UPPORTING INFORMATION FOR:

Two Unexpected Roles of Water: Assisting and Preventing Functions in the Oxidation of Methane and Methanol Catalyzed by Porphyrin-Fe and Porphyrin-SH-Fe

Xingbang Hu, Congmin Wang, Yong Sun, Hang Sun and Haoran Li*

Department of Chemistry, Zhejiang University, Hangzhou 310027, P. R. China

LANL2DZ(6-31G): The LANL2DZ basis set was used for Fe and the 6-31G basis set for other atoms
LANL2DZ(6-31+G*): The LANL2DZ basis set was used for Fe and the 6-31+G* basis set for other atoms
CEP-121G(6-31+G*): The LANL2DZ basis set was used for Fe and the 6-31+G* basis set for other atoms

1) The coordinates of the optimized structures (Optimized with LANL2DZ(6-31G))

1) ^{L}Porph-CH_4
Total spin density: 2.0
Absolute energy: -1227.29840264 Hartree

C 0	-3.712082	-3.112488	-1.018661
C 0	-2.590103	-2.463303	-1.656448
C 0	-2.678300	-1.712600	-2.814255
C 0	1.795517	-0.144500	-3.859283
C 0	3.507019	-2.400864	0.083633
C 0	-0.966171	-3.972916	1.125763
O 0	0.103700	-0.499008	-0.335175
Fe 0	0.371536	-1.843307	-1.224700
N 0	-0.286957	-1.138733	-2.990845
N 0	2.253174	-1.420044	-1.799393

*Corresponding author. Fax: +86-571-8795-1895

Email Address: lihr@zju.edu.cn

N 0	1.119568	-2.994904	0.246292
N 0	-1.421661	-2.711395	-0.942719
C 0	-1.604965	-1.101120	-3.435623
C 0	-1.698883	-0.331772	-4.654648
C 0	-0.440994	0.108871	-4.948547
C 0	0.435150	-0.386185	-3.912308
C 0	2.639557	-0.628479	-2.876831
C 0	4.062759	-0.384781	-2.832733
C 0	4.543777	-1.018646	-1.723572
C 0	3.419785	-1.656509	-1.078293
C 0	2.436188	-3.025711	0.695953
C 0	2.533890	-3.815033	1.901794
C 0	1.276123	-4.256622	2.194900
C 0	0.396408	-3.742538	1.170929
C 0	-1.809677	-3.494217	0.140320
C 0	-3.230820	-3.748077	0.089172
H 0	-4.727539	-3.077805	-1.385193
H 0	-3.656128	-1.599976	-3.269424
H 0	2.231171	0.463440	-4.644440
H 0	4.483368	-2.505829	0.543777
H 0	-1.402649	-4.574509	1.915482
H 0	-2.614624	-0.162811	-5.202011
H 0	-0.118759	0.711900	-5.784775
H 0	4.606491	0.195572	-3.563644
H 0	5.561081	-1.062164	-1.363113
H 0	3.452347	-3.998123	2.440018
H 0	0.956909	-4.874756	3.021255
H 0	-3.772812	-4.339035	0.812927
C 0	2.020996	2.631104	-0.353638
H 0	1.628464	3.351089	-1.077850
H 0	1.360413	1.761368	-0.304825
H 0	2.080353	3.103714	0.631027
H 0	3.019989	2.310974	-0.664215

2) ^{L}Porph-CH_4-TS

Total spin density: 2.0

Absolute energy: -1227.2501748 Hartree

C 0	-2.694107	-1.285721	-3.600372
C 0	-1.361557	-1.335266	-3.040176
C 0	-0.201111	-1.096100	-3.755966
C 0	3.544418	-1.912766	-0.771271
C 0	0.433426	-2.444122	2.924835
C 0	-3.297791	-2.146637	-0.165451
O 0	0.029541	0.058990	-0.038925

Fe 0	0.109055	-1.671219	-0.393997
N 0	1.401535	-1.551651	-1.936142
N 0	1.660600	-2.123459	0.807083
N 0	-1.162781	-2.228333	1.060196
N 0	-1.420807	-1.690002	-1.697250
C 0	1.082458	-1.219498	-3.248611
C 0	2.288345	-1.082748	-4.034286
C 0	3.341293	-1.345215	-3.204285
C 0	2.791336	-1.629929	-1.898575
C 0	3.017120	-2.128235	0.491150
C 0	3.804062	-2.355408	1.681519
C 0	2.929260	-2.471832	2.724380
C 0	1.597137	-2.332443	2.180923
C 0	-0.847183	-2.415848	2.400300
C 0	-2.053741	-2.627228	3.170547
C 0	-3.101471	-2.570251	2.297394
C 0	-2.547455	-2.311325	0.986298
C 0	-2.771942	-1.844803	-1.410370
C 0	-3.562912	-1.607178	-2.597488
H 0	-2.917847	-1.040955	-4.628571
H 0	-0.302963	-0.831116	-4.802994
H 0	4.623276	-1.944077	-0.879623
H 0	0.535324	-2.605713	3.992691
H 0	-4.375626	-2.234772	-0.081848
H 0	0.941010	0.625854	-0.108109
H 0	2.309494	-0.833969	-5.085449
H 0	4.395706	-1.349991	-3.439697
H 0	4.882690	-2.413528	1.701263
H 0	3.149689	-2.647812	3.767242
H 0	-2.077469	-2.802841	4.236252
H 0	-4.155151	-2.686798	2.505264
H 0	-4.640274	-1.675247	-2.639282
C 0	2.140823	1.582611	-0.153015
H 0	1.670502	2.481354	0.237167
H 0	2.842239	1.075424	0.503952
H 0	2.376907	1.578156	-1.213821

