

Supporting Information for

The Mechanism for Catalytic Hydrosilylation by Bis(imino)pyridine Iron Olefin Complexes Supported by Broken Symmetry Density Functional Theory

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Cartesian Coordinates and Electronic Energy of Species Mentioned in Manuscript

The electronic energy cited here is that of the lowest energy spin state in hartrees, uncorrected for “broken-symmetry”.

^{(MePDI)Fe(C₄H₈), A}			E: -1414.3430
Fe1	-0.7621038157	0.6878237939	-0.0264895540
C2	-1.6052495235	-0.9951650126	-2.4366841660
N3	-1.3960389047	0.2664066883	-2.1661549941
N4	-1.3929419205	-1.2555341593	-0.0902024918
N5	-1.3843589046	0.2287624389	2.0056017558
C6	-1.8270707289	-1.5441239141	-3.8238329585
C7	-1.6292950883	-1.0489971435	2.2487298612
C8	-1.6751336654	-1.8753643921	-1.2768567295
C9	-2.0599915359	-3.2085834194	-1.3209416726
C10	-2.2257910703	-3.9191344688	-0.1184382052
C11	-2.0690691982	-3.2446542552	1.0903403690
C12	-1.6893839148	-1.8980263855	1.0883738358
C13	-1.8772846804	-1.6107863755	3.6265607127

C14	-1.3227995012	1.2552756841	-3.1734149785
C15	-2.3757236902	2.1899762469	-3.2487606325
C16	-0.1886013297	1.3682717572	-4.0040064815
C17	-2.2833987745	3.2307745350	-4.1743989313
C18	-3.5770806374	2.0371325979	-2.3509494146
C19	-1.1698703481	3.3556698017	-5.0041792090
C20	-0.1331999797	2.4306090098	-4.9124698499
C21	0.9471016959	0.3784784195	-3.9089140851
C22	-1.2986396296	1.1730438352	3.0549371394
C23	-0.1450471628	1.2529728484	3.8604352331
C24	-2.3544145770	2.0950578906	3.2046857221
C25	-0.0683355882	2.2719417833	4.8156728720
C26	0.9828657602	0.2641124459	3.6912450125
C27	-1.1100303785	3.1810244279	4.9839521009
C28	-2.2471832282	3.0862008346	4.1821603358
C29	-3.5540180436	2.0063665125	2.2964078271
C30	0.5159198324	2.2699390894	0.5761343299
C31	0.8612006220	1.7938818386	-0.6999672896
H32	-1.8341968315	-0.7467794858	-4.5674604884
H33	-2.7833653231	-2.0745991625	-3.8802601050
H34	-2.5197750883	-4.9637497760	-0.1336348454
H35	-2.8391261576	-2.1332049036	3.6664015400
H36	-1.8886462120	-0.8213802878	4.3787842759
H37	-3.0931151532	3.9540401785	-4.2402234452
H38	-1.1074787883	4.1760409110	-5.7143305331
H39	0.7425583905	2.5332430390	-5.5496368100
H40	-3.2684271307	1.8629147281	-1.3146519363
H41	1.1169483690	0.0729492235	-2.8739234603
H42	0.8244069895	2.3514938855	5.4324366085
H43	-1.0332748050	3.9658362732	5.7318809240
H44	-3.0591465334	3.7993781774	4.3057715894
H45	1.1493702772	0.0290215328	2.6355305618
H46	-3.2431958998	2.0401288148	1.2453586810
H47	1.0902700096	1.9028360243	1.4250952871
H48	0.6177682620	2.3634653674	-1.5933262973
H49	1.6956373213	1.1029989366	-0.8139847438
H50	-2.2586934602	-3.7551204649	2.0294663746
H51	-1.1033488330	-2.3365220464	3.9027483674
H52	-2.2537906244	-3.6938341426	-2.2719623062
H53	-1.0426298895	-2.2610294201	-4.0913127170
C54	-0.1291375447	3.6224973342	0.8313312357
H55	-0.6182114371	3.6039448172	1.8103314639
H56	0.6762571354	4.3693840664	0.9145440600
C57	-1.1322487259	4.0944063565	-0.2262962418
H58	-0.6845902800	4.1690953314	-1.2222759025
H59	-1.9721857028	3.3957807961	-0.3017306923

H60	-1.5361822258	5.0790069024	0.0326588303
H62	0.7642041847	-0.6851020427	4.1958461330
H63	1.9126633824	0.6542949043	4.1144428593
H64	-4.2541125818	2.8258544007	2.4811543059
H65	-4.0891571333	1.0585211286	2.4253712871
H66	-4.1819136196	1.1686787472	-2.6396572992
H67	-4.2158610615	2.9236949288	-2.3877611929
H68	1.8724730924	0.8091650523	-4.3014964612
H69	0.7390022117	-0.5317752712	-4.4850501356

(^{Me}PDI)Fe(C₄H₈)₂, A'

E: -1571.626865

Fe1	-1.2833499940	0.8014041662	-0.0177585976
C2	-1.3629485054	-1.1459636083	-2.5604538219
N3	-0.8884124361	0.0381938627	-2.3419926541
N4	-1.6580595412	-1.2306988855	-0.2036490163
N5	-0.8890185670	-0.0498874386	1.9761834095
C6	-1.3387627840	-1.8348523762	-3.9030512412
C7	-1.4518367631	-1.2429335409	2.1568431009
C8	-1.8858607702	-1.8612798370	-1.3868382065
C9	-2.4835033522	-3.1099382688	-1.4545058106
C10	-2.8699108914	-3.7498009839	-0.2572057685
C11	-2.5873288850	-3.1389180940	0.9529173249
C12	-1.9490434014	-1.8844491139	0.9769720828
C13	-1.5097405091	-1.9379170288	3.4962644757
C14	-0.1016600969	0.7035395151	-3.3110419683
C15	-0.6353691983	1.7372573086	-4.1000092034
C16	1.2673697313	0.3591263605	-3.3896522793
C17	0.2229547186	2.4303031051	-4.9613765576
C18	-2.1034287764	2.0789664896	-4.0434555399
C19	1.5743132369	2.1110110529	-5.0435104235
C20	2.0878970012	1.0776527713	-4.2597647045
C21	1.8193175634	-0.7597909755	-2.5400553651
C22	0.0163772594	0.4499437055	2.9430288759
C23	1.3196543000	-0.0981797096	2.9845222909
C24	-0.3340474146	1.5173245549	3.7931557647
C25	2.2616085494	0.4608535639	3.8509375805
C26	1.6852610853	-1.2655156033	2.0991298875
C27	1.9276969128	1.5260984447	4.6856543977
C28	0.6335084956	2.0377787975	4.6587332526
C29	-1.7247267884	2.0991905748	3.7719506880
C30	-3.1964123298	1.5166682122	0.7212681243
C31	-3.4384546735	1.4046131237	-0.6315846124
C32	-0.5932616839	2.7902600905	-0.6175314795
C33	0.3062732572	2.2964425079	0.3091228733
H34	-0.9094778704	-1.1882877930	-4.6687765829
H35	-2.3549398679	-2.1071673797	-4.2080176996

H36	-3.3555647202	-4.7203647130	-0.2854898309
H37	-2.5428880975	-2.1956034100	3.7578016391
H38	-1.1131897580	-1.2968734904	4.2850183500
H39	-0.1831262610	3.2346623391	-5.5712721914
H40	2.2275703324	2.6647625875	-5.7124553417
H41	3.1440925311	0.8246648003	-4.3189110579
H42	-2.5587657412	1.6898532079	-3.1344328039
H43	1.4805725838	-0.6721023726	-1.5035649726
H44	3.2703760529	0.0536762273	3.8703041110
H45	2.6703403763	1.9502801150	5.3564319378
H46	0.3622629179	2.8583204232	5.3200959428
H47	1.2536676498	-1.1546443593	1.0995434919
H48	-2.4801244585	1.3312047935	3.5895670373
H49	-2.9549482785	2.4713041401	1.1763385541
H50	-1.3987479223	3.4560627598	-0.3188713974
H51	-0.3522225240	2.7894893689	-1.6761493370
H52	-3.3045494652	2.2870814870	-1.2531190544
H53	-3.5422258460	0.7472047279	1.4083289086
H54	0.1570869974	2.5408751133	1.3603922177
H55	-2.8360863837	-3.6337286667	1.8867104470
H56	-0.9356065773	-2.8726657767	3.4983631954
H57	-2.6498553217	-3.5934658102	-2.4107142699
H58	-0.7558146976	-2.7609971440	-3.8584385878
H61	-1.8265117070	2.8416140256	2.9720576346
H62	-1.9542499683	2.6009401565	4.7166512621
H63	1.2980411537	-2.2097269337	2.5018623146
H64	2.7707134118	-1.3647625916	2.0094472519
H65	2.9122835922	-0.7575770594	-2.5513858756
H66	1.4840313792	-1.7407138064	-2.8986240381
H67	-2.6422110758	1.6497886712	-4.8977117606
H68	-2.2577299973	3.1624887347	-4.0738877347
C69	1.7049585219	1.8373470600	-0.0306208085
H70	1.7987364658	1.7313992500	-1.1160392153
H71	1.9032397510	0.8559553426	0.4105269214
C72	2.7590367266	2.8238716492	0.4960548031
H73	2.7035437763	2.8985345085	1.5880324584
H74	3.7712473462	2.4962442029	0.2323903789
H75	2.6044216312	3.8248681396	0.0779314427
C76	-4.2592234088	0.2993850903	-1.2410327599
H77	-4.2769341543	-0.5598084328	-0.5625602588
H78	-3.7976724395	-0.0508044197	-2.1717961725
C79	-5.6949091562	0.7595768307	-1.5399747483
H80	-5.7004429405	1.6116985890	-2.2296264492
H81	-6.2799398852	-0.0465237900	-1.9968707036
H82	-6.2028952537	1.0733564838	-0.6217192271

(^{Me}PDI)Fe(HSiEt₃), **B**

E: -2312.8589

Fe1	3.2494891765	6.5261260347	8.9510835207
H2	1.8706778081	5.8665912100	8.0212265501
Si3	1.7575834985	5.3453945842	6.5873259593
N4	3.8905248149	4.8582764324	9.7196428047
N5	4.4775813092	7.2342386440	10.1519313887
N6	2.9998005014	8.4138446089	8.5427347550
C7	4.8415016388	5.0216540393	10.6902979565
C8	5.1888720298	6.3713814677	10.9438487541
C9	6.1254821640	6.8940954158	11.8629423123
H10	6.7037245431	6.2260352827	12.4908423391
C11	6.2927090695	8.2786271274	11.9351854105
H12	7.0150089506	8.6909651337	12.6355075743
C13	5.5568069852	9.1448450872	11.1242602015
H14	5.6967548460	10.2185726955	11.1793350614
C15	4.6268327971	8.5953574311	10.2135822363
C16	3.7734324049	9.2550657786	9.2955347342
C17	5.4625897918	3.8909434042	11.4583030139
H18	4.9188917162	2.9561476361	11.3113915928
H19	5.4736361008	4.1141270915	12.5314472023
H20	6.5064786520	3.7199681912	11.1607889705
C21	3.7274706451	10.7514776985	9.1870853166
H22	2.7982578992	11.0919032627	8.7256466470
H23	4.5575745675	11.1484083668	8.5858418968
H24	3.8045410468	11.2114740441	10.1778315558
C25	3.5155365863	3.5383947707	9.3586689025
C26	4.3355847129	2.7773110341	8.5013518379
C27	3.9391161446	1.4758708983	8.1731847500
H28	4.5631784333	0.8825049102	7.5082379698
C29	2.7643084842	0.9325892052	8.6906152577
H30	2.4724004953	-0.0816920210	8.4307902580
C31	1.9577902650	1.6986719398	9.5312952325
H32	1.0345659963	1.2795182870	9.9252424867
C33	2.3131796033	3.0069778324	9.8688423217
C34	5.6251104745	3.3533892389	7.9715277636
H35	5.5031278907	4.4043328145	7.6959488885
C36	1.4434391470	3.8515996785	10.7651853756
H37	1.9778679935	4.1472649215	11.6745806819
C38	2.1567557243	8.9857569000	7.5554175664
C39	0.7879080917	9.1572615208	7.8459172581
C40	-0.0398384706	9.7345329297	6.8794251870
H41	-1.0964455073	9.8723845098	7.0974434635
C42	0.4712756694	10.1253098596	5.6422948764
H43	-0.1848417396	10.5669401734	4.8967472241
C44	1.8233905938	9.9377268470	5.3600541733
H45	2.2205909021	10.2344788546	4.3916512736

