	2.5704397180	1.2680789965
H	-2.7322415863	2.2530713394	2.2172573831
H	-1.5599512413	3.3598736979	1.4851132460
H	-3.0879528071	2.9744194272	0.6424414867
C	-4.5175079736	-1.0267472023	-0.4349418137
C	-5.6102596385	-1.1665090356	-1.2809057696
C	-5.8876013907	-0.1845074217	-2.2477493846
C	-5.0480238580	0.9373163018	-2.3587990490
C	-3.9460905326	1.0852827524	-1.5229761983
H	-4.3195152079	-1.7811400474	0.3210966516
H	-6.2575742087	-2.0318213361	-1.1877997630
H	-6.7481707157	-0.2891941616	-2.8992272656
H	-5.2685270455	1.6997594890	-3.0995803063
H	-3.2980853672	1.9465395118	-1.6227059526

ts3a

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C	1.4014407825	2.0601140951	1.6412133340
C	1.6161659278	2.7416261273	2.8399972568
C	1.6359851270	4.1412564531	2.8315440323
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C	1.2721663722	4.0839911173	0.4479978853
C	1.2391534493	4.7171870087	-0.9303906287
N	0.2976085558	3.8903724884	-1.7968725592
C	-1.1185060789	4.3135990233	-1.4892373762
C	0.4838405831	3.9563397616	-3.3117844012
N	2.8024128001	2.3590214918	-2.0660263781
C	3.4803519427	3.4975647241	-1.3421774316
C	2.6910572403	4.8075387448	-1.5021639735
C	2.6177184677	5.1536222785	-2.9791622648
C	1.9766782804	4.0187292139	-3.7581613575
C	2.7533133971	2.7052990338	-3.5311576960
C	-0.1956129908	2.7393321368	-3.8915188220
C	-0.8704495751	2.7378663178	-5.1114282129
C	-1.4130812466	1.5357036101	-5.5840819679
C	-1.2721956265	0.3764517306	-4.8139676037
C	-0.5959968241	0.4480053217	-3.5950014904
N	-0.0527599009	1.6046317474	-3.1502673698
C	3.5927339060	1.0996202650	-1.8317126289
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H	-1.2889749489	4.2577719042	-0.4180559293
H	-1.8104746189	3.6365049449	-1.9837046992
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H	4.4942803762	3.6358253323	-1.7472386611
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H	3.2133172580	5.6086296683	-0.9698983099
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H	-1.6880070673	-0.5673877384	-5.1440190365
H	-0.4924085499	-0.4148643494	-2.9551777230

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H	4.3414933271	-1.5142585341	-1.8760658731
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H	0.6136872435	-3.1131261752	-0.4119458829
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O	-1.0470787652	1.4633101921	-0.7461943209
C	-1.6532943432	1.1447298676	0.5673608684
C	-2.6888087784	0.0913797176	0.3081178458
H	-0.8837626244	0.6994520872	1.2135310757
H	-2.5255884235	-0.8643697832	0.8059073277
C	-3.8620331651	0.1828027250	-0.4802981607
C	-2.2056945827	2.3857920485	1.2899570946
H	-2.6415310699	2.0893475881	2.2503137632
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C	-5.9874102348	-0.8605532404	-1.1418290270
C	-6.3129982874	0.2751874525	-1.9023364649
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H	-4.5409192244	-1.7866518915	0.1473073669
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H	-7.2543407785	0.3175210354	-2.4391236923
H	-5.6654953816	2.2240929699	-2.5712808065

H -3.5035550094 2.1308838441 -1.3686643923

cis-epoxide (S=1)

Fe 0.7557585135 1.8994318392 -1.2408584385

N 1.3297798925 2.7541170728 0.4790378829

C 1.5102196737 2.1458440552 1.6775244626

C 1.8064307862 2.8713109314 2.8322905870

C 1.9120824773 4.2645949109 2.7498662573

C 1.7232619360 4.8932095774 1.5113000169

C 1.4362181431 4.1142026411 0.3907368889

C 1.3021225577 4.6819396915 -1.0077967772

N 0.2905340968 3.8148917712 -1.7481136361

C -1.0927450703 4.2165731132 -1.3065567789

C 0.3290569371 3.8244555511 -3.2752391100

N 2.8693208976 2.3320818871 -2.2590293097

C 3.5517300705 3.4909889388 -1.6001132808

C 2.6984421085 4.7711482118 -1.7102018577

C 2.4622299689 5.0855299599 -3.1768152605

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C 2.6290440791 2.6432082914 -3.7044445208