3) ^{H}Porph-CH_4

Total spin density: 4.0

Absolute energy: -1227.28049392 Hartree

C 0	1.910583	-3.861557	2.707092
C 0	1.910583	-2.411865	2.707092
C 0	3.044907	-1.604828	2.707092
C 0	1.606293	3.046829	2.805756

C 0	-3.045639	1.606598	2.837997
C 0	-1.606903	-3.045029	2.738892
N 0	1.949326	0.604889	2.747772
N 0	-0.603363	1.950775	2.805481
N 0	-1.950500	-0.602676	2.776169
N 0	0.602585	-1.949020	2.721741
C 0	3.070236	-0.213104	2.729034
C 0	4.266434	0.605331	2.752747
C 0	3.862442	1.911682	2.780228
C 0	2.412903	1.912582	2.774155
C 0	0.214600	3.071838	2.824341
C 0	-0.603928	4.266754	2.880737
C 0	-1.910385	3.862305	2.890182
C 0	-1.911118	2.413513	2.839600
C 0	-3.071075	0.214828	2.811905
C 0	-4.266769	-0.604523	2.833176
C 0	-3.862640	-1.910828	2.805527
C 0	-2.413528	-1.910767	2.766586
C 0	-0.215027	-3.070221	2.722153
C 0	0.604156	-4.266083	2.716522
H 0	2.798004	-4.477768	2.704117
H 0	4.005081	-2.111145	2.697372
H 0	2.113022	4.006592	2.826019
H 0	-4.005524	2.112595	2.868393
H 0	-2.113434	-4.005142	2.738815
H 0	5.276108	0.220840	2.751694
H 0	4.479034	2.798477	2.805969
H 0	-0.219330	5.275909	2.912125
H 0	-2.797302	4.477875	2.930939
H 0	-5.276108	-0.220840	2.868759
H 0	-4.478714	-2.798340	2.814178
H 0	0.220078	-5.275894	2.722641
O 0	-0.028732	0.034332	0.654602
Fe 0	-0.005997	0.008804	2.315659
C 0	0.423203	2.382294	-2.051590
H 0	0.098679	3.382584	-1.749451
H 0	0.253052	1.677475	-1.232864
H 0	1.488556	2.405472	-2.299316
H 0	-0.145874	2.067169	-2.930954

4) ^{H}Porph-CH_4-TS

Total spin density: 4.0

Absolute energy: -1227.24461721 Hartree

C 0	1.895004	-3.835220	2.013718

C 0	1.895004	-2.389359	2.013718
C 0	3.036774	-1.605530	2.013718
C 0	1.609665	3.038666	2.255280
C 0	-3.033676	1.613342	2.029633
C 0	-1.607895	-3.033188	2.036530
O 0	-0.075394	-0.045303	-0.146698
Fe 0	0.003754	0.012634	1.770660
N 0	1.916641	0.594513	2.085495
N 0	-0.585510	1.921814	2.106476
N 0	-1.915665	-0.586000	2.030700
N 0	0.589844	-1.914230	2.034027
C 0	3.044144	-0.221054	2.066727
C 0	4.237534	0.586807	2.155136
C 0	3.836487	1.891159	2.240829
C 0	2.393250	1.897202	2.196900
C 0	0.224716	3.046753	2.212845
C 0	-0.590836	4.238495	2.266525
C 0	-1.894867	3.837845	2.187027
C 0	-1.892685	2.396210	2.092010
C 0	-3.041458	0.228287	2.014633
C 0	-4.237320	-0.582947	2.008820
C 0	-3.836533	-1.889100	2.022888
C 0	-2.391251	-1.890533	2.031448
C 0	-0.222916	-3.039948	2.038055
C 0	0.589630	-4.236191	2.032379
H 0	2.784744	-4.447739	2.004623
H 0	3.995209	-2.112823	1.999680
H 0	2.116760	3.993469	2.341034
H 0	-3.991577	2.121658	2.018280
H 0	-2.115891	-3.991287	2.034805
H 0	5.243790	0.193863	2.162476
H 0	4.450195	2.775803	2.329498
H 0	-0.202698	5.242767	2.355392
H 0	-2.785461	4.449081	2.199646
H 0	-5.243790	-0.190704	2.000351
H 0	-4.449860	-2.778381	2.026321
H 0	0.197464	-5.242752	2.039505
H 0	0.561951	0.757629	-0.714874
C 0	1.313828	1.709045	-1.306778
H 0	1.049393	1.572998	-2.355408
H 0	0.977509	2.650833	-0.877000
H 0	2.342117	1.445938	-1.064224