C46	2.6850101533	9.3735203021	6.3074297041
C47	4.1540627481	9.2002937284	6.0121077323
H48	4.5323572542	8.2641002339	6.4305666452
C49	0.4775220708	6.4138427166	5.7266599080
H50	5.9778495104	2.7941198467	7.1000970265
H51	6.4152045167	3.3204283305	8.7309379689
H52	0.5328422805	3.3184622563	11.0528496188
H53	1.1626439325	4.7862483750	10.2653315889
H54	4.7469310590	10.0040403401	6.4645080157
H55	4.3443001572	9.2119354151	4.9353422595
H56	0.4152295325	6.0454646204	4.6923194163
H57	0.8325219528	7.4431604064	5.6538337594
C58	1.1210971640	3.5831432216	6.7128150333
H59	0.3001963872	3.5403999498	7.4389922019
H60	1.9123746994	2.9476526172	7.1151960624
C61	3.4638298731	5.4412852544	5.7761901790
H62	4.1205319297	6.0722122486	6.3890440228
H63	3.9034239102	4.4371427684	5.8137772280
C64	-0.9157830037	6.3735042394	6.3782083650
H65	-1.6209032611	7.0172221417	5.8410693621
H66	-0.8822577425	6.7272958878	7.4139610569
C67	3.4474086785	5.9717838790	4.3300128046
H68	2.8472562672	5.3337390863	3.6710136152
H69	4.4593123076	6.0140568311	3.9120539834
C70	0.6530862123	3.0286617162	5.3520683185
H71	1.4581943039	3.0505399170	4.6073089755
H72	0.3292128557	1.9859604512	5.4445190452
H73	-0.1881338763	3.5982975356	4.9417376311
H74	3.0261790612	6.9810537967	4.2825739095
H75	-1.3327552225	5.3596745018	6.3873150260
C76	0.2511206240	8.7290639907	9.1883889041
H77	-0.8330916233	8.8615509924	9.2439195644
H78	0.4906048089	7.6779734969	9.3868184317
H79	0.7142318621	9.2997910496	10.0010599991

Anti-Markovnikov Hydride Migration TS, $\text{TS}(\text{A} \rightarrow \text{D}_{\text{AM}})$, $^{\text{Me}}\text{PDI}$

E: -1414.343026

Fe1	2.6142025536	6.1913856240	8.5839800672
H2	1.6733092259	5.8230177702	7.3659366404
Si3	3.4717743594	5.8145982017	6.2871057966
N4	3.3718222589	4.3590883444	9.6251725684
N5	4.3633821890	6.7361624483	9.2345319722
N6	2.5702903542	8.5474985016	8.5762328481
C7	4.6414922057	4.4810085267	9.9376605276
C8	5.2488397997	5.7646990107	9.6596730949
C9	6.5958006948	6.0637892048	9.8614000532
H10	7.2827061647	5.2819348462	10.1694833933

C11	7.0564374091	7.3682507966	9.6762872701
H12	8.1036454726	7.6108140921	9.8245409794
C13	6.1358072524	8.3657076593	9.3263156924
H14	6.4663018829	9.3937420410	9.2203218053
C15	4.8000811790	8.0401342008	9.1183945073
C16	3.7597632784	9.0187189587	8.8300492286
C17	5.4492407822	3.3883962472	10.5940579825
H18	6.3131922967	3.1260834555	9.9730218972
H19	4.8472419039	2.4903872701	10.7375987530
H20	5.8345730316	3.7061096546	11.5691346745
C21	4.0920660829	10.4921851996	8.8538204366
H22	4.5296061839	10.7921969966	9.8118093318
H23	3.2006196632	11.0946559236	8.6755412072
H24	4.8260347706	10.7256751390	8.0739233151
C25	2.5903196609	3.3037170138	10.1528279269
C26	2.1714687562	2.2358585647	9.3347528966
C27	1.3231777349	1.2669487646	9.8766098305
H28	0.9997696056	0.4401276666	9.2479825170
C29	0.8869627489	1.3474159906	11.1971440119
H30	0.2218580496	0.5884719988	11.6006093286
C31	1.3053761051	2.4094026739	11.9950115506
H32	0.9635958493	2.4809349468	13.0253411349
C33	2.1598941739	3.3963394260	11.4953742284
C34	2.6333880722	2.1516706356	7.9055399166
H35	2.3642385989	3.0597646399	7.3579201578
C36	2.6023290761	4.5508227026	12.3615698613
H37	2.5187680850	5.4986352934	11.8204934354
C38	1.4114862212	9.3534955331	8.5746064028
C39	0.9155481517	9.8359526299	9.8091833338
C40	-0.3011135681	10.5235361500	9.8209052782
H41	-0.6919711039	10.8848460236	10.7696003467
C42	-1.0193730272	10.7389394347	8.6478738317
H43	-1.9663499829	11.2712848083	8.6755021518
C44	-0.5217984505	10.2555539158	7.4402585748
H45	-1.0806128534	10.4154910457	6.5207649025
C46	0.6858811870	9.5564359842	7.3816454846
C47	1.6644306318	9.5814509212	11.0964641562
H48	2.0317726154	8.5511662720	11.1432668570
C49	1.2070459987	9.0382160639	6.0673279015
H50	1.4880050422	7.9861730953	6.1478053192
C51	2.2568760007	5.3436482711	4.8763051066
H52	2.1870984067	1.2942227566	7.3941302792
H53	3.7224230560	2.0614644722	7.8410735137
H54	3.6519897870	4.4512190299	12.6640616740
H55	2.0004185965	4.6086495120	13.2723335361
H56	1.0196189820	9.7608518450	11.9609178312

H57	2.5390022718	10.2353236061	11.1981360178
H58	2.1041982616	9.5778078851	5.7434192535
H59	0.4550446348	9.1375496482	5.2800657191
H60	1.6275435360	6.2151319031	4.6463943797
H61	1.5681289907	4.5933843052	5.2881882947
C62	4.7806955585	4.4142651366	6.3478261473
H63	4.2753239712	3.4753171719	6.0956522773
H64	5.1298037357	4.2970302578	7.3790570000
C65	4.3963332062	7.4333387229	5.8460890956
H66	3.8637330987	8.2653013008	6.3097600702
H67	5.3614829630	7.3885204972	6.3679319058
C68	2.8628739105	4.7805928593	3.5773901305
H69	2.0824609728	4.5127473665	2.8538618547
H70	3.5285935144	5.4968862565	3.0874410644
H71	3.4464703539	3.8739508903	3.7725731153
C72	4.6173809971	7.7499795315	4.3577962431
H73	5.2200734401	6.9845012202	3.8590852077
H74	3.6656551407	7.8200448678	3.8186700089
H75	5.1357260973	8.7086133985	4.2248785160
C76	5.9979542473	4.5946362428	5.4212742407
H77	6.5556598360	5.5072982581	5.6569039584
H78	6.6978704715	3.7540283101	5.5160240731
H79	5.7053256481	4.6543608928	4.3676894121
C80	0.7667865324	6.1918885227	9.5988156641
C81	0.4293151859	5.9359762964	8.2430278184
H82	0.7219062636	5.3651907475	10.3020542465
H83	0.0333396539	6.7894216854	7.6891347294
H85	0.5853429817	7.1768048300	10.0120494505
C86	-0.2035799283	4.6072947018	7.8506875176
H87	0.3033750399	3.7996332388	8.3856904714
H88	-0.0673565302	4.4194962327	6.7794187741
C89	-1.6997147846	4.5860393743	8.1866315808
H90	-2.2355119018	5.3871274675	7.6636895608
H91	-2.1525996266	3.6321231713	7.8951571169
H92	-1.8576222679	4.7254504909	9.2609880392

Markovnikov Hydride Migration TS, $\text{TS}(\text{A} \rightarrow \text{D}_M)$

Fe1	2.5198719931	6.3018233097	8.6525741570
H2	1.7041634210	5.7654094800	7.3870981700
Si3	3.4279243104	5.8879444753	6.3365233913
N4	3.2740108347	4.3326114036	9.6374009490
N5	4.3061841788	6.7319762736	9.3227917232
N6	2.5826364766	8.5890107264	8.6244596401
C7	4.5321842422	4.4375872615	9.9676628193
C8	5.1649421258	5.7236664898	9.7127602247
C9	6.5230454439	5.9665075657	9.8849992484

E: -1942.2177

H10	7.1840441194	5.1593965285	10.1831516726
C11	7.0386181086	7.2514803944	9.6704752291
H12	8.0987261814	7.4483749909	9.7921237925
C13	6.1619772358	8.2756012589	9.3101561886
H14	6.5382126310	9.2811796581	9.1535509738
C15	4.8021574901	8.0101980103	9.1472814051
C16	3.8142392762	9.0123137602	8.8187449470
C17	5.3223313883	3.3255599166	10.6144021968
H18	6.1649624611	3.0362225655	9.9762364428
H19	4.6970349853	2.4460804532	10.7722575212
H20	5.7371723254	3.6363262198	11.5790673370
C21	4.2337411631	10.4570035694	8.6762177119
H22	4.7320607887	10.8308575027	9.5766838088
H23	3.3767885223	11.0975439084	8.4672883755
H24	4.9435615783	10.5573345316	7.8465224609
C25	2.4620316754	3.2767911974	10.1125574065
C26	1.9970378338	2.2762877488	9.2361776942
C27	1.1050166488	1.3182802374	9.7240714569
H28	0.7497565775	0.5404227215	9.0515820446
C29	0.6661917688	1.3471492789	11.0455998835
H30	-0.0346516784	0.5986908902	11.4055530678
C31	1.1247797839	2.3468523590	11.8997729269
H32	0.7750162463	2.3835217458	12.9291367208
C33	2.0232421163	3.3205875771	11.4561942247
C34	2.4703165532	2.2366597310	7.8081890909
H35	2.2756960534	3.1862213462	7.3020205887
C36	2.4841719503	4.4252959177	12.3760568376
H37	2.4217985858	5.3986619576	11.8777459214
C38	1.5030136145	9.5043359224	8.6054004498
C39	1.1475400009	10.1702305571	9.8030482211
C40	0.0138827253	10.9864043475	9.8106515180
H41	-0.2694276859	11.4847543861	10.7351636164
C42	-0.7646623240	11.1525263281	8.6684631526
H43	-1.6471028353	11.7864999359	8.6927321188
C44	-0.4122491200	10.4845362178	7.4989410638
H45	-1.0216966257	10.5994061088	6.6049789590
C46	0.7109937687	9.6547041511	7.4469236212
C47	1.9331298633	9.9544060292	11.0744215089
H48	2.2113509013	8.9022411937	11.1896303712
C49	1.0580800665	8.9329803094	6.1719751805
H50	1.2986653298	7.8877657715	6.3745939854
C51	2.1903339107	5.4033955942	4.9447121767
H52	1.9753476958	1.4386959170	7.2480165974
H53	3.5517294296	2.0742971990	7.7511846827
H54	3.5287388354	4.2934417686	12.6825054407
H55	1.8747477912	4.4556852041	13.2829427119