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C -1.1059031277 2.5057172926 -4.9361192092

C	-1.6449950082	1.2773100668	-5.3401759575
C	-1.4328318925	0.1436463543	-4.5473129707
C	-0.6930947910	0.2695554199	-3.3719016727
N	-0.1645240183	1.4559954208	-2.9835584767
C	3.6434839209	1.0688720163	-2.0796986656
C	2.8525963048	-0.1104128331	-1.5415923787
C	3.4457348208	-1.3808588757	-1.5357795310
C	2.7764054264	-2.4602823459	-0.9587454010
C	1.5122038168	-2.2476559752	-0.3911442804
C	0.9639693713	-0.9707014349	-0.4390615962
N	1.6154779939	0.0825379827	-1.0105332347
H	1.4182490681	1.0681306420	1.6884864862
H	1.9513471617	2.3546727171	3.7730747668
H	2.1363447002	4.8532605826	3.6319216804
H	1.7972050171	5.9712314847	1.4214153741
H	0.9109394088	5.7068199524	-0.9585582788
H	-1.2890714047	5.2583941162	-1.5893261819
H	-1.1757474136	4.1048657485	-0.2268220015
H	-1.8219572985	3.5628737414	-1.7796729191
H	-0.2154402023	4.7091565638	-3.6309365903
H	4.5314231045	3.6795736424	-2.0686752607
H	3.7303453827	3.2395177659	-0.5526451044
H	3.2450481108	5.6012036620	-1.2514901598
O	2.7559113524	6.1502396932	-3.7225919361
H	1.6770872198	4.1446304560	-4.9340262808

H	3.5885569772	2.7984805955	-4.2244374850
H	2.1377413582	1.7860622157	-4.1696325490
H	-1.2607513714	3.3999927058	-5.5293626220
H	-2.2231948435	1.2095258365	-6.2545031210
H	-1.8390058185	-0.8195972700	-4.8295880421
H	-0.5115776050	-0.5748535786	-2.7220106140
H	4.1211008162	0.7792610821	-3.0254975456
H	4.4666536371	1.2614878834	-1.3792821388
H	4.4282745350	-1.5134398107	-1.9756071927
H	3.2300647238	-3.4446494501	-0.9480340085
H	0.9642643479	-3.0575005573	0.0747110549
H	-0.0100303015	-0.7433921502	-0.0300943943
O	-1.3761182760	1.2584253051	-0.1013277067
C	-2.1756469374	1.1018828123	1.1899168636
C	-2.5640055369	0.2919846628	0.0003330764
H	-1.5915188627	0.5695832030	1.9401436365
H	-2.2274080677	-0.7431959480	0.0336694876
C	-3.7420363531	0.4790424227	-0.8844231166
C	-2.9232889993	2.2886680956	1.7216077422
H	-3.5642870696	1.9614140244	2.5489619402
H	-2.2299868866	3.0358931245	2.1242251100
H	-3.5630451230	2.7601491105	0.9753949739
C	-4.4808740103	-0.6740027383	-1.2150628034
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C	-6.0405684234	0.6579661883	-2.5036516951

C	-5.3030401388	1.8084480959	-2.1967819217
C	-4.1619756275	1.7215680579	-1.3935379528
H	-4.1674573971	-1.6424677375	-0.8344662181
H	-6.1913939774	-1.4803154078	-2.2444994070
H	-6.9303362593	0.7299210621	-3.1193419312
H	-5.6228209593	2.7731341696	-2.5764818720
H	-3.6017669744	2.6191281013	-1.1645895092

cis-epoxide (S=2)