5) ^{L}Porph-CH_4-W1

Total spin density: 2.0
Absolute energy: -1303.349244 Hartree

C 0	-3.513702	-0.855942	-3.187363
C 0	-2.124237	-1.096512	-2.877548
C 0	-1.087234	-0.947098	-3.778854
C 0	3.017151	-2.093414	-1.455444
C 0	0.480957	-2.967239	2.591187
C 0	-3.624527	-1.830978	0.263229
O 0	-0.097565	-0.135132	-0.075455
Fe 0	-0.274338	-1.703522	-0.522018
N 0	0.735092	-1.611267	-2.255554
N 0	1.379959	-2.434082	0.356552
N 0	-1.345505	-2.332687	1.061035
N 0	-1.989151	-1.503952	-1.553162
C 0	0.241806	-1.190536	-3.488495
C 0	1.320755	-1.050110	-4.437164
C 0	2.474182	-1.373932	-3.783920
C 0	2.113663	-1.715210	-2.428909
C 0	2.673462	-2.429200	-0.159927
C 0	3.617096	-2.836533	0.852676
C 0	2.904160	-3.081863	1.991180
C 0	1.516479	-2.827316	1.686310
C 0	-0.850388	-2.739777	2.297409
C 0	-1.931595	-2.900223	3.240402
C 0	-3.085831	-2.580368	2.585526
C 0	-2.722458	-2.221161	1.235397
C 0	-3.281372	-1.500229	-1.033981
C 0	-4.227203	-1.105209	-2.050781
H 0	-3.878220	-0.539719	-4.153671
H 0	-1.333206	-0.620972	-4.783340
H 0	4.066956	-2.118195	-1.723100
H 0	0.729584	-3.282806	3.598434
H 0	-4.673050	-1.786026	0.535645
H 0	1.194382	-0.741165	-5.464218
H 0	3.484238	-1.379700	-4.165375
H 0	4.682312	-2.919662	0.695724
H 0	3.268188	-3.409103	2.954102
H 0	-1.806915	-3.218719	4.264832
H 0	-4.096802	-2.583664	2.965759
H 0	-5.294022	-1.034012	-1.898254
O 0	2.433716	1.062912	-0.160751
H 0	1.504623	0.761795	-0.295761
H 0	2.642532	0.956116	0.785126
C 0	5.315400	1.198242	-2.113373

H 0	6.001511	0.427704	-1.745743
H 0	5.077286	1.000549	-3.163574
H 0	5.802902	2.174866	-2.036926
H 0	4.394928	1.195663	-1.520905

6) ^{L}Porph-CH_4-W1-TS

Total spin density: 2.0

Absolute energy: -1303.296321 Hartree

C 0	-2.654205	0.320969	-4.051483
C 0	-1.384842	-0.159698	-3.546646
C 0	-0.155243	0.129257	-4.113754
C 0	3.231445	-2.322540	-1.625839
C 0	-0.183975	-3.769974	1.509888
C 0	-3.610046	-1.706024	-1.243271
O 0	-0.028076	-0.286987	-0.209412
Fe 0	-0.160156	-1.740265	-1.242920
N 0	1.237793	-1.240997	-2.602188
N 0	1.230667	-2.828873	-0.277176
N 0	-1.599197	-2.619370	-0.149933
N 0	-1.587860	-0.983368	-2.446945
C 0	1.057770	-0.390671	-3.689484
C 0	2.321243	-0.156418	-4.350418
C 0	3.271439	-0.866287	-3.670151
C 0	2.600342	-1.534119	-2.578262
C 0	2.593216	-2.916214	-0.548325
C 0	3.255585	-3.698624	0.471313
C 0	2.298859	-4.078735	1.367920
C 0	1.038925	-3.543945	0.899400
C 0	-1.408417	-3.355881	1.012543
C 0	-2.684097	-3.659744	1.624725
C 0	-3.649017	-3.100952	0.837677
C 0	-2.972595	-2.440369	-0.257600
C 0	-2.962189	-1.018433	-2.255692
C 0	-3.627518	-0.214035	-3.258698
H 0	-2.767563	0.972900	-4.905487
H 0	-0.143219	0.782455	-4.979950
H 0	4.300964	-2.475204	-1.725632
H 0	-0.185364	-4.345444	2.429443
H 0	-4.692413	-1.645752	-1.205368
H 0	0.906662	-0.128159	0.083511
H 0	2.448288	0.460098	-5.228638
H 0	4.328629	-0.942963	-3.879791
H 0	4.313416	-3.917145	0.486282
H 0	2.416900	-4.674026	2.261673

H 0	-2.806931	-4.228439	2.535004
H 0	-4.720352	-3.118362	0.975266
H 0	-4.697800	-0.086136	-3.331161
C 0	1.735916	2.534790	-1.021561
H 0	0.695419	2.213959	-1.045593
H 0	1.925446	3.432617	-0.432663
H 0	2.226303	2.529968	-1.994644
O 0	2.690048	0.541718	0.179153
H 0	3.079636	0.045761	-0.583740
H 0	2.285568	1.604980	-0.325089