H56	1.3460726825	10.2576453005	11.9455687737
H57	2.8637805391	10.5338608523	11.0897217440
H58	1.9361075736	9.3677490947	5.6817599429
H59	0.2280983081	8.9697618008	5.4608885683
H60	1.6112664920	6.2980402618	4.6757753838
H61	1.4552851377	4.7077383177	5.3760902876
C62	4.7519624593	4.5046784534	6.3940960608
H63	4.2563313929	3.5546236803	6.1672710362
H64	5.1238545055	4.4092271523	7.4194118931
C65	4.3191303896	7.5115040938	5.8549887170
H66	3.7706790532	8.3439277846	6.2984924244
H67	5.2897834221	7.5027651441	6.3678386518
C68	2.7730344957	4.7633389433	3.6714963531
H69	1.9834092192	4.5029772168	2.9552052759
H70	3.4701828560	5.4322723387	3.1583529775
H71	3.3169757188	3.8406903177	3.9025767974
C72	4.5181691798	7.7851272003	4.3546266578
H73	5.1328090261	7.0181728662	3.8734430649
H74	3.5600122500	7.8165041665	3.8233564179
H75	5.0128778378	8.7504732966	4.1866901572
C76	5.9483077399	4.6855765072	5.4407266275
H77	6.4958519039	5.6111638949	5.6478028164
H78	6.6629235436	3.8578180000	5.5377194584
H79	5.6333839174	4.7196135004	4.3925062597
C81	0.6112915839	5.9891385853	9.5312066866
C82	0.5189790955	5.5719314422	8.1635770846
H83	0.7590544464	5.1885778498	10.2508360998
H84	0.4676702614	4.5035656498	7.9572982158
H85	-0.1215085347	6.1647707768	7.5086263484
C86	-0.2464172765	7.1205196252	10.0507680391
H87	-0.3650643125	7.8889420718	9.2830116295
H88	0.2403300052	7.6072484623	10.9032253043
C89	-1.6372034056	6.6262116795	10.4840263891
H90	-1.5596922024	5.8630687225	11.2674527862
H91	-2.2477159673	7.4503521742	10.8716731690
H92	-2.1708777127	6.1773297021	9.6381489522

(^{Me}PDI)Fe(CH₂CH₂Et)(SiEt₃), **D**_{AM} E: -1942.2553

Fe1	15.5091426424	5.1950720898	2.9039291138
N2	14.5070918231	7.1896867961	2.6416601130
N3	15.6365028488	5.6265026327	0.9306843362
N4	15.7588015253	3.1936104096	1.8166947057
C5	14.1722249929	9.1101970111	1.0877551686
H6	13.5734641475	9.5393120379	1.8923469661
H7	13.5571108857	9.0748658149	0.1831306830
H8	15.0102516596	9.7876560561	0.8886809542

C9	14.6590580079	7.7318046529	1.4583891970
C10	15.2841804920	6.8768355752	0.4688234169
C11	15.9778975056	4.6591935593	0.0124839582
C12	16.0494221610	3.3094881453	0.5471543686
H13	16.2404893282	1.1982983287	0.1550569782
C14	13.9226811637	7.8533520565	3.7428955645
C15	14.5680415025	8.9276196905	4.3943166306
C16	14.0239569003	9.4046697997	5.5927757499
H17	14.5324901082	10.2138604504	6.1125344736
C18	12.8604692981	8.8623937443	6.1279311961
H19	12.4616495518	9.2397820886	7.0657792922
C20	12.2056196524	7.8349535293	5.4494456693
H21	11.2857509437	7.4185867918	5.8535098698
C22	12.7171999099	7.3214766376	4.2581270303
C23	11.9715304729	6.2501162048	3.5019291352
H24	12.6489640759	5.4942817406	3.0987069394
C25	15.7780017603	1.9587434959	2.5061639307
C26	14.5481532453	1.4771213935	3.0086949052
C27	14.5453137033	0.3304848260	3.8026861824
C28	13.2603583836	2.1728471443	2.6474583608
H29	13.3216844210	3.2462419736	2.8410534073
Si30	17.7212780114	5.5090688771	3.7193529528
C31	15.4659513452	7.2283545019	-0.8672338734
H32	15.2142684257	8.2291355774	-1.2030847984
C33	15.9474744236	6.2830577149	-1.7761168508
H34	16.1006221087	6.5450005429	-2.8179317800
C35	16.1657233742	4.9746951083	-1.3297063203
H36	16.4630575615	4.2031741267	-2.0321659656
C37	16.3633391816	2.1488084398	-0.3648770213
H38	17.3910939760	2.2061475880	-0.7403874403
H39	15.6980951268	2.1524275703	-1.2343280712
C40	15.8075515853	9.5817104018	3.8340507807
H41	16.3579810194	8.9137198343	3.1716901738
C42	16.9832618259	1.2744447180	2.7760992553
C43	16.9345377169	0.1359138632	3.5891322386
C44	18.3090051540	1.7292731170	2.2145882954
C45	15.7325375302	-0.3353053348	4.1052855678
H46	17.8629238884	-0.3821699381	3.8199876816
H47	18.3455161374	2.8109920199	2.0820581374
H48	15.7186629865	-1.2179545039	4.7393154197
H49	13.6001443313	-0.0416864338	4.1914873960
C50	18.3210889463	4.0250971834	4.7670026377
H51	17.7819547278	3.1348844312	4.4301875850
H52	17.9547721186	4.2017028290	5.7870386441
C53	17.9351897619	7.1077719365	4.7505518402
H54	16.9703869834	7.3701929459	5.1959288735

H55	18.1635197890	7.9142987777	4.0422901812
C56	19.8285140330	3.7240856983	4.8089611016
H57	20.4060031156	4.5693322642	5.1969471801
H58	20.0466703895	2.8592737674	5.4491196856
H59	20.2190014652	3.4936346585	3.8118461163
C60	19.0112419702	7.0819699945	5.8504237368
H61	20.0115095691	6.9119776953	5.4369902290
H62	19.0436362340	8.0292751301	6.4038002829
H63	18.8231324186	6.2873230372	6.5807829297
C64	18.7788352084	5.7589489478	2.1383135044
H65	18.7753236834	4.8369390370	1.5424477119
H66	18.2237434774	6.4864687102	1.5312209475
C67	20.2222190976	6.2567008162	2.3410122433
H68	20.2457793087	7.1890390929	2.9170499779
H69	20.8361166289	5.5290548575	2.8802603255
H70	20.7182062588	6.4567737682	1.3822128595
C71	15.1021793242	4.6082043830	4.7749955315
H72	15.4920091966	3.5988002251	4.9517777699
H73	14.0390658830	4.4793766654	4.4833537337
C74	15.1508736715	5.4440480583	6.0502499301
H75	14.9109885092	6.4893062747	5.8298181083
H76	16.1692623261	5.4443128965	6.4591949442
C77	14.1850380941	4.9448687787	7.1349351139
H78	14.4153967528	3.8973324719	7.3745143944
H79	13.1641230408	4.9513771783	6.7281957537
C80	14.2339880144	5.7999619180	8.4042002736
H81	13.9706256073	6.8396249390	8.1767943239
H82	13.5399932659	5.4350713601	9.1697188310
H83	15.2405489234	5.8013492931	8.8398601698
H84	11.4395062345	6.6766989662	2.6422391902
H85	11.2359502341	5.7541529418	4.1408088316
H86	16.4825061763	9.8915940782	4.6361238283
H87	15.5460971286	10.4793783842	3.2598784384
H88	18.5049616286	1.2710618943	1.2375642783
H89	19.1291901490	1.4433008888	2.8778842782
H90	12.4186166733	1.7655560210	3.2138173850
H91	13.0379640325	2.0638401714	1.5790032034

(^{Me}PDI)Fe(CHMeEt)(SiEt₃), **D_M**

E: -1942.221757

Fe1	2.4954813270	6.2881609469	8.5381487937
H2	1.4100554247	5.7583001255	7.3236545705
Si3	3.6702966332	5.9226626765	6.3299426114
N4	3.1931462530	4.3180660291	9.5105477280
N5	4.2036648069	6.7346454341	9.3099941353
N6	2.5136749836	8.5615454021	8.4718718444
C7	4.4207641526	4.4378213193	9.9412664267

C8	5.0462971086	5.7372767954	9.7630652013
C9	6.3835777226	6.0030698031	10.0385021730
H10	7.0331208639	5.2049439465	10.3826969300
C11	6.8941187717	7.2948730845	9.8651868504
H12	7.9387664976	7.5076715731	10.0666117673
C13	6.0320095364	8.3055516418	9.4356760479
H14	6.4047485617	9.3159172681	9.3035391396
C15	4.6936155992	8.0206507262	9.1702547622
C16	3.7196468532	9.0042762012	8.7562122465
C17	5.1884968871	3.3212058886	10.6059936617
H18	6.0622032837	3.0527131294	10.0012658392
H19	4.5660373806	2.4329741582	10.7172542356
H20	5.5550217660	3.6169210459	11.5943380180
C21	4.1318046026	10.4519370667	8.6257270072
H22	4.5450930942	10.8462156922	9.5596290943
H23	3.2891584290	11.0774315548	8.3312964714
H24	4.9100615373	10.5458454071	7.8594114500
C25	2.3687542932	3.2345159630	9.8946731953
C26	1.9288972322	2.2961975376	8.9386326852
C27	1.0259701487	1.3063100604	9.3333758176
H28	0.6919133452	0.5768828303	8.5986205180
C29	0.5486557389	1.2442007462	10.6403277125
H30	-0.1595516121	0.4717101171	10.9278981580
C31	0.9753794970	2.1867431332	11.5718287599
H32	0.5911560247	2.1557144060	12.5889774529
C33	1.8832200509	3.1903634796	11.2227941799
C34	2.4384969669	2.3522496621	7.5242492684
H35	2.3394238776	3.3593126847	7.1125298793
C36	2.2984711145	4.2354314288	12.2306837431
H37	2.2775482492	5.2361890633	11.7867249409
C38	1.4272985746	9.4618662269	8.3547735543
C39	0.9800332546	10.1533966830	9.5062281676
C40	-0.1588291415	10.9567147582	9.4094715689
H41	-0.5138334026	11.4745601626	10.2976945501
C42	-0.8529079800	11.0850192348	8.2094178720
H43	-1.7403363057	11.7098428264	8.1526198943
C44	-0.4090283944	10.3928783183	7.0857508669
H45	-0.9499372811	10.4816914428	6.1459408139
C46	0.7227582928	9.5752070564	7.1372960457
C47	1.6704282377	9.9785564397	10.8378710283
H48	1.9715135675	8.9381380416	10.9905786805
C49	1.1795020883	8.8358740421	5.9083210029
H50	1.4171920328	7.7982307030	6.1484260175
C51	2.4986303991	5.3902444203	4.8941910118
H52	1.8956304713	1.6565959840	6.8787326040
H53	3.5032829060	2.1004631514	7.4743494644