Fe	0.6945949621	1.7610715925	-1.1352334593
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C	1.3541209978	3.5214238381	2.9339464143
C	1.4312285184	4.8899078151	2.6450940606
C	1.3439757299	5.3127577948	1.3131793086
C	1.1854615522	4.3598635178	0.3030641449
C	1.1891374966	4.7395950578	-1.1703747476
N	0.2717420738	3.8010514562	-1.9176389352
C	-1.1517025780	4.1753582118	-1.6150244663
C	0.4470897599	3.7098828953	-3.4149252073
N	2.8708703993	2.2681095771	-1.9864900492
C	3.4781050464	3.5075462449	-1.3930475999
C	2.6527941475	4.7639885191	-1.7242850712
C	2.5871902254	4.9190353297	-3.2322645696
C	1.9467193206	3.6937174740	-3.8593165845

C	2.7444380953	2.4261163253	-3.4753088628
C	-0.2785984748	2.4759528798	-3.9181807045
C	-0.9066850553	2.4409745076	-5.1655147962
C	-1.4962470311	1.2474673613	-5.5987854527
C	-1.4447629012	0.1219010428	-4.7680611981
C	-0.8107774745	0.2289206093	-3.5301934913
N	-0.2334360267	1.3820903261	-3.1113730228
C	3.7232444085	1.0908438753	-1.6354002004
C	2.9652821243	-0.2079341468	-1.5020795144
C	3.5922595196	-1.4354130094	-1.7428583771
C	2.9102304267	-2.6241379164	-1.4681868692
C	1.6082969396	-2.5590374248	-0.9543813599
C	1.0303409003	-1.3079032875	-0.7579608637
N	1.6896245018	-0.1501351666	-1.0322879743
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H	1.4251035807	3.1597348739	3.9525155253
H	1.5556059673	5.6146258356	3.4415746878
H	1.3978918379	6.3667442385	1.0633884046
H	0.8028721050	5.7642977735	-1.2732538674
H	-1.3723185710	5.1819854139	-1.9951412633
H	-1.3118532264	4.1542492590	-0.5370427569
H	-1.8260479016	3.4577694297	-2.0794347587
H	-0.0032129724	4.5992839595	-3.8808624443
H	4.5005340304	3.6484944127	-1.7794114458
H	3.5503796055	3.3694262044	-0.3124468101

H	3.1549258130	5.6371019049	-1.2959417918
O	2.9618412202	5.9142974084	-3.8544899571
H	1.9670539886	3.7981630444	-4.9487068162
H	3.7473388132	2.5043341827	-3.9261958039
H	2.2690015322	1.5298839779	-3.8804927430
H	-0.9382512118	3.3307921331	-5.7847163066
H	-1.9897952125	1.1994821822	-6.5626844639
H	-1.8923905572	-0.8168736148	-5.0702703797
H	-0.7528672455	-0.6135360699	-2.8537279918
H	4.5465206140	0.9770387052	-2.3548559560
H	4.1876161426	1.3008586652	-0.6633697885
H	4.6043055445	-1.4559263469	-2.1308677122
H	3.3860280521	-3.5816816127	-1.6465387398
H	1.0549405671	-3.4590467676	-0.7159540417
H	0.0257239472	-1.2017418238	-0.3731612224
O	-1.2019603869	1.1341845976	-0.1621016773
C	-1.8688663769	0.7228111452	1.1520650964
C	-2.4185603287	0.1894471368	-0.1281218159
H	-1.2276858795	0.0344579661	1.7020207702
H	-2.1211381492	-0.8324104035	-0.3558493878
C	-3.6819143850	0.5819467650	-0.7991784840
C	-2.5116994466	1.7816390199	1.9969588967
H	-3.0854910860	1.2905559069	2.7925792034
H	-1.7561540090	2.4107485627	2.4782556432
H	-3.1990059786	2.4153017921	1.4372200833

C	-4.5070662038	-0.4642425436	-1.2575114905
C	-5.7438736170	-0.1900154623	-1.8472914543
C	-6.1645516531	1.1355678741	-2.0054813307
C	-5.3419525636	2.1835378846	-1.5728247491
C	-4.1095082965	1.9111838058	-0.9720801935
H	-4.1895471953	-1.4964476626	-1.1352460195
H	-6.3749327166	-1.0062073914	-2.1811554073
H	-7.1242991356	1.3505758521	-2.4620479747
H	-5.6652610099	3.2114803075	-1.6969588395
H	-3.4808282355	2.7308231867	-0.6483008011

ts4 (S=1)