7) ^{H}Porph-CH_4-W1

Total spin density: 4.0

Absolute energy: -1303.335268 Hartree

C 0	-3.028061	-1.098221	-3.551529
C 0	-1.625702	-1.029160	-3.192154
C 0	-0.622696	-0.440720	-3.959366
C 0	3.608505	-0.967957	-1.612808
C 0	1.326385	-3.362289	1.959793
C 0	-2.914215	-2.792023	-0.364380
N 0	1.309204	-0.897629	-2.496094
N 0	2.125320	-2.117538	-0.014145
N 0	-0.611832	-2.873322	0.515335
N 0	-1.428818	-1.651566	-1.968445
C 0	0.731873	-0.375137	-3.645584
C 0	1.756531	0.239700	-4.465881
C 0	2.944519	0.094147	-3.805054
C 0	2.664810	-0.613785	-2.572052
C 0	3.368225	-1.667740	-0.433182
C 0	4.374725	-2.050964	0.535629
C 0	3.734848	-2.726608	1.538513
C 0	2.326797	-2.764557	1.198227
C 0	-0.030914	-3.419403	1.650772
C 0	-1.049118	-4.066315	2.453445
C 0	-2.240982	-3.904190	1.801605
C 0	-1.968277	-3.156708	0.590729
C 0	-2.673019	-2.101486	-1.549164
C 0	-3.672211	-1.757507	-2.540878
H 0	-3.452377	-0.695358	-4.459702
H 0	-0.928085	0.009842	-4.898605
H 0	4.633194	-0.666565	-1.802353
H 0	1.636139	-3.837234	2.885620
H 0	-3.941360	-3.085236	-0.170639
H 0	1.578506	0.719300	-5.417313

H 0	3.922653	0.435928	-4.109558
H 0	5.428436	-1.829193	0.449020
H 0	4.166382	-3.163956	2.427170
H 0	-0.865800	-4.577164	3.387573
H 0	-3.216904	-4.257141	2.101898
H 0	-4.723236	-1.995987	-2.465744
O 0	0.060211	-0.007782	0.008011
Fe 0	0.281006	-1.480789	-0.770996
O 0	2.311707	1.586288	0.135071
H 0	1.440262	1.138336	-0.005829
H 0	2.502502	1.579010	1.090698
C 0	4.735367	3.230560	-1.698730
H 0	5.664856	2.655685	-1.628159
H 0	4.454712	3.335938	-2.751495
H 0	4.898392	4.225113	-1.272339
H 0	3.935364	2.719894	-1.153198

8) ^{H}Porph-CH_4-W1-TS

Total spin density: 4.0

Absolute energy: -1303.302863 Hartree

C 0	-4.411972	0.245636	-2.124496
C 0	-3.087616	-0.299530	-2.324036
C 0	-2.332169	-0.121979	-3.472626
C 0	1.849457	-2.527252	-2.851974
C 0	0.345459	-3.989182	1.537003
C 0	-3.810867	-1.545242	0.933456
N 0	-0.364716	-1.437332	-2.775208
N 0	0.746445	-3.023926	-0.698914
N 0	-1.602249	-2.638016	0.855042
N 0	-2.702408	-1.028946	-1.208008
C 0	-1.072952	-0.659058	-3.683365
C 0	-0.302200	-0.491394	-4.895248
C 0	0.874466	-1.164520	-4.720688
C 0	0.834793	-1.754333	-3.400482
C 0	1.797897	-3.130066	-1.602676
C 0	2.834045	-3.977722	-1.057037
C 0	2.409927	-4.388504	0.175140
C 0	1.111084	-3.795944	0.398987
C 0	-0.916306	-3.454147	1.742920
C 0	-1.715195	-3.676208	2.928665
C 0	-2.882202	-2.987747	2.760223
C 0	-2.810013	-2.338440	1.469406
C 0	-3.761215	-0.945557	-0.314987
C 0	-4.826874	-0.151947	-0.885132

H 0	-4.942337	0.847794	-2.847794
H 0	-2.764450	0.472153	-4.270523
H 0	2.732758	-2.700943	-3.457443
H 0	0.759918	-4.613968	2.320618
H 0	-4.704437	-1.392700	1.528824
H 0	-0.633789	0.064316	-5.760345
H 0	1.695404	-1.270004	-5.415161
H 0	3.756134	-4.222488	-1.563889
H 0	2.917023	-5.035309	0.876160
H 0	-1.408936	-4.281967	3.768997
H 0	-3.722794	-2.917343	3.435089
H 0	-5.764145	0.060303	-0.391815
O 0	-0.100113	-0.260590	-0.061203
Fe 0	-0.852081	-1.771988	-0.822708
H 0	0.869781	-0.096756	0.008835
C 0	1.413071	2.110962	-1.878677
H 0	0.431519	1.877975	-1.468200
H 0	1.829758	3.068054	-1.563309
H 0	1.510681	1.913986	-2.946136
O 0	2.658691	0.249496	-0.739090
H 0	2.557785	-0.453445	-1.429413
H 0	2.159103	1.254379	-1.273926