H54	3.3183648653	4.0701912534	12.5976690522
H55	1.6315679050	4.2235262783	13.0966685268
H56	1.0067147960	10.2719531208	11.6557207350
H57	2.5768070291	10.5904147019	10.9171617311
H58	2.0894125635	9.2736031399	5.4833273341
H59	0.4097555814	8.8479317635	5.1317510700
H60	1.9455863242	6.2793862780	4.5616934677
H61	1.7335200698	4.7166176707	5.3051857626
C62	5.0363537424	4.5818930581	6.4630163295
H63	4.5710999643	3.6066979511	6.2835182856
H64	5.3969186387	4.5512677072	7.4972970635
C65	4.5510527126	7.5546659508	5.8415529262
H66	3.9651198166	8.3886638565	6.2348073925
H67	5.4991265924	7.5828115840	6.3954809631
C68	3.1435232860	4.7031717457	3.6764533438
H69	2.3907835651	4.4202541609	2.9293475695
H70	3.8690968541	5.3526966196	3.1776399543
H71	3.6708109605	3.7879345644	3.9675658711
C72	4.8107904536	7.7915553780	4.3436671659
H73	5.4571241197	7.0218494818	3.9109299461
H74	3.8759185463	7.7905264091	3.7713408709
H75	5.2963910389	8.7602859633	4.1675769905
C76	6.2455513498	4.7426597464	5.5222563143
H77	6.7639105260	5.6934437433	5.6868458331
H78	6.9814841885	3.9425989825	5.6772475694
H79	5.9503619791	4.7103650834	4.4684165872
C80	0.6287377295	6.0040263460	9.4079323665
C81	0.4378088432	5.6064128364	7.9954628998
H82	0.2554680230	4.5429506335	7.8272665029
H83	-0.2799535737	6.2246494191	7.4501293868
C84	-0.2782321664	7.0735217087	9.9727168178
H85	-0.3501401801	7.9168517147	9.2822789316
H86	0.1451345187	7.4660184424	10.9047005131
C87	-1.6935344519	6.5387079234	10.2527050371
H88	-1.6665367241	5.6952443924	10.9526175836
H89	-2.3362950308	7.3166221081	10.6810145074
H90	-2.1648175555	6.1846235152	9.3282612368
H91	0.7228920945	5.1560224391	10.0821630723

Reductive Elimination TS, $\text{TS}(\text{D}_{\text{AM}} \rightarrow \text{B})$

E: -1942.2430

Fe1	15.4941634238	5.2117055313	3.0647727151
N2	14.7499906090	7.1729909828	2.7578876731
N3	15.6385909878	5.4619624981	1.0249336118
N4	15.7270044718	3.0275547007	1.9759317865
C5	14.5767927972	9.0865688586	1.1515174095
H6	14.0479116830	9.5915303747	1.9616511483

H7	13.9352671374	9.1097819868	0.2636574462
H8	15.4735767355	9.6740654481	0.9180533713
C9	14.9298467642	7.6715945634	1.5366957433
C10	15.4282762560	6.7456362839	0.5590349274
C11	15.8998935473	4.4679933641	0.1298843375
C12	15.9257050313	3.1143841425	0.6972615080
H13	15.9619829029	0.9900920556	0.3232287769
C14	14.1455362776	7.9243568625	3.7942205342
C15	14.8701810083	8.8947536255	4.5181043605
C16	14.2657332802	9.4880114786	5.6318021556
H17	14.8278854993	10.2203359432	6.2075422593
C18	12.9674343332	9.1573115467	6.0108951097
H19	12.5185492929	9.6208500183	6.8856956373
C20	12.2427998400	8.2363814525	5.2557624474
H21	11.2212164466	7.9888242962	5.5361682924
C22	12.8114198512	7.6177100178	4.1409676849
C23	12.0125445422	6.6552282730	3.2967624901
H24	12.5953399442	5.7647353969	3.0404715284
C25	15.7364968982	1.8101907355	2.6821405372
C26	14.5273935170	1.4136322004	3.2977722294
C27	14.5286971787	0.2880147056	4.1205337278
C28	13.2701198287	2.2113483171	3.0568697443
H29	13.4062107492	3.2590624318	3.3488150125
Si30	17.4921454314	5.4513473618	4.3043153458
C31	15.6390908110	7.0541201404	-0.7949299115
H32	15.5140836706	8.0752899621	-1.1414581494
C33	15.9908076618	6.0528443877	-1.6882286487
H34	16.1602931870	6.2813305705	-2.7361376407
C35	16.0917376479	4.7288472404	-1.2216228344
H36	16.3176394545	3.9238794549	-1.9120621757
C37	16.1119127154	1.9261953061	-0.2158847442
H38	17.1189050777	1.9189621421	-0.6471540119
H39	15.4023654797	1.9665569324	-1.0481523155
C40	16.2546921295	9.3141962767	4.0899018386
H41	16.8105351923	8.4815633111	3.6592946554
C42	16.9292665250	1.0860397556	2.8932905405
C43	16.8862494961	-0.0287810904	3.7379050470
C44	18.2307122009	1.4898095884	2.2417115898
C45	15.7023801621	-0.4304360547	4.3482799603
H46	17.8041528756	-0.5836822228	3.9198163336
H47	18.2876853587	2.5678822891	2.0739168660
H48	15.6932614222	-1.2972590080	5.0035431724
H49	13.6006130686	-0.0213002548	4.5958320562
C50	18.5578323177	3.9232450744	4.7617685274
H51	18.0483533123	3.0435367564	4.3553409078
H52	18.5073736792	3.7917276202	5.8507940463

C53	17.4974721809	6.6764014557	5.7838065828
H54	16.5246969954	7.1805925170	5.8103009199
H55	18.2244108781	7.4650669082	5.5573871192
C56	20.0308925459	3.9112295940	4.3301642124
H57	20.6065364120	4.6955220259	4.8347132857
H58	20.5117377591	2.9544169360	4.5698497849
H59	20.1429688548	4.0699641678	3.2522628683
C60	17.8077491437	6.1188489065	7.1858018209
H61	18.8045197690	5.6661408490	7.2340290565
H62	17.7751859275	6.9121585742	7.9433532727
H63	17.0882142968	5.3529874050	7.5001456878
C64	18.3362775477	6.3080002916	2.7996455097
H65	18.5999026190	5.4975575056	2.1072456266
H66	17.5969706774	6.9074250818	2.2591468341
C67	19.5625465162	7.1781809936	3.1175964358
H68	19.2743436521	8.0681235702	3.6875765124
H69	20.3088200774	6.6409908526	3.7106300354
H70	20.0554457066	7.5242722709	2.2009835336
C71	15.6422852379	4.3479400265	4.9599102371
H72	16.3492437850	4.2490256196	5.7870347075
H73	15.4897397823	3.3104865431	4.6447846688
C74	14.3702489599	4.9452511890	5.5723977060
H75	13.5706136996	5.0601337352	4.8312378981
H76	14.5721924756	5.9573176413	5.9401900560
C77	13.8328790945	4.0703873836	6.7093720895
H78	14.6087517337	3.9737569608	7.4815482367
H79	13.6594153158	3.0570859667	6.3223037164
C80	12.5486051497	4.6351897091	7.3163929208
H81	11.7642897792	4.7170428640	6.5542294493
H82	12.1690844563	4.0023312152	8.1252894518
H83	12.7171717268	5.6407399492	7.7186190807
H84	11.7272777954	7.1143587561	2.3421844128
H85	11.0977989993	6.3435732053	3.8089479874
H86	16.8243298039	9.7094032331	4.9351958628
H87	16.2063555752	10.1005903596	3.3260773419
H88	18.3495026361	0.9991342777	1.2678852285
H89	19.0836012533	1.2004299658	2.8621647738
H90	12.4284625443	1.8059366283	3.6248365456
H91	12.9965918300	2.2258251438	1.9958577348

(^{Me}PDI)Fe, **B** E: -1257.023182

Fe1	0.0035068265	-0.2395157521	-0.0636125448
C2	-0.3683351064	-1.8289440563	-2.3684097155
N3	-0.0952714300	-0.5339576345	-2.0140721322
N4	-0.3575427466	-2.1676915908	-0.0697283279
N5	-0.1054715616	-0.6195457480	1.8939478480

C6	-0.5629637776	-2.2777469543	-3.7889181813
C7	-0.3603054203	-1.9049404146	2.2245061394
C8	-0.5124495831	-2.7568596574	-1.2893277044
C9	-0.8081600254	-4.1361882775	-1.3267796309
C10	-0.9459389923	-4.8268289670	-0.1189139748
C11	-0.8091031999	-4.1833849934	1.1199502282
C12	-0.5108143178	-2.8084178871	1.1119596896
C13	-0.5191312053	-2.3944593495	3.6351204417
C14	0.0675062711	0.4564032492	-3.0201745988
C15	-0.9818509478	1.3707808208	-3.2482175946
C16	1.2692838083	0.5395016623	-3.7529224150
C17	-0.8203082304	2.3501166222	-4.2319625338
C18	-2.2568489524	1.2725661621	-2.4485189025
C19	0.3543265184	2.4289078762	-4.9773170375
C20	1.3910422589	1.5310537455	-4.7310943239
C21	2.3937877716	-0.4272334416	-3.4804118160
C22	0.0423996773	0.3555214923	2.9212665775
C23	1.2803722363	0.5103066568	3.5730282967
C24	-1.0613468166	1.1676103066	3.2463773516
C25	1.3892165328	1.4801642935	4.5744596514
C26	2.4471903411	-0.3701190508	3.2012416999
C27	0.3011885428	2.2793865176	4.9198762962
C28	-0.9132401357	2.1247146996	4.2539728656
C29	-2.3736593110	0.9793702816	2.5262478275
H32	-0.5275592913	-1.4407031619	-4.4875769614
H33	-1.5314877019	-2.7793601604	-3.9088914046
H34	-1.1733367427	-5.8895341671	-0.1414529849
H35	-1.4987224020	-2.8688972648	3.7709335183
H36	-0.4273828109	-1.5864513187	4.3618642759
H37	-1.6298277880	3.0520253517	-4.4203577642
H38	0.4621219698	3.1888358642	-5.7469478385
H39	2.3113972681	1.5960177828	-5.3074849084
H40	-2.0626050824	1.4021481296	-1.3748215333
H41	2.5804820997	-0.5149743804	-2.4043345394
H42	2.3378383946	1.6036246634	5.0921081152
H43	0.3996028689	3.0222929496	5.7071027287
H44	-1.7624308974	2.7490838257	4.5225539667
H45	2.6057062317	-0.3784558735	2.1170200096
H46	-2.2509312300	1.0874588204	1.4409040676
H50	-0.9352898202	-4.7247044825	2.0511804218
H51	0.2345730003	-3.1557846548	3.8720402614
H52	-0.9309306710	-4.6496680444	-2.2746839196
H53	0.2055242135	-3.0017648962	-4.0911319620
H62	2.2722155623	-1.4117046579	3.4958646015
H63	3.3666427680	-0.0325169963	3.6866788362
H64	-3.1179688060	1.7062645456	2.8623944647

H65	-2.7775418982	-0.0268233913	2.6869847467
H66	-2.7209961342	0.2860070104	-2.5535228027
H67	-2.9792993938	2.0322906665	-2.7595276402
H68	3.3156124380	-0.1069970872	-3.9736054442
H69	2.1549966316	-1.4358165764	-3.8370114018