Fe	0.8195519069	1.9386523840	-1.3382241451
N	1.3175257004	2.7060060438	0.4344319576
C	1.5849070485	2.0354383471	1.5814422316
C	1.7592827849	2.7025082290	2.7948594895
C	1.6377622153	4.0966103123	2.8279603479
C	1.3711299048	4.7890613785	1.6384903057
C	1.2246662326	4.0704999863	0.4520830362
C	1.1180524636	4.7304297134	-0.9086764639
N	0.2491428775	3.8424345649	-1.7940006450
C	-1.2009358315	4.1463031548	-1.4869963372
C	0.4251161940	3.9608374328	-3.3039436168
N	2.8379647155	2.5244141712	-2.0827654451
C	3.4412959406	3.6990327367	-1.3383124863

C	2.5584841417	4.9512274561	-1.4732780557
C	2.4573849841	5.3286165930	-2.9405058382
C	1.9079036514	4.1652627455	-3.7468737900
C	2.7901164220	2.9168519376	-3.5436684495
C	-0.1137780046	2.6933717967	-3.9186120478
C	-0.7679239967	2.6489349177	-5.1482018421
C	-1.0774652948	1.4021938063	-5.7079821656
C	-0.7061975595	0.2399855222	-5.0246262513
C	-0.0712716945	0.3529063088	-3.7865015863
N	0.2097384902	1.5572267731	-3.2360578369
C	3.7365423425	1.3242118059	-1.8881352579
C	3.0093447746	0.0643094961	-1.4990177849
C	3.6781205346	-1.1650597532	-1.5068374042
C	3.0153421761	-2.3153962141	-1.0736863439
C	1.6853070757	-2.2081483352	-0.6479694950
C	1.0638433498	-0.9631301666	-0.6758417483
N	1.7151978999	0.1616847294	-1.0902906231
H	1.6511844747	0.9589922463	1.5098400923
H	1.9763379083	2.1385611794	3.6936198020
H	1.7522732249	4.6375939943	3.7602856119
H	1.2831712318	5.8697744914	1.6347431830
H	0.6409587009	5.7137954584	-0.8231245243
H	-1.4476597165	5.1421113838	-1.8737440668
H	-1.3539948188	4.1236333517	-0.4130067044
H	-1.8334766428	3.3855646263	-1.9376623782

H	-0.1418727791	4.8314810428	-3.6546531495
H	4.4373966492	3.9090273475	-1.7537490330
H	3.5726170369	3.4209773206	-0.2931069934
H	3.0175590105	5.7755932312	-0.9188041226
O	2.7476906080	6.4318431627	-3.4025781136
H	1.9070938275	4.4305417905	-4.8087705724
H	3.8106602515	3.1401757055	-3.8872257844
H	2.4221522568	2.0708706388	-4.1232761641
H	-1.0273663933	3.5680475801	-5.6613496617
H	-1.5916008825	1.3425883513	-6.6602770059
H	-0.9130516698	-0.7399802938	-5.4360365514
H	0.2187324401	-0.5202402764	-3.2214162769
H	4.3240708802	1.1526656622	-2.7980070686
H	4.4603071988	1.5624087220	-1.0994587611
H	4.7068548772	-1.2141770488	-1.8463384158
H	3.5225217142	-3.2733313314	-1.0726964252
H	1.1296549745	-3.0743358102	-0.3107483141
H	0.0299756799	-0.8470284229	-0.3956310064
O	-0.8719466938	1.4457395509	-0.8142678240
C	-1.4414820616	1.0661692162	0.5040471863
C	-2.6888547304	0.2239082150	0.3789110232
H	-0.6601579769	0.5001075783	1.0449780309
H	-3.3961959256	0.4137570881	1.1839708947
C	-3.0552223783	-0.8299019179	-0.4985113368
C	-1.8094810875	2.2980292882	1.3596545111