9) ^{L}Porph-CH_4-W2

Total spin density: 2.0

Absolute energy: -1303.69946961 Hartree

C 0	1.892303	-3.828200	2.389313
C 0	1.892303	-2.384827	2.389313
C 0	3.033539	-1.605118	2.389313
C 0	1.603394	3.033386	2.438263
C 0	-3.034912	1.603394	2.397659
C 0	-1.605606	-3.034622	2.387360
O 0	-0.003036	0.013306	0.492142
Fe 0	-0.001389	0.000961	2.133362
N 0	1.902237	0.585434	2.423340
N 0	-0.587738	1.902115	2.427353
N 0	-1.902176	-0.587326	2.406326
N 0	0.584808	-1.903152	2.400040
C 0	3.036057	-0.223083	2.409485
C 0	4.229324	0.588943	2.428680
C 0	3.826813	1.893280	2.443939
C 0	2.383377	1.892242	2.433319
C 0	0.221481	3.035492	2.437119
C 0	-0.590607	4.229141	2.451355

C 0	-1.895126	3.827057	2.437210
C 0	-1.894104	2.383575	2.415771
C 0	-3.036392	0.221527	2.397263
C 0	-4.229477	-0.591064	2.398834
C 0	-3.826950	-1.894897	2.398438
C 0	-2.384094	-1.894287	2.395569
C 0	-0.224167	-3.036438	2.390533
C 0	0.587250	-4.229462	2.391129
H 0	2.783096	-4.439163	2.391556
H 0	3.991989	-2.112320	2.380371
H 0	2.110138	3.991974	2.445480
H 0	-3.993713	2.109680	2.389175
H 0	-2.112427	-3.992233	2.365433
H 0	5.235596	0.196350	2.432480
H 0	4.436966	2.784378	2.462189
H 0	-0.197556	5.235046	2.470734
H 0	-2.786300	4.437302	2.442963
H 0	-5.235596	-0.198380	2.398682
H 0	-4.436218	-2.786453	2.393875
H 0	0.193146	-5.235031	2.391953
C 0	-0.359802	2.972443	-1.682983
H 0	-0.705200	3.780106	-1.031036
H 0	-0.231689	2.060257	-1.094147
H 0	0.594833	3.254044	-2.136993
H 0	-1.098602	2.799713	-2.470749
O 0	-1.072357	-2.217361	-0.849640
H 0	-0.861542	-1.344604	-0.443832
H 0	-0.234848	-2.589905	-1.182770

10) ^{L}Porph-CH_4-W2-TS
Total spin density: 2.0
Absolute energy: -1303.65528517 Hartree

C 0	-4.350600	-1.279144	-1.091248
C 0	-2.960526	-1.352020	-1.480148
C 0	-2.498489	-1.161346	-2.770309
C 0	2.277756	-2.042419	-2.737228
C 0	2.146255	-2.348907	2.112106
C 0	-2.696930	-2.038223	2.002060
O 0	0.011414	0.089539	-0.076843
Fe 0	-0.169861	-1.662628	-0.312790
N 0	-0.118103	-1.630127	-2.327881
N 0	1.783585	-2.148132	-0.322113
N 0	-0.262619	-2.129227	1.637985
N 0	-2.172379	-1.677155	-0.379990

C 0	-1.180557	-1.314789	-3.168610
C 0	-0.725235	-1.236618	-4.538071
C 0	0.611420	-1.519638	-4.534393
C 0	0.991013	-1.757095	-3.160889
C 0	2.648071	-2.209259	-1.413467
C 0	4.002167	-2.430740	-0.963333
C 0	3.968109	-2.482605	0.401489
C 0	2.590561	-2.309860	0.800537
C 0	0.818741	-2.287125	2.498734
C 0	0.352478	-2.437515	3.859039
C 0	-1.011902	-2.381027	3.824280
C 0	-1.393906	-2.180710	2.444916
C 0	-3.054810	-1.786636	0.690063
C 0	-4.409027	-1.556046	0.243881
H 0	-5.162949	-1.046768	-1.764191
H 0	-3.228500	-0.914139	-3.533493
H 0	3.053741	-2.115356	-3.491592
H 0	2.890778	-2.480957	2.889816
H 0	-3.489655	-2.087219	2.739900
H 0	-1.360138	-1.010803	-5.382431
H 0	1.289032	-1.566956	-5.374390
H 0	4.856918	-2.527237	-1.616867
H 0	4.789368	-2.633896	1.086823
H 0	0.995956	-2.580490	4.714935
H 0	-1.707809	-2.463333	4.646317
H 0	-5.277466	-1.588928	0.884964
H 0	0.620895	0.672226	-0.780792
C 0	1.412476	1.570511	-1.636185
H 0	1.318146	2.508682	-1.094360
H 0	2.391251	1.097473	-1.608185
H 0	0.878998	1.509445	-2.581757
O 0	-1.593200	1.233154	1.820831
H 0	-1.073456	1.030884	2.620468
H 0	-1.073395	0.904602	1.042953

11) ^{H}Porph-CH_4-W2

Total spin density: 4.0

Absolute energy: -1303.68292503 Hartree

C 0	-2.854263	-2.653168	-3.200119
C 0	-1.486191	-2.610397	-2.723175
C 0	-0.351639	-2.547913	-3.527542
C 0	3.568604	-2.486771	-0.641678
C 0	0.685577	-2.746445	3.273727
C 0	-3.235200	-2.755859	0.387756