(^{Me}PDI)Fe(H)(CHEtCH₂SiEt₃), E_{AM} E: -1942.2438

Fe1	14.9759200756	5.3957735006	1.9873547803
N2	14.3580508568	7.3467312002	1.9303401950
N3	15.0065455165	5.7600875960	0.1130343834
N4	14.6876392416	3.5280767572	1.1952691932
C5	14.3033208880	9.4266207509	0.5369946022
H6	13.6588204200	9.8490363215	1.3107721935
H7	13.8489369071	9.6257367176	-0.4364119670
H8	15.2571188627	9.9653821320	0.5724878113
C9	14.4963582049	7.9509154091	0.7524200142
C10	14.7884128657	7.0505713203	-0.3248865477
C11	14.9309004918	4.7107447517	-0.7808753246
C12	14.8363787573	3.4383329472	-0.1227543392
H13	14.4236785554	1.3363211193	-0.3084200796
H14	14.4486714306	5.0528007220	3.3821032689
C15	14.0072663360	8.0915291673	3.0932300886
C16	14.9019801610	8.9857699798	3.7136371507
C17	14.4988606743	9.6115877090	4.9006760960
H18	15.1936561653	10.2852506667	5.3977341428
C19	13.2415677116	9.3883402070	5.4469493573
H20	12.9516974905	9.8806903601	6.3714688298
C21	12.3551464597	8.5244534968	4.8050714674
H22	11.3686274571	8.3460332284	5.2261253737
C23	12.7219936335	7.8626492713	3.6347394937
C24	11.7734569678	6.9148387373	2.9506527647
H25	12.2311294179	5.9264669882	2.8593866296
C26	14.6381806874	2.3529399603	2.0014102546
C27	13.4314237630	2.0791599324	2.6842667721
C28	13.3642383752	0.9579668945	3.5097948129
C29	12.2460239017	2.9953906430	2.5380119653
H30	12.4582817537	3.9471439352	3.0350800286
C31	14.7641421329	7.3284562045	-1.6905205438
H32	14.6351756322	8.3486907165	-2.0368365680
C33	14.8574485851	6.2806173984	-2.6125864123
H34	14.8284079527	6.4860109015	-3.6776109712
C35	14.8988084590	4.9588760402	-2.1500928223
H36	14.8763563752	4.1332547252	-2.8538745450
C37	14.8848343880	2.1418408583	-0.8826047313
H38	15.9173164244	1.8448818540	-1.1002680697
H39	14.3598627614	2.2304402750	-1.8373997370

C40	16.2647364298	9.3118193610	3.1485486718
H41	16.5999123390	8.5738405613	2.4212398675
C42	15.7620309912	1.5170866112	2.1619243143
C43	15.6489308209	0.4029746902	3.0033811446
C44	17.0893051054	1.7793310090	1.4921056356
C45	14.4662118325	0.1190234766	3.6730282959
H46	16.5163270426	-0.2396518693	3.1379976695
H47	17.1345521715	2.7630849085	1.0303758727
H48	14.4017828114	-0.7468535558	4.3267587552
H49	12.4368667870	0.7439589075	4.0358307925
Si50	16.2227814195	5.0624891238	5.6721018252
H51	17.3466392900	1.4182130870	5.0598563806
H52	18.0905696736	2.9179541257	4.4968649022
C53	16.9385336744	4.7367153923	8.4657162424
H54	16.8707842113	3.6451570449	8.3815642812
H55	17.6275007534	4.9568911491	9.2910014628
H56	15.9472439683	5.0984242763	8.7651214153
C57	13.3924650925	4.7896312786	6.3700706250
H58	13.2299428264	4.1553050847	5.4911646965
H59	13.6118064234	4.1237460340	7.2137324260
H60	12.4446655886	5.2967995592	6.5924793468
C61	16.8969840449	5.3750969400	2.7759818157
H62	17.1171673711	4.3002551959	2.8108791361
C63	17.0001466434	5.9629139587	4.1943138495
H64	16.5857925638	6.9765175721	4.2169667683
H65	18.0701323796	6.0928058738	4.4414411246
C66	17.8748462031	6.0641184702	1.8065969874
H67	18.7873348274	6.3411147033	2.3621650862
H68	17.4534522643	7.0151336051	1.4525655254
C69	18.2910339319	5.2314371768	0.5925147910
H70	17.4236346572	4.9552374879	-0.0115426086
H71	18.9833153959	5.7859715265	-0.0510639444
H72	18.7967209693	4.3109819099	0.9058979467
C73	17.3928869635	5.3738502295	7.1405067239
H74	18.3965647381	5.0107228756	6.8784792320
H75	17.4976938968	6.4615166656	7.2684871696
C76	16.1072309458	3.1951255783	5.3924433817
H77	15.5225665788	2.7505532990	6.2089519312
H78	15.5226538991	3.0206292010	4.4836553997
C79	14.5277233044	5.7972204371	6.1213356850
H80	14.6555892196	6.4340683168	7.0085552701
H81	14.2354044257	6.4723626446	5.3133270045
C82	17.4673508303	2.4835677389	5.2881170694
H83	18.0361789725	2.5590380674	6.2226507955
H84	17.0134804065	9.3597406083	3.9448300147
H85	16.2541591395	10.2928173085	2.6573845092

H86	11.5380859847	7.2444815322	1.9322832985
H87	10.8385659931	6.8180633950	3.5088317711
H88	11.3505881686	2.5597867608	2.9902643244
H89	12.0331562490	3.2267570910	1.4895140117
H90	17.2934397944	1.0300772792	0.7171904054
H91	17.9001288147	1.7159005113	2.2247091750

(MePDI)Fe(O₂)

E: -1407.4755

Fe1	-1.2053472628	0.7508173420	-0.0385908562
C2	-1.6232421199	-0.9967081081	-2.4196894138
N3	-1.3615019520	0.2548937774	-2.1248932773
N4	-1.6332659280	-1.2257960188	-0.0695414140
N5	-1.3664665876	0.1813838601	2.0368781462
C6	-1.7598673938	-1.5224645090	-3.8225571416
C7	-1.6254201877	-1.0778170601	2.2879841408
C8	-1.7861958462	-1.8700856351	-1.2717399867
C9	-2.0764697468	-3.2313995055	-1.3138763581
C10	-2.2221302728	-3.9435844766	-0.1174478539
C11	-2.0811956946	-3.2715630089	1.1044529361
C12	-1.7898597459	-1.9112995016	1.1082346844
C13	-1.7557535486	-1.6540147878	3.6714078732
C14	-1.1699804138	1.2502014142	-3.1195410674
C15	-2.2393896153	2.1116860609	-3.4243607960
C16	0.1020101982	1.4216235899	-3.6936690971
C17	-2.0232802798	3.1318578671	-4.3539432760
C18	-3.5670545042	1.9441329013	-2.7293582761
C19	-0.7763670307	3.3036237503	-4.9517952362
C20	0.2776478275	2.4562038970	-4.6170326048
C21	1.2448939571	0.5286075849	-3.2810380001
C22	-1.1552707229	1.1412498380	3.0615679837
C23	0.1257947016	1.2798455939	3.6246718465
C24	-2.2089785478	2.0081196650	3.4022613426
C25	0.3264318823	2.2858551743	4.5738810779
C26	1.2535231207	0.3885530129	3.1686421451
C27	-0.7115009620	3.1386385601	4.9433722564
C28	-1.9674409960	3.0000284158	4.3560016314
C29	-3.5462767412	1.8782292447	2.7181897393
H32	-1.6784317306	-0.7142000700	-4.5502355366
H33	-2.7258935922	-2.0195164476	-3.9611437151
H34	-2.4471649268	-5.0049237548	-0.1357278434
H35	-2.7275183560	-2.1426193153	3.8001430538
H36	-1.6564429420	-0.8743740535	4.4275303878
H37	-2.8409500322	3.8050869048	-4.6008031253
H38	-0.6227442810	4.1057665115	-5.6689043034
H39	1.2562367405	2.6031724623	-5.0681690055
H40	-3.4439185682	2.0838042851	-1.6489205278

H41	1.3729402950	0.5514028178	-2.1924940450
H42	1.3124676813	2.4076437780	5.0162411602
H43	-0.5380191466	3.9196836437	5.6790072378
H44	-2.7722998390	3.6782820303	4.6296701256
H45	1.3740691328	0.4546110432	2.0808558938
H46	-3.4302543663	2.0340981389	1.6394197836
H50	-2.1992405258	-3.8064317338	2.0414734414
H51	-0.9851520040	-2.4118599021	3.8526595488
H52	-2.1901920304	-3.7345831926	-2.2688747112
H53	-0.9805455456	-2.2618966028	-4.0399115267
H62	1.0671687191	-0.6655661310	3.4060303849
H63	2.1976860805	0.6777566411	3.6373894769
H64	-4.2574887130	2.6164837598	3.0980799508
H65	-3.9805087225	0.8811458663	2.8551095192
H66	-3.9831450695	0.9412157096	-2.8786714108
H67	-4.2963680980	2.6746718743	-3.0893680525
H68	2.1814885627	0.8488603748	-3.7447534090
H69	1.0699428145	-0.5173435876	-3.5600282377
O70	-0.1117710704	2.3382283049	0.0380850985
O72	-1.4554405336	2.6670371035	0.0192733193

(^{Me}PDI)Fe(OH)(OSiEt₃)

E: -1935.5707

Fe1	15.5132829041	5.1370574543	2.8144359986
N2	14.6421761021	7.1617017197	2.7221347661
N3	15.0435663124	5.4650768667	0.8570479561
N4	15.8647931332	3.2355243455	1.7907309041
C5	13.7986556565	8.9995692837	1.2845777161
H6	13.7077605884	9.5581940530	2.2165854838
H7	12.8117879810	8.9485474940	0.8120880823
H8	14.4574715002	9.5545902137	0.6081686120
C9	14.3399986557	7.6187761965	1.5402838103
C10	14.5476571776	6.6781363750	0.4517089802
C11	15.2301532955	4.4725347508	-0.0715935632
C12	15.7068716972	3.2236419946	0.4956285319
H13	16.3319759233	1.1850004765	0.2179527891
C14	14.4581484249	7.9250213036	3.9056490664
C15	15.5096408265	8.7269885108	4.3839390792
C16	15.3289002524	9.3851201062	5.6047788920
H17	16.1356311536	10.0015394424	5.9945534067
C18	14.1447056077	9.2519311753	6.3260144445
H19	14.0268827560	9.7627784854	7.2780253731
C20	13.1133299759	8.4579625774	5.8275086854
H21	12.1882912774	8.3509243987	6.3893070488
C22	13.2499067026	7.7814419995	4.6124256624
C23	12.1575430446	6.8990963597	4.0655619481
H24	12.5434054605	5.8879197506	3.9012203620