H	-2.1447696562	1.9595489908	2.3459416616
H	-0.9724394364	2.9780205393	1.5119679557
H	-2.6389909121	2.8435011969	0.9004630876
C	-4.2158851492	-1.6035882862	-0.1720892540
C	-4.6228200364	-2.6672592797	-0.9673634825
C	-3.9039159394	-3.0025271817	-2.1276920775
C	-2.7770052200	-2.2437551184	-2.4845066694
C	-2.3605093326	-1.1778969172	-1.6934575935
H	-4.7766025513	-1.3532228589	0.7233159728
H	-5.5010053081	-3.2406977430	-0.6913109272
H	-4.2245971756	-3.8321641232	-2.7478638924
H	-2.2370047756	-2.4881838235	-3.3952011997
H	-1.5329663693	-0.5560377593	-1.9958836580

trans-epoxide (S=1)

Fe	0.7128001619	1.8050892487	-1.0884593784
N	1.3463835842	2.8430221679	0.4995247434
C	1.6661784926	2.3490341608	1.7209464223
C	1.9748206453	3.1868246780	2.7938755701
C	1.9413076586	4.5733576835	2.6039455373
C	1.6078994477	5.0831250814	1.3413685508
C	1.3197275472	4.1958416318	0.3044218639
C	1.0493484441	4.6394057338	-1.1198141100
N	0.0751958668	3.6363239677	-1.7280653133
C	-1.3134522969	3.9624483362	-1.2413088418

C	0.0388401986	3.5164674583	-3.2492798291
N	2.7503956156	2.3347992210	-2.2507739296
C	3.3630023560	3.6045219966	-1.7477916172
C	2.3908492434	4.7898721318	-1.9147431759
C	2.0567042838	4.9434937272	-3.3872929897
C	1.4409784856	3.6646587226	-3.9286365501
C	2.4073757214	2.4795678732	-3.7000661787
C	-0.5795197024	2.1764478863	-3.5871622744
C	-1.3452314509	1.9612581409	-4.7331536021
C	-1.8020607329	0.6672983654	-5.0143957309
C	-1.4868620964	-0.3733908811	-4.1329920956
C	-0.7268244357	-0.0943198217	-2.9967794815
N	-0.2718842098	1.1557110018	-2.7308845624
C	3.6409082158	1.1668646218	-1.9921932518
C	2.9514491844	-0.0588629790	-1.4234633244
C	3.6181193208	-1.2910153286	-1.4423907955
C	3.0448087239	-2.4028395432	-0.8223405895
C	1.8033092843	-2.2583470505	-0.1897928074
C	1.1768124371	-1.0162191962	-0.2152892080
N	1.7345405688	0.0669750786	-0.8272954444
H	1.6728542051	1.2714907287	1.8154727466
H	2.2353838015	2.7608201863	3.7549842846
H	2.1706444956	5.2473427623	3.4213052051
H	1.5749238058	6.1530581737	1.1682505664
H	0.5730998600	5.6286048021	-1.1193802273

H	-1.6358052383	4.9310376647	-1.6435320268
H	-1.3117659424	4.0001604592	-0.1538886494
H	-2.0046189147	3.1841328819	-1.5624036637
H	-0.5881112180	4.3254770262	-3.6476555219
H	4.2923567930	3.8303332737	-2.2959487181
H	3.6255231850	3.4712744289	-0.6965342260
H	2.8810807890	5.7031511249	-1.5629191505
O	2.2302000242	5.9712236038	-4.0441939769
H	1.2720774076	3.7782780227	-5.0041961304
H	3.3202705299	2.6571217325	-4.2922809865
H	1.9653053603	1.5443749938	-4.0507656942
H	-1.5808526463	2.7878651356	-5.3941732738
H	-2.3955980047	0.4787031655	-5.9016373148
H	-1.8263887966	-1.3848546772	-4.3183133455
H	-0.4750406718	-0.8636016806	-2.2811251058
H	4.1854858945	0.8881760285	-2.9050602468
H	4.4074118277	1.4768043455	-1.2701709919
H	4.5808205094	-1.3703537998	-1.9354681359
H	3.5548357563	-3.3593065417	-0.8323183304
H	1.3213094013	-3.0926148424	0.3045098842
H	0.2092213885	-0.8495688649	0.2361407229
O	-1.1239972028	1.0982463208	0.3074745169
C	-1.8670778763	1.1692754093	1.6324929776
C	-2.5048690979	0.3980720802	0.5446640839
H	-1.3426653900	0.6052863438	2.3999100896