N 0	1.376419	-2.527985	-1.768921
N 0	1.810303	-2.604797	1.083588
N 0	-1.043320	-2.728989	1.514404
N 0	-1.477142	-2.649475	-1.335449
C 0	0.972412	-2.511749	-3.095612
C 0	2.137009	-2.463181	-3.956940
C 0	3.238571	-2.444809	-3.146271
C 0	2.763382	-2.482132	-1.777603
C 0	3.137207	-2.547928	0.681351
C 0	3.999054	-2.583557	1.845581
C 0	3.189194	-2.659409	2.945587
C 0	1.820633	-2.670135	2.469574
C 0	-0.637711	-2.774841	2.841934
C 0	-1.801559	-2.864807	3.700531
C 0	-2.903061	-2.864532	2.888855
C 0	-2.428833	-2.776627	1.522888
C 0	-2.803665	-2.702927	-0.933945
C 0	-3.663895	-2.708511	-2.099716
H 0	-3.144989	-2.639191	-4.240463
H 0	-0.515213	-2.528091	-4.600540
H 0	4.641373	-2.449066	-0.803589
H 0	0.849930	-2.794189	4.345810
H 0	-4.307556	-2.783752	0.549957
H 0	2.105087	-2.448242	-5.036728
H 0	4.278488	-2.411697	-3.437408
H 0	5.078629	-2.557648	1.814636
H 0	3.481216	-2.707474	3.984634
H 0	-1.769409	-2.922394	4.778885
H 0	-3.942581	-2.920242	3.177582
H 0	-4.742920	-2.745270	-2.068024
O 0	0.057129	-0.482742	-0.065460
Fe 0	0.147110	-2.161774	-0.112320
C 0	2.533478	2.083847	0.584412
H 0	3.306717	1.629898	1.211472
H 0	1.766434	1.339508	0.352951
H 0	2.984940	2.446152	-0.343811
H 0	2.081696	2.924988	1.118317
O 0	-2.485016	0.485000	0.492584
H 0	-1.596924	0.237213	0.135559
H 0	-2.357452	0.758789	1.420029

12) ^{H}Porph-CH_4-W2-TS
Total spin density: 4.0
Absolute energy: -1303.65131023 Hartree

C 0	-1.426682	-0.924530	-4.461960
C 0	-0.321320	-1.071655	-3.543411
C 0	0.993744	-0.755997	-3.840881
C 0	3.655319	-1.780807	0.102081
C 0	-0.340576	-3.329636	2.393585
C 0	-3.014800	-2.203247	-1.507080
O 0	-0.149490	-0.002258	0.174118
Fe 0	0.274918	-1.739273	-0.606200
N 0	1.963425	-1.360794	-1.649811
N 0	1.423904	-2.462540	0.902115
N 0	-1.329086	-2.616882	0.247055
N 0	-0.775757	-1.571228	-2.328110
C 0	2.054489	-0.899719	-2.961914
C 0	3.427719	-0.599274	-3.283783
C 0	4.174515	-0.879211	-2.172745
C 0	3.267807	-1.358078	-1.158539
C 0	2.796661	-2.304626	1.053558
C 0	3.208923	-2.779510	2.354218
C 0	2.086304	-3.220551	2.995285
C 0	0.974533	-3.018051	2.095032
C 0	-1.408981	-3.143250	1.532272
C 0	-2.776947	-3.483612	1.840302
C 0	-3.528885	-3.161987	0.744278
C 0	-2.629486	-2.624039	-0.246277
C 0	-2.150421	-1.726822	-2.475296
C 0	-2.553223	-1.325806	-3.802551
H 0	-1.336578	-0.557648	-5.473877
H 0	1.209579	-0.378250	-4.834091
H 0	4.708450	-1.717834	0.352615
H 0	-0.548584	-3.753738	3.369659
H 0	-4.069200	-2.249374	-1.752350
H 0	3.764740	-0.229080	-4.241043
H 0	5.242767	-0.784485	-2.042877
H 0	4.227463	-2.771790	2.714005
H 0	2.002426	-3.645065	3.985062
H 0	-3.105072	-3.914047	2.775177
H 0	-4.594162	-3.274109	0.605804
H 0	-3.570190	-1.349670	-4.165100
H 0	0.507980	0.903931	-0.236465
C 0	1.202591	1.907150	-0.760727
H 0	0.786316	2.770752	-0.242203
H 0	2.239578	1.688522	-0.509781
H 0	0.984116	1.879807	-1.826721
O 0	-2.768433	0.737717	-0.004120