C25	16.2926523453	2.0829801290	2.5052919484
C26	15.3157906300	1.2148371227	3.0252517883
C27	15.7434182351	0.1070228107	3.7614864602
C28	13.8530428110	1.5155445130	2.8229591355
H29	13.6232751547	2.5106522145	3.2196739523
C30	14.2599538992	6.9299790632	-0.8854400928
H31	13.8719801560	7.8986654400	-1.1830980941
C32	14.4670506140	5.9268423088	-1.8394829888
H33	14.2455802684	6.1070538942	-2.8860949016
C34	14.9532148102	4.6846048923	-1.4189058675
H35	15.1109582143	3.8858728968	-2.1362850404
C36	15.9755575958	2.0265162616	-0.3762421702
H37	16.7296324642	2.2621149988	-1.1348208951
H38	15.0660500813	1.7184748692	-0.9032473378
C39	16.7919322130	8.8429245947	3.6008190823
H40	17.2076680838	7.8495410309	3.3970954459
C41	17.6666073118	1.8758913557	2.7243963699
C42	18.0485697784	0.7624295370	3.4801736526
C43	18.6811703118	2.8348131377	2.1554534469
C44	17.0986881613	-0.1193137344	3.9922680663
H45	19.1061278225	0.5889603759	3.6656635514
H46	18.4576374509	3.8608553695	2.4689931989
H47	17.4147064829	-0.9781770360	4.5788344136
H48	15.0009818159	-0.5708249539	4.1759917545
H49	17.4337752995	5.4909432496	4.2712977594
Si50	14.6543685285	4.3289986916	5.8703134037
C51	15.8877963319	5.6069911966	6.5448541362
H52	15.8250905553	6.4933762646	5.9026000492
H53	16.9037778472	5.2007834538	6.4171827937
C54	15.6957079206	6.0412386418	8.0093717678
H55	15.7777386109	5.1966496130	8.7026611150
H56	16.4414299894	6.7864070772	8.3119180669
H57	14.7095949539	6.4949059297	8.1562827520
H58	11.7847071251	7.2713584383	3.1036558533
H59	11.3136831011	6.8440917908	4.7574964661
H60	17.5303492404	9.4363119282	4.1464644481
H61	16.6238372942	9.3263233479	2.6303546860
H62	18.6678745519	2.8222664080	1.0581016031
H63	19.6916397317	2.5712129743	2.4796673907
H64	13.2278356641	0.7773908569	3.3323640640
H65	13.5798309382	1.5151935908	1.7608010833
O66	17.2622019497	5.5598733556	3.3226795676
O67	14.5078385999	4.5023180325	4.2426218964
C68	12.9394077995	4.5990607090	6.6322332787
H69	12.7567490643	5.6814506808	6.6663259053
H70	12.2123535359	4.1999023802	5.9116318055

C71	12.6825945983	3.9803522260	8.0183198463
H72	12.7979802660	2.8907051504	7.9975091552
H73	13.3776926160	4.3652211341	8.7725097295
H74	11.6670411504	4.1914210986	8.3763373602
C75	15.3141460792	2.5943547897	6.2379438013
H76	14.5245700983	1.8607304857	6.0240805305
H77	16.0925511281	2.3983736719	5.4890122520
C78	15.8912792956	2.3517998149	7.6450720892
H79	16.7203725234	3.0360278699	7.8602264232
H80	15.1422838797	2.4956674023	8.4313983124
H81	16.2805813556	1.3313411428	7.7491820444

(^{Me}PDI)Fe(OH)(H)

E: -1333.5151

Fe1	15.2901849376	5.1022209992	2.7621282093
N2	14.5415598240	7.1699081688	2.6672354027
N3	15.1727691727	5.5118526546	0.8182421533
N4	15.7612000763	3.2579857472	1.8344467324
C5	14.1029067312	9.1300032894	1.1719043120
H6	13.7795241260	9.6349864934	2.0945366592
H7	13.2831729298	9.1888227740	0.4349862336
H8	14.9604350875	9.6900784426	0.7561428695
C9	14.4747723221	7.6964473191	1.4516123278
C10	14.8082433486	6.7759456096	0.3728097816
C11	15.5159900245	4.5281687648	-0.1083031572
C12	15.8538219417	3.2648442234	0.4976239705
H13	16.3607484210	1.1769007146	0.3091959860
C14	14.3210080676	7.9219121138	3.8679906851
C15	15.3738186493	8.7112900996	4.4027118676
C16	15.1504105772	9.3784332293	5.6239774833
H17	15.9581473954	9.9831139318	6.0495223489
C18	13.9231220128	9.2677315951	6.2951607234
H19	13.7668186372	9.7932741296	7.2425521982
C20	12.8994955975	8.4732254199	5.7540751009
H21	11.9435506779	8.3752665244	6.2793135092
C22	13.0794362682	7.7797135422	4.5416925807
C23	12.0080847866	6.8753218686	3.9832737164
H24	12.3868167533	5.8354455767	3.9597153111
C25	16.0829934114	2.1039068960	2.6262942380
C26	15.0215318055	1.2964447619	3.1144356524
C27	15.3428926182	0.2020113121	3.9407373340
C28	13.5893914085	1.6365619199	2.7802854088
H29	13.3343399515	2.6164326589	3.2268546288
C30	14.8011726319	7.0847755321	-0.9918595443
H31	14.5191398973	8.0876847440	-1.3211412231
C32	15.1589122140	6.0964929694	-1.9372771404
H33	15.1549608673	6.3275010599	-3.0048597059

C34	15.5154798022	4.8160609024	-1.4863831803
H35	15.7921157774	4.0346526659	-2.1986521055
C36	16.2739187902	2.0729815158	-0.3234907744
H37	17.2527240966	2.2416578781	-0.8090993307
H38	15.5424779789	1.8612830454	-1.1226604061
C39	16.7080679686	8.7977031697	3.6987059120
H40	17.0914250705	7.7874334645	3.4651864880
C41	17.4360146743	1.8404518045	2.9680490238
C42	17.7083120092	0.7401821587	3.8059524157
C43	18.5472559513	2.7339374493	2.4685638605
C44	16.6743491769	-0.0770305540	4.2883703735
H45	18.7475408605	0.5327737757	4.0826138628
H46	18.3156693414	3.7948835854	2.6740428200
H47	16.9051717200	-0.9272034776	4.9382270454
H48	14.5312144101	-0.4285101245	4.3188617681
H49	11.7313338859	7.1468119906	2.9485133547
H50	11.0973904221	6.9109744200	4.6023162219
H51	17.4491185857	9.3179635835	4.3258320226
H52	16.6388805839	9.3454094112	2.7401260376
H53	18.6911748322	2.6438135699	1.3753808709
H54	19.5032248178	2.4797314415	2.9531536773
H55	12.8984759877	0.8726630975	3.1720164452
H56	13.4274534792	1.7226897146	1.6906439865
H57	16.8246942044	5.4685689812	3.2171643523
O58	14.2670479898	4.5122651009	4.1948453373
H59	14.5990540266	4.4370532023	5.1176978242

(MePDI)Fe(OSiEt₃)(H)

E: -1860.2856

Fe1	15.4621149191	5.1595620569	2.7626458439
N2	14.5760550469	7.1495485892	2.6692663916
N3	15.1032868500	5.5052549900	0.7941589081
N4	15.7954250844	3.2403934597	1.7486401364
C5	13.9392531652	9.0630631204	1.2190042568
H6	13.6829318249	9.5640728351	2.1531155639
H7	13.0625629350	9.0772535786	0.5634901568
H8	14.7284869256	9.6399647336	0.7234789336
C9	14.3920793838	7.6520946428	1.4782776746
C10	14.6597993164	6.7340701841	0.3847461469
C11	15.3510305150	4.5322028361	-0.1342384096
C12	15.7695536110	3.2625904432	0.4470136234
H13	16.3389301278	1.2083898532	0.1752764792
C14	14.3746679288	7.9045522372	3.8573095543
C15	15.3980034096	8.7423001438	4.3378530851
C16	15.1955371003	9.3933208100	5.5590207764
H17	15.9825153132	10.0328855250	5.9515987628
C18	14.0180111634	9.2180384390	6.2810872141

H19	13.8826872247	9.7242884747	7.2332311557
C20	13.0198854776	8.3800141815	5.7876680478
H21	12.1040797235	8.2321276245	6.3550701624
C22	13.1811492992	7.7044111512	4.5753951838
C23	12.1335558939	6.7592727982	4.0480385328
H24	12.5714446332	5.7643582145	3.9163109254
C25	16.1821899603	2.0823652985	2.4794363194
C26	15.1685130064	1.2631320750	3.0086053394
C27	15.5476555420	0.1445414320	3.7540301048
C28	13.7211477627	1.6292887055	2.8085701937
H29	13.5411108715	2.6271537402	3.2244159455
C30	14.4992777145	7.0245311293	-0.9692473840
H31	14.1575269326	8.0077271813	-1.2758352855
C32	14.7760572635	6.0430762506	-1.9232248921
H33	14.6530950380	6.2525007344	-2.9806233028
C34	15.2031866256	4.7802381351	-1.4946381115
H35	15.4145373722	3.9982425969	-2.2165078695
C36	16.1348882052	2.0939496828	-0.4270270785
H37	17.0257631516	2.3212421752	-1.0232202602
H38	15.3240043900	1.8626365690	-1.1252365902
C39	16.6902408772	8.8882892748	3.5759193562
H40	17.1181860757	7.9038252463	3.3566716367
C41	17.5443991615	1.8305933456	2.7227980346
C42	17.8776873629	0.7094263291	3.4905034702
C43	18.6046587324	2.7582660932	2.1853777328
C44	16.8912039118	-0.1344959057	3.9954570488
H45	18.9255316540	0.5033014903	3.6960609734
H46	18.3824887632	3.7964509942	2.4552187885
H47	17.1688490793	-0.9997697859	4.5917884423
H48	14.7761231540	-0.4985301223	4.1706828562
Si50	14.8193315610	4.3680096410	5.8985132569
C51	16.0530273886	5.6788345574	6.4895220605
H52	15.8895415978	6.5660412529	5.8665079482
H53	17.0645405284	5.3268473562	6.2406987492
C54	15.9799594680	6.0873132485	7.9716989450
H55	16.1524332805	5.2389344138	8.6436158976
H56	16.7245868549	6.8542640392	8.2188734880
H57	14.9963957281	6.5042764177	8.2164202292
H58	11.7499639414	7.0850938190	3.0739603722
H59	11.2908326871	6.6820214086	4.7393933671
H60	17.4174415172	9.4677830881	4.1501096864
H61	16.5402232605	9.3955980360	2.6150715306
H62	18.6608971078	2.7164245567	1.0903195787
H63	19.5893411440	2.4945933037	2.5798657616
H64	13.0635310298	0.9128939223	3.3080536137
H65	13.4489946677	1.6597357514	1.7469510410

H66	17.0441781148	5.5990004381	2.9869556286
O67	14.6046342792	4.5135612975	4.2771585437
C68	13.1317189901	4.6187296675	6.7306541590
H69	12.9198634516	5.6962258147	6.7424732981
H70	12.3815809341	4.1769402623	6.0598302952
C71	12.9614202851	4.0361590571	8.1456437391
H72	13.1098779518	2.9502201281	8.1517189301
H73	13.6810423975	4.4641955809	8.8520932701
H74	11.9588669842	4.2277576809	8.5488589404
C75	15.4904747783	2.6372201179	6.2756740842
H76	14.6747218356	1.9095563815	6.1605484040
H77	16.2004851830	2.3976612332	5.4746453331
C78	16.1809576367	2.4411625247	7.6382466698
H79	17.0425250167	3.1100451878	7.7471814321
H80	15.5074793432	2.6436768384	8.4784160983
H81	16.5514132067	1.4152654004	7.7587108583