C	-2.5836454471	-1.0777241908	0.4589580975
H	-3.2711704676	0.9246530175	-0.0187595647
C	-2.3881793062	2.5065343665	2.0790850479
C	-3.2882103181	-1.6446229531	-0.6216344404
C	-3.4058043118	-3.0313749009	-0.7494542112
C	-2.8199556998	-3.8730065918	0.2043067485
C	-2.1232219141	-3.3216569933	1.2883832859
C	-2.0056630337	-1.9343809475	1.4169781777
H	-3.7655947285	-0.9937047267	-1.3492772495
H	-3.9663619475	-3.4543257142	-1.5760775969
H	-2.9216387805	-4.9490242783	0.1150322940
H	-1.6948441485	-3.9713217446	2.0441703212
H	-1.4905198284	-1.5280973083	2.2816388440
H	-3.0652478745	2.3667571344	2.9301148039
H	-1.5751903222	3.1607588008	2.4125362276
H	-2.9497624388	3.0096804744	1.2868781511

trans-epoxide (S=2)

Fe	0.6967858543	1.7136152048	-0.9408741777
N	1.2235544761	3.0857395416	0.6659696858
C	1.4529209399	2.7398573287	1.9577726445
C	1.7155649056	3.6922473110	2.9430197160
C	1.7227093584	5.0467069276	2.5855417621
C	1.4790366300	5.4032236844	1.2534941955
C	1.2408691447	4.3993762293	0.3104303998

C	1.0701081111	4.7086059976	-1.1700525398
N	0.1084513986	3.7088712093	-1.7683418514
C	-1.2857688784	4.0584273265	-1.3294562484
C	0.1240509818	3.5482723071	-3.2692497275
N	2.7454904239	2.2552273239	-2.0586352867
C	3.3667453112	3.5401629482	-1.5927020871
C	2.4624659201	4.7516255980	-1.8845917125
C	2.2263407308	4.8303061361	-3.3812392433
C	1.5651678695	3.5565107103	-3.8766980349
C	2.4458979914	2.3347074417	-3.5280695508
C	-0.6075199296	2.2691301075	-3.6311069713
C	-1.3511464388	2.1468802408	-4.8075880942
C	-1.9426455140	0.9159744285	-5.1146393332
C	-1.7796634590	-0.1571239277	-4.2300342531
C	-1.0345694941	0.0359379690	-3.0660266870
N	-0.4532312903	1.2260360953	-2.7727772789
C	3.6752032354	1.1230841149	-1.7558179613
C	2.9786961123	-0.1920867589	-1.5065179060
C	3.6045425885	-1.4102435924	-1.7877632834
C	2.9846359731	-2.6061156838	-1.4104537219
C	1.7486464774	-2.5545763567	-0.7546939114
C	1.1646123218	-1.3118703448	-0.5196356970
N	1.7632912934	-0.1499938389	-0.8957779561
H	1.4258949333	1.6808934684	2.1841548725
H	1.9058272139	3.3820878620	3.9632983413

H	1.9129059720	5.8115823398	3.3297903524
H	1.4748913709	6.4451340113	0.9523609881
H	0.6400904806	5.7157756028	-1.2737179349
H	-1.6031710132	5.0106957176	-1.7758926786
H	-1.3126363145	4.1470772276	-0.2442869707
H	-1.9759548231	3.2717633859	-1.6338114340
H	-0.4058199396	4.3988405417	-3.7242887196
H	4.3343988337	3.6964630753	-2.0966380631
H	3.5633897199	3.4566283713	-0.5219038742
H	2.9759056643	5.6603904126	-1.5552247543
O	2.4966082708	5.8038569136	-4.0864070697
H	1.4614537910	3.6083024507	-4.9651047549
H	3.3876655175	2.4202574216	-4.0947315059
H	1.9603444132	1.4048715497	-3.8338180529
H	-1.4685409995	2.9982317808	-5.4690988983
H	-2.5231145270	0.7994214170	-6.0227208065
H	-2.2244114023	-1.1230871034	-4.4359440441
H	-0.8956317758	-0.7609458799	-2.3475133012
H	4.4272213591	1.0121056040	-2.5499487937
H	4.2232064264	1.3861100908	-0.8420441604
H	4.5668646447	-1.4195888091	-2.2868149906
H	3.4599523590	-3.5575560640	-1.6204038576
H	1.2423797093	-3.4569806416	-0.4351577514
H	0.2081346394	-1.2166157442	-0.0251890050
O	-0.9847572535	1.0099090368	0.3005596148