H 0	-3.053146	0.788666	0.927124
H 0	-1.797485	0.514130	-0.009827

13) ^{L}Porph-CH_3OH

Total spin density: 2.0

Absolute energy: -1302.145295 Hartree

C 0	1.885941	-1.847763	3.836456
C 0	0.914352	-1.718323	2.776642
C 0	-0.454025	-1.702300	2.970840
C 0	-2.521423	-1.235962	-1.396530
C 0	1.868179	-1.138687	-3.463776
C 0	3.936691	-1.591110	0.903778
O 0	0.740570	0.481873	-0.069595
Fe 0	0.712158	-1.151428	-0.221695
N 0	-1.094116	-1.468246	0.600174
N 0	-0.141357	-1.243423	-2.037827
N 0	2.508560	-1.386536	-1.095978
N 0	1.555527	-1.618300	1.544600
C 0	-1.386536	-1.587891	1.957062
C 0	-2.815338	-1.582413	2.161911
C 0	-3.396362	-1.449188	0.933487
C 0	-2.329422	-1.373138	-0.035217
C 0	-1.502274	-1.180100	-2.326630
C 0	-1.706039	-1.051712	-3.749252
C 0	-0.472153	-1.024170	-4.330994
C 0	0.500092	-1.135178	-3.269700
C 0	2.801224	-1.258072	-2.450867
C 0	4.229996	-1.274765	-2.657578
C 0	4.811569	-1.402008	-1.429276
C 0	3.744461	-1.464355	-0.458862
C 0	2.916687	-1.665955	1.833786
C 0	3.120621	-1.814987	3.255035
H 0	1.638733	-1.950668	4.882919
H 0	-0.821167	-1.788818	3.987518
H 0	-3.540146	-1.160812	-1.758530
H 0	2.234344	-1.044708	-4.480042
H 0	4.956924	-1.640625	1.267776
H 0	-3.294724	-1.671494	3.125748
H 0	-4.447281	-1.405914	0.688232
H 0	-2.674149	-0.985367	-4.222992
H 0	-0.224915	-0.934631	-5.378525
H 0	4.708496	-1.199800	-3.623016
H 0	5.862656	-1.452087	-1.185516
H 0	4.088486	-1.886002	3.729309

C 0	-2.018051	2.600784	0.288071
O 0	-1.497116	1.958145	-0.896225
H 0	-2.941406	3.104904	-0.007767
H 0	-2.255203	1.881012	1.085403
H 0	-1.328430	3.354919	0.695023
H 0	-0.647491	1.502808	-0.680954

14) ^{L}Porph-CH_3OH-TS

Total spin density: 2.0

Absolute energy: -1302.118172 Hartree

C 0	-4.357391	-1.768372	0.030900
C 0	-3.047424	-1.872818	-0.572083
C 0	-2.816376	-1.979492	-1.932510
C 0	1.962692	-2.582047	-2.557770
C 0	2.646881	-1.774750	2.183228
C 0	-2.158417	-1.701553	2.869293
O 0	-0.012085	-0.026474	-0.084534
Fe 0	-0.081070	-1.782364	0.113907
N 0	-0.362411	-2.220505	-1.822815
N 0	1.880615	-2.150360	-0.133133
N 0	0.183624	-1.792892	2.108215
N 0	-2.066437	-1.888580	0.412918
C 0	-1.571396	-2.162720	-2.510361
C 0	-1.352142	-2.383896	-3.921463
C 0	-0.012894	-2.586334	-4.093552
C 0	0.604218	-2.474960	-2.792740
C 0	2.557922	-2.412888	-1.320190
C 0	3.982071	-2.450455	-1.083405
C 0	4.175034	-2.192047	0.244431
C 0	2.869186	-2.009186	0.836288
C 0	1.398911	-1.694900	2.776566
C 0	1.175323	-1.543533	4.196930
C 0	-0.176071	-1.551086	4.392975
C 0	-0.792252	-1.694153	3.093414
C 0	-2.748749	-1.778351	1.620056
C 0	-4.173584	-1.718170	1.382736
H 0	-5.285660	-1.743973	-0.521225
H 0	-3.677002	-1.955292	-2.592316
H 0	2.608124	-2.779388	-3.406600
H 0	3.515564	-1.686630	2.827026
H 0	-2.811417	-1.614166	3.730881
H 0	0.383072	0.313660	-0.963303
H 0	-2.132950	-2.391037	-4.667984
H 0	0.523026	-2.787003	-5.009720

H 0	4.724258	-2.646957	-1.843384
H 0	5.106796	-2.140854	0.789032
H 0	1.959381	-1.453171	4.934662
H 0	-0.719650	-1.464508	5.322510
H 0	-4.920883	-1.641373	2.158997
C 0	2.477280	1.556381	-1.239227
O 0	1.480927	0.791870	-1.910400
H 0	2.998230	2.131851	-2.023529
H 0	2.046814	2.268173	-0.524231
H 0	3.220261	0.917221	-0.746094