(^{Me}PDI)Fe(H₂) E: -1258.2194

Fe1	15.3176238612	5.1894819382	2.5397263182
N2	14.7343476551	7.0075119267	2.6439694562
N3	15.1308300337	5.5269056213	0.7029631878
N4	15.7995033056	3.4586165411	1.8842891649
C5	14.0224041631	9.0354952596	1.3610654610
H6	13.0657236168	9.1736367454	1.8798813200
H7	13.8911853709	9.3464265149	0.3231301509
H8	14.7321091569	9.7247008576	1.8351406860
C9	14.4943375432	7.6159134555	1.4513957327
C10	14.7248064008	6.7737601687	0.3166197307
C11	15.4034490706	4.5092828293	-0.1681068797
C12	15.7817200028	3.3184535485	0.5313091768
H13	15.4926886694	1.2052510166	0.2157377200
C14	14.4976062258	7.7245107404	3.8491502152
C15	15.5505774003	8.4394211471	4.4473905710
C16	15.3058504475	9.1018891053	5.6541046870
H17	16.1110126285	9.6590187992	6.1279731183
C18	14.0492173706	9.0518732719	6.2548625766
H19	13.8738247045	9.5717236158	7.1931807224
C20	13.0196431707	8.3275593644	5.6564045654
H21	12.0424282667	8.2801170140	6.1318580664
C22	13.2270701132	7.6524352711	4.4502369340
C23	12.1343830072	6.8388202574	3.8017389899
H24	12.4599619461	5.8011706959	3.6563128996
C25	16.1149412384	2.3335027294	2.6954232638
C26	15.0751289355	1.4909899116	3.1312607775
C27	15.3926827018	0.4129753592	3.9623741899
C28	13.6528976997	1.7758678762	2.7158640441

H29	13.3606752843	2.7921584242	3.0083956071
C30	14.5893683603	7.0425483518	-1.0583353658
H31	14.2724631503	8.0207865965	-1.4019734491
C32	14.8707596985	6.0215555973	-1.9708342301
H33	14.7699318076	6.2191159037	-3.0348180760
C34	15.2771057183	4.7521902808	-1.5487090892
H35	15.4901811753	3.9708886900	-2.2695174958
C36	16.1279006658	2.0246264468	-0.1415048707
H37	17.1628355080	1.7267870502	0.0695226814
H38	16.0113113816	2.0950830546	-1.2243916799
C39	16.9105560568	8.4590355191	3.7952027708
H40	17.2836562015	7.4377277780	3.6506896010
C41	17.4460166871	2.1192231864	3.0952596817
C42	17.7255130912	1.0309790180	3.9274465927
C43	18.5283764188	3.0665052853	2.6411560682
C44	16.7090397766	0.1795044457	4.3566009655
H45	18.7507683602	0.8530628629	4.2442518850
H46	18.2858887997	4.0964767543	2.9299228654
H47	16.9416376766	-0.6623927987	5.0035537568
H48	14.5985390592	-0.2461363754	4.3062003504
H49	11.8802694533	7.2203252450	2.8063031071
H50	11.2260609634	6.8361876587	4.4103898408
H51	17.6335707350	9.0129862072	4.4001558298
H52	16.8749803191	8.9141548707	2.7988070664
H53	18.6296571262	3.0718036907	1.5498712701
H54	19.4964795388	2.8006417446	3.0743330758
H55	12.9560598898	1.0682941833	3.1734046292
H56	13.5298454685	1.7249272857	1.6280039824
H57	15.9289203433	5.0472173305	4.0684963921
H58	15.1467868986	4.7940448653	4.1420678808

(ⁱPrPDI)Fe(C₄H₈), A

E: -1728.9684

Fe1	-0.5496082931	0.6768945977	0.0407252933
C2	-1.5974829455	-0.9822592870	-2.4733444870
N3	-1.2906918115	0.2627702624	-2.2650640210
N4	-1.3473820707	-1.2141695333	-0.1011639415
N5	-1.2735031881	0.2596891513	2.0404646065
C6	-1.9682619990	-1.5631657189	-3.8194878055
C7	-1.6268037167	-1.0062407995	2.2480178149
C8	-1.6608467893	-1.8380492596	-1.2792523395
C9	-2.0923435166	-3.1576875494	-1.3181432309
C10	-2.2735996907	-3.8648621701	-0.1097445531
C11	-2.0999349930	-3.1873291894	1.0902128124
C12	-1.6776934539	-1.8452599625	1.0829099842
C13	-2.0343832767	-1.5690508475	3.5909599047
C14	-1.2733970555	1.2256478753	-3.3074666756

C15	-2.3198788943	2.1853339055	-3.3148732529
C16	-0.2194687846	1.2869046342	-4.2496277297
C17	-2.3085227032	3.1767703663	-4.3002290663
C18	-3.4464772291	2.0850716364	-2.2915781660
C19	-1.2861192888	3.2380251133	-5.2493443390
C20	-0.2538071699	2.3050034050	-5.2138446341
C21	0.9442443332	0.2986437566	-4.2465748757
C22	-4.1344284179	3.4248551271	-1.9920535984
C23	-4.4978834096	1.0400228318	-2.7202471386
C24	2.2968206021	1.0109458014	-4.0484693722
C25	0.9851085461	-0.5438218206	-5.5388681093
C26	-1.2964070045	1.1908018382	3.1173206833
C27	-0.1920054980	1.3123130192	3.9931723672
C28	-2.4271032236	2.0372698845	3.2449227442
C29	-0.2707947512	2.2459268875	5.0356338595
C30	1.0638741386	0.4611990626	3.8252335162
C31	-1.3940639744	3.0533294175	5.2008702047
C32	-2.4566772610	2.9543192733	4.3015300865
C33	-3.5817598958	1.9355104684	2.2514462081
C34	1.1641418867	-0.6374254996	4.9031837571
C35	2.3512658315	1.3087873049	3.8436013568
C36	-4.6090268893	0.8670276207	2.6772681443
C37	-4.2946641499	3.2743300528	2.0042623149
C38	0.6848154270	2.2837689479	0.5740903530
C39	0.9246906279	1.8665757057	-0.7504703984
H40	-2.0118762301	-0.7853986547	-4.5815319503
H41	-2.9473746094	-2.0500455643	-3.7712974440
H42	-2.5961922196	-4.9008807786	-0.1211139956
H43	-3.0485470431	-1.9819169676	3.5488226201
H44	-2.0169913587	-0.8023419180	4.3652936697
H45	-3.1043381674	3.9136212174	-4.3311994655
H46	-1.2940296728	4.0149829608	-6.0086668818
H47	0.5435626445	2.3654731109	-5.9493484547
H48	-2.9925384289	1.7200002889	-1.3603569999
H49	-4.7298796114	3.7745685995	-2.8435446501
H50	-3.4109796061	4.2045995532	-1.7372685117
H51	-4.8189042073	3.3087469103	-1.1457419932
H52	-5.2775415955	0.9435249829	-1.9555163847
H53	-4.0503926503	0.0546019767	-2.8675380061
H54	-4.9758903408	1.3395635737	-3.6607113200
H55	0.8094339883	-0.3825568901	-3.4011049987
H56	2.5308272460	1.6583301947	-4.9010417468
H57	3.1044798718	0.2749047702	-3.9595320058
H58	2.2957949553	1.6302597909	-3.1491210996
H59	0.0388035266	-1.0579737481	-5.7250073513
H60	1.7776376272	-1.2989406971	-5.4785833852

H61	1.1934725178	0.0874902396	-6.4101892954
H62	0.5607721710	2.3432153246	5.7278237275
H63	-1.4376504950	3.7670799873	6.0187741268
H64	-3.3167717082	3.6045140364	4.4255490011
H65	0.9978171199	-0.0275713774	2.8473036690
H66	2.0553582069	-1.2550101360	4.7402052812
H67	0.2927883142	-1.2944116738	4.9020696204
H68	1.2416425561	-0.1903979696	5.9013501952
H69	2.2924144407	2.1557071615	3.1546704764
H70	3.2117373004	0.6930975843	3.5578408987
H71	2.5528864292	1.7093833172	4.8434222707
H72	-3.1483717282	1.6031987613	1.2990956309
H73	-4.1531387949	-0.1215063265	2.7547538732
H74	-5.4232319110	0.8041904184	1.9455253288
H75	-5.0447213443	1.1184688156	3.6519263510
H76	-4.8656447856	3.5999977583	2.8814033118
H77	-5.0069748649	3.1684174973	1.1792676674
H78	-3.5875461645	4.0668714209	1.7435252393
H79	1.3597462834	1.9080435997	1.3406833880
H80	0.5529192959	2.4366285319	-1.5997351528
H81	1.7731784236	1.2189345946	-0.9698094488
H82	-2.3075123991	-3.6864613113	2.0306929613
H83	-1.3694821256	-2.3847915868	3.8966185776
H84	-2.3119386386	-3.6386160128	-2.2642074935
H85	-1.2406094840	-2.3195423693	-4.1333783060
C87	-0.0128470912	3.5819476021	0.9502534714
H88	-0.3841814244	3.4985388159	1.9770270899
H89	0.7416560322	4.3845730214	0.9620100088
C90	-1.1674743495	3.9945643816	0.0314867462
H91	-0.8464545787	4.1199980678	-1.0076697984
H92	-1.9535028286	3.2328749334	0.0401622549
H93	-1.6117287354	4.9401301990	0.3612933884

Anti-Markovnikov Hydride Migration TS, $\text{TS}(\text{A} \rightarrow \text{D}_{\text{AM}})$, ${}^i\text{PrPDI}$ E: -2256.8338

Fe1	2.6501351188	6.2250869506	8.5556321309
H2	1.7262142859	5.8472297687	7.3379921229
Si3	3.5669253164	5.8429433016	6.2887254572
N4	3.4655773891	4.4254456269	9.6633702306
N5	4.4021385748	6.7955830024	9.1632642050
N6	2.5259561219	8.5228571680	8.5449620980
C7	4.7388270539	4.5684929640	9.9298899497
C8	5.3178494996	5.8576787455	9.5926759217
C9	6.6646305740	6.1884405966	9.7208259178
H10	7.3820579844	5.4361903979	10.0334359290
C11	7.0922350850	7.4909936546	9.4423652888
H12	8.1411071105	7.7567114949	9.5267522425

C13	6.1427969277	8.4551344132	9.0806946633
H14	6.4537153580	9.4783762801	8.8959095234
C15	4.8020989917	8.1006219477	8.9609468050
C16	3.7240096565	9.0348264326	8.6710730055
C17	5.5924309424	3.5143187086	10.5908282923
H18	6.4068892420	3.2102919506	9.9229596215
H19	5.0028113586	2.6302294358	10.8348902624
H20	6.0525933256	3.8902188098	11.5104532190
C21	4.0297552161	10.5050524956	8.5195505250
H22	4.5972420681	10.8955956920	9.3690105909
H23	3.1128836415	11.0858085942	8.4155482459
H24	4.6384438658	10.6626107573	7.6208441645
C25	2.6810811512	3.3541364817	10.1605130837
C26	2.2581516510	2.3393742885	9.2578177345
C27	1.3702178391	1.3596631881	9.6992967270
H28	1.0490979905	0.5811053513	9.0140939216
C29	0.8773880397	1.3714475200	11.0011197207
H30	0.1722606677	0.6126202193	11.3307544236
C31	1.2895790183	2.3702252653	11.8695415011
H32	0.8931920274	2.3867679392	12.8831811753
C33	2.1963338299	3.3756940085	11.4925343841
C34	2.7992060112	2.3011414407	7.8353557872
C36	2.5399657373	4.3653467296	12.6235543397
C38	1.3474604674	9.3103906633	8.5875925554
C39	0.8940419598	9.8027704409	9.8397896119
C40	-0.3063590122	10.5198867503	9.8761717188
H41	-0.6574687504	10.9127281315	10.8267847874
C42	-1.0639922165	10.7327853976	8.7306648567
H43	-1.9921457948	11.2960745114	8.7842767001
C44	-0.6317065340	10.2066662318	7.5177650321
H45	-1.2326767158	10.3609250767	6.6260590882
C46	0.5600148981	9.4845719699	7.4229084240
C47	1.6527828640	9.5580513937	11.1433069338
C49	1.0246161866	8.9401302725	6.0802662750
H50	1.7155005830	8.1226820031	6.2947952917
C51	2.3847548229	5.1573698575	4.9434383879
H53	3.0007063769	3.3362333018	7.5515979293
H55	1.5803178322	4.5345842468	13.1309212209
H57	2.4560962697	8.8449670062	10.9410218898
H60	1.6746746283	5.9571914199	4.6885322825
H61	1.7779169834	4.3794842712	5.4248540928
C62	5.0287102975	4.5921157471	6.4320297368
H63	4.7967705965	3.7405587629	5.7804028735
H64	5.0583491292	4.1811482081	7.4432141603
C65	4.3248884339	7.5065703861	5.7026847340
H66	3.7403368703	8.3291966490	6.1162808410