C	-1.7653065006	1.1225270107	1.5986532167
C	-2.3738230064	0.2983399606	0.5318840386
H	-1.2553741142	0.5945382370	2.4006744829
C	-2.4442136102	-1.1773733531	0.5158097666
H	-3.1221752490	0.7973789314	-0.0778232423
C	-2.3241355222	2.4645609250	1.9795561121
C	-3.2073853760	-1.7955165764	-0.4956531449
C	-3.3402237706	-3.1860254048	-0.5403315533
C	-2.7088815928	-3.9791546111	0.4257934091
C	-1.9495147778	-3.3766477425	1.4389365893
C	-1.8184611955	-1.9860765267	1.4868061883
H	-3.7195587480	-1.1812183634	-1.2313334855
H	-3.9453738673	-3.6483479692	-1.3123526601
H	-2.8216876257	-5.0574859393	0.4013412878
H	-1.4808369299	-3.9885939549	2.2019756857
H	-1.2484040691	-1.5394588710	2.2951602127
H	-3.0420605552	2.3332596116	2.7982202065
H	-1.5405811122	3.1403902874	2.3358395979
H	-2.8516867923	2.9351343464	1.1455327322

cis-rad_{heptet}

Fe	0.4451789639	2.0938613419	-1.2220848011
N	1.2664047482	3.0012177010	0.5808655568
C	1.2374505318	2.4142009020	1.8036704877
C	1.5650270597	3.1190717238	2.9623278542

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C	1.9104711707	4.4721317328	2.8541865366
C	1.9342396982	5.0756411994	1.5897957978
C	1.6137455498	4.3119123049	0.4652594245
C	1.7247067534	4.8466007289	-0.9509923846
N	0.6137758270	4.2384804983	-1.7846420793
C	-0.6820185095	4.9229989293	-1.4289082803
C	0.7943013148	4.2765150459	-3.2883665584
N	2.7363239556	2.1381940444	-2.0165741033
C	3.6367931317	3.1227321667	-1.3185344878
C	3.1579664204	4.5719297824	-1.5138688030
C	3.1649113321	4.8859031285	-2.9982895303
C	2.2495831497	3.9283061896	-3.7401415733
C	2.6904772002	2.4682535277	-3.4859985344
C	-0.1948645033	3.3191446038	-3.9151793989
C	-0.8273239662	3.5688439112	-5.1338784181
C	-1.6688127574	2.5886605871	-5.6754871680
C	-1.8574436996	1.3886988410	-4.9791499768
C	-1.2057180621	1.2047147538	-3.7595683546
N	-0.3834548846	2.1523270271	-3.2429381657
C	3.2745615452	0.7570424893	-1.7910178903
C	2.2175147744	-0.3169740257	-1.7726010261
C	2.5252114724	-1.6453899601	-2.0786013754
C	1.5528599598	-2.6352119242	-1.8982971150
C	0.2909660890	-2.2713036584	-1.4118183938
C	0.0324895322	-0.9291269034	-1.1442706896

N	0.9796271803	0.0336379140	-1.3305028326
H	0.9493747692	1.3706067113	1.8335965714
H	1.5424459832	2.6223165279	3.9245378399
H	2.1553233863	5.0491902327	3.7386010254
H	2.1967413245	6.1221660763	1.4815926129
H	1.5923454566	5.9374085223	-0.9393426183
H	-0.6562510129	5.9727244706	-1.7485522178
H	-0.8297933905	4.8772491586	-0.3510930652
H	-1.5143245767	4.4135090828	-1.9118467121
H	0.5878393088	5.2962603914	-3.6435390182
H	4.6603339406	3.0322086817	-1.7149636622
H	3.6709015101	2.8654282875	-0.2589705365
H	3.8519617216	5.2450905378	-1.0008354941
O	3.7929674698	5.8064711112	-3.5219097417
H	2.3178527243	4.1285787668	-4.8140486501
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