H67	5.3071097804	7.5923132638	6.1818992174
C68	3.0003468164	4.5724083495	3.6602299779
H69	2.2264298440	4.1905744225	2.9822742027
H70	3.5837687578	5.3125145429	3.1052912379
H71	3.6712925962	3.7354573589	3.8847855949
C72	4.4716890112	7.7148639782	4.1862099487
H73	5.1384083655	6.9740679265	3.7314287562
H74	3.5061028255	7.6385510684	3.6736854009
H75	4.8826791033	8.7063091091	3.9558569636
C76	6.4310480298	5.1245862747	6.0884045040
H77	6.7420056555	5.9134028798	6.7816511171
H78	7.1822334443	4.3260048568	6.1511306127
H79	6.4815783771	5.5384793939	5.0752804840
C80	0.8074383557	6.1633551344	9.6036361188
C81	0.4457104300	5.9582277744	8.2543097492
H82	0.7929362125	5.3150383357	10.2820371290
H83	0.0690983130	6.8373244387	7.7325948233
H85	0.6642849011	7.1369858544	10.0512533805
C86	-0.2141672609	4.6603202789	7.8189685450
H87	0.2663849608	3.8263088891	8.3377092933
H88	-0.0734337351	4.5002269017	6.7440806027
C89	-1.7151851210	4.6746522299	8.1395852067
H90	-2.2200884088	5.5086530736	7.6372139669
H91	-2.1952343856	3.7457557168	7.8122288370
H92	-1.8820466617	4.7852586304	9.2160377091
C92	1.8246501941	1.7213297822	6.7975549826
H93	0.8405518798	2.1936138103	6.8506046174
H94	2.2224782951	1.8827140951	5.7896962059
H95	1.6879089201	0.6407394319	6.9203991420
C95	4.1262805418	1.5189264299	7.7874965906
H96	3.9613601090	0.4773463276	8.0883328232
H97	4.5451038221	1.5206458960	6.7755571029
H98	4.8733507820	1.9465643763	8.4599952452
C98	3.0879244634	5.7649674365	12.2987504382
H99	4.1538854255	5.7491343094	12.0604999528
H100	2.5748640912	6.2412329557	11.4651999357
H101	2.9678543150	6.3981065821	13.1855545609
C101	3.4646908365	3.6795330909	13.6533843948
H102	4.4417175874	3.4602468327	13.2108347772
H103	3.6275686347	4.3331906669	14.5182138859
H104	3.0439558401	2.7357628050	14.0132613038
C104	-0.1088916461	8.3604970555	5.2182402774
H105	-0.8038862651	9.1339815698	4.8732109101
H106	0.3091300810	7.8827203186	4.3254210699
H107	-0.6888973118	7.6081135702	5.7622807291
C107	1.7916957093	10.0224270929	5.2965755080

H108	1.1262518386	10.8579843878	5.0491159972
H109	2.6254669991	10.4234910947	5.8812566398
H110	2.1969181219	9.6184356437	4.3627832373
C110	0.7609723770	8.9334631989	12.2351163968
H111	0.2821756250	8.0116767314	11.8940154494
H112	1.3639746299	8.6916995507	13.1174517788
H113	-0.0296352432	9.6209734636	12.5554610892
C113	2.2840961305	10.8588222142	11.6749468215
H114	1.5070634502	11.5868407264	11.9364866680
H115	2.8754655862	10.6621336560	12.5764140328
H116	2.9368928012	11.3270025667	10.9342566418

(ⁱPrPDI)Fe(CH₂CH₂Et)(SiEt₃), **D_{AM}** E: -2256.8680

Fe1	15.1012991081	5.1439646529	2.5942277999
N2	14.7892952208	7.3598182279	2.3596851389
N3	14.6905291698	5.4455912599	0.6260772146
N4	15.9732882154	3.3439783616	1.4496746020
C5	13.8934832699	9.1223511298	0.8175111370
H6	13.9298150307	9.7926273767	1.6747585151
H7	12.8844677644	9.1548922279	0.3965876514
H8	14.5709210656	9.5157670287	0.0514230030
C9	14.2904839084	7.7122697180	1.1934860128
C10	14.2297096369	6.6663647561	0.1980041304
C11	14.8666321009	4.4464361428	-0.2956919427
C12	15.5574562552	3.2746299642	0.2091765299
H13	16.3612401992	1.3158556896	-0.2211797283
C14	14.9372669185	8.3466415643	3.3746622954
C15	16.2155149591	8.9212042808	3.5551061993
C16	16.3588735933	9.9194440957	4.5226256510
H17	17.3285640007	10.3825328893	4.6770391374
C18	15.2787907373	10.3241066456	5.3029792885
H19	15.4080727866	11.1064753416	6.0465138913
C20	14.0445319578	9.7003391064	5.1542949936
H21	13.2216285106	9.9907935212	5.8010653547
C22	13.8489708803	8.6901583493	4.2070385907
C23	12.5229537509	7.9375194421	4.1308481251
H24	12.7447955316	6.9667712776	3.6846944644
C25	16.6716384102	2.2492017715	2.0321748814
C26	15.9651270454	1.1285687756	2.5273360813
C27	16.7059315054	0.0909342658	3.1051352949
C28	14.4433030154	1.0136162366	2.4500847008
H29	14.0496220764	1.9860266105	2.1438410978
Si30	16.1479185783	4.9676288717	4.8076504000
C31	13.8138869547	6.8615320547	-1.1186636241
H32	13.4402367226	7.8302407137	-1.4334115359
C33	13.9037217102	5.8138935392	-2.0368635406

H34	13.5835340726	5.9502283172	-3.0647504064
C35	14.4625288512	4.6005206756	-1.6185962715
H36	14.5979900598	3.7920394390	-2.3288151964
C37	15.8094107132	2.1111388159	-0.7193335261
H38	16.3916405676	2.4356532761	-1.5879439867
H39	14.8681209528	1.7027094766	-1.0988329029
C40	17.4015269416	8.4309811287	2.7306985718
H41	17.2226074921	7.3658639807	2.5366773685
C42	18.0815591777	2.3410704769	2.1379879337
C43	18.7669000116	1.2758879999	2.7272272682
C44	18.8235648148	3.5645408123	1.6030718007
C45	18.0899264527	0.1561684163	3.2042284292
H46	19.8473995944	1.3179003999	2.8182371050
H47	18.2013957441	4.4366479870	1.8391990191
H48	18.6436384426	-0.6614365241	3.6583573181
H49	16.1833435922	-0.7820331667	3.4871283608
C50	15.8621151667	3.2454781050	5.5771532832
H51	15.8782313306	2.5306252318	4.7490930328
H52	14.8405784989	3.2213364628	5.9809146949
C53	15.4956882155	6.3011166969	6.0056660334
H54	14.4458786412	6.4654016921	5.7496058939
H55	15.9933909676	7.2503244477	5.7743596373
C56	16.8601963374	2.7666955635	6.6458434934
H57	16.8840921687	3.4266766238	7.5187888013
H58	16.6064677352	1.7602813937	7.0025291308
H59	17.8773151269	2.7150172761	6.2422469471
C60	15.6006466453	6.0070907466	7.5127902825
H61	16.6405681904	5.8979935102	7.8382005075
H62	15.1570809295	6.8170757804	8.1067746976
H63	15.0764431083	5.0827787369	7.7811395853
C64	18.0420293518	5.1604151294	4.6116999253
H65	18.4072948407	4.1658117306	4.3342972959
H66	18.2749473159	5.8103977772	3.7616087087
C67	18.7994161970	5.6643636210	5.8545890872
H68	18.4256800168	6.6382976079	6.1894159964
H69	18.6977319128	4.9742760992	6.6981628915
H70	19.8725208269	5.7786702180	5.6513442525
C71	13.4650061411	4.4202163904	3.5673115555
H72	13.6365533251	3.3959341536	3.9063752469
H73	13.1956593959	5.0035122537	4.4556741978
C74	12.3220104019	4.4550784838	2.5470823663
H75	12.1981749345	5.4688584762	2.1420004545
H76	12.5724359037	3.8261644040	1.6820497076
C77	10.9815281382	3.9898221447	3.1381029393
H78	11.0956812765	2.9658670493	3.5200960013
H79	10.7412862553	4.6149102724	4.0096389800

C80	9.8329605679	4.0466362692	2.1263696856
H81	9.6860699695	5.0695914810	1.7581855202
H82	10.0433289134	3.4126073920	1.2562099752
H83	8.8860213101	3.7100383789	2.5634190504
C91	18.9858569251	3.5218773739	0.0696410325
H92	18.0257895884	3.5528166373	-0.4452428635
H93	19.5721133345	4.3820225724	-0.2741900314
H94	19.5117183114	2.6103360547	-0.2371665292
C94	20.2085851609	3.7761587953	2.2371260294
H95	20.9315388244	3.0353408766	1.8756399133
H96	20.5934481775	4.7641522890	1.9629489465
H97	20.1833566661	3.7192337487	3.3277935944
C97	13.8037720241	0.6591895734	3.8071527471
H98	14.0452903948	-0.3669500360	4.1062478994
H99	14.1340825047	1.3246270815	4.6057556216
H100	12.7126570908	0.7304545417	3.7352653763
C100	14.0049088506	-0.0369487252	1.4106770370
H101	14.3798375362	-1.0288746925	1.6875298006
H102	12.9115458303	-0.0949232728	1.3624704016
H103	14.3744083013	0.1860236663	0.4089622250
C103	11.4784892723	8.6321174152	3.2377137500
H104	11.3112234475	9.6652301914	3.5643059847
H105	11.7831863768	8.6538771485	2.1915737985
H106	10.5207815351	8.1019344516	3.2916660341
C106	11.9046384707	7.6815315009	5.5177529038
H107	11.4859064071	8.5981246199	5.9486861195
H108	11.0848203630	6.9601534335	5.4305142927
H109	12.6340415975	7.2819696674	6.2270928153
C109	17.4952959064	9.1308200039	1.3616687015
H110	16.6188006143	8.9298016198	0.7438405724
H111	17.5841150964	10.2161272990	1.4880891099
H112	18.3769013278	8.7805259555	0.8120999614
C112	18.7429792717	8.5579232858	3.4694484757
H113	19.0698796827	9.6020515530	3.5373801706
H114	18.6888237794	8.1543478902	4.4833006487
H115	19.5221280951	8.0096750093	2.9287059952