15) ^{L}Porph-CH_3OH-W1

Total spin density: 2.0

Absolute energy: -1378.533652 Hartree

C 0	1.892090	-3.056030	2.174622
C 0	1.892090	-1.611954	2.174622
C 0	3.031418	-0.830582	2.174622
C 0	1.599045	3.792313	1.796707
C 0	-3.033173	2.370071	2.086945
C 0	-1.602814	-2.270416	2.077591
O 0	-0.018967	0.625000	0.129761
Fe 0	-0.003448	0.748642	1.770538
N 0	1.898500	1.354065	2.012619
N 0	-0.587936	2.665405	1.960037
N 0	-1.899796	0.178925	2.107819
N 0	0.584610	-1.130783	2.138275
C 0	3.032303	0.549484	2.092697
C 0	4.224838	1.361252	2.049210
C 0	3.822632	2.659592	1.921707
C 0	2.379639	2.656464	1.895813
C 0	0.217377	3.795654	1.839981
C 0	-0.595444	4.987503	1.809174
C 0	-1.897324	4.588562	1.910889
C 0	-1.894638	3.148010	1.994629
C 0	-3.033951	0.988617	2.133118
C 0	-4.225266	0.175690	2.180267
C 0	-3.822830	-1.129303	2.155991
C 0	-2.381332	-1.128815	2.110184
C 0	-0.221832	-2.266968	2.099030
C 0	0.590271	-3.459442	2.109497
H 0	2.783752	-3.664993	2.199997
H 0	3.990295	-1.335098	2.216980
H 0	2.104630	4.747314	1.706253
H 0	-3.991592	2.876923	2.109497

H 0	-2.096939	-3.229050	1.988068
H 0	5.230865	0.972183	2.106049
H 0	4.432785	3.548447	1.855728
H 0	-0.205124	5.991470	1.729080
H 0	-2.787720	5.199814	1.928360
H 0	-5.230881	0.568039	2.220856
H 0	-4.430069	-2.022141	2.172500
H 0	0.188126	-4.457352	2.040848
C 0	-1.351593	-4.992844	-1.407730
O 0	-1.481918	-4.064285	-0.313889
H 0	-1.559891	-5.991455	-1.013824
H 0	-2.066528	-4.790848	-2.220856
H 0	-0.339172	-4.996170	-1.839233
H 0	-1.285904	-3.133575	-0.620193
O 0	-1.073654	-1.542938	-1.189987
H 0	-0.547882	-0.844406	-0.721024
H 0	-1.845291	-1.123459	-1.607986

16) ^{L}Porph-CH_3OH-W1-TS
Total spin density: 2.0
Absolute energy: -1378.49555 Hartree

C 0	4.070496	0.399719	-1.807083
C 0	3.223602	-0.598358	-1.208496
C 0	3.624435	-1.465347	-0.208557
C 0	-0.161392	-4.313568	0.836227
C 0	-2.876221	-1.850220	-2.343842
C 0	0.990265	0.805527	-3.598740
O 0	-0.121658	-0.385406	0.037109
Fe 0	0.331467	-1.537170	-1.159149
N 0	1.498077	-2.691269	0.005096
N 0	-1.176300	-2.840256	-0.860458
N 0	-0.696762	-0.740509	-2.682877
N 0	1.956909	-0.579041	-1.804794
C 0	2.826157	-2.449463	0.343002
C 0	3.266418	-3.388092	1.349854
C 0	2.206116	-4.199051	1.631348
C 0	1.103470	-3.759216	0.806091
C 0	-1.225021	-3.876877	0.066254
C 0	-2.553268	-4.439896	0.119186
C 0	-3.320953	-3.738998	-0.766525
C 0	-2.467529	-2.744827	-1.372620
C 0	-2.048279	-0.932434	-2.964539
C 0	-2.466492	-0.049805	-4.027771
C 0	-1.375320	0.684250	-4.395782

C 0	-0.279602	0.264084	-3.556717
C 0	2.024460	0.422226	-2.767715
C 0	3.331635	1.036331	-2.765167
H 0	5.094650	0.583923	-1.518021
H 0	4.642426	-1.377609	0.154694
H 0	-0.336227	-5.138565	1.517990
H 0	-3.912918	-1.887711	-2.660675
H 0	1.178802	1.612869	-4.295868
H 0	-0.015945	0.666367	-0.217285
H 0	4.260849	-3.411636	1.770920
H 0	2.155060	-5.018951	2.332825
H 0	-2.843842	-5.263458	0.754776
H 0	-4.367142	-3.872482	-1.000366
H 0	-3.467209	-0.013916	-4.433273
H 0	-1.302185	1.443344	-5.160660
H 0	3.622330	1.845215	-3.415909
C 0	2.715866	3.908981	-0.713898
O 0	1.877945	3.212219	-1.627487
H 0	3.570724	4.354050	-1.242752
H 0	2.161942	4.743103	-0.245361
H 0	3.092621	3.267593	0.098511
O 0	0.050415	1.992859	-0.563263
H 0	0.893509	2.498962	-1.035507
H 0	-0.805267	2.418716	-0.733536

17) ^{L}Porph-CH_3OH-W2

Total spin density: 2.0

Absolute energy: -1378.523066 Hartree

C 0	-2.460281	-0.444565	-4.165787
C 0	-1.168762	-0.701157	-3.576600
C 0	0.032883	-0.305771	-4.131668
C 0	3.556091	-1.839355	-1.165649
C 0	0.222031	-3.692169	1.834305
C 0	-3.298431	-2.207657	-1.159256
O 0	0.036118	-0.334961	-0.207458
Fe 0	0.114838	-1.770782	-1.019150
N 0	1.494629	-1.249756	-2.383575
N 0	1.571091	-2.640335	0.057419
N 0	-1.236969	-2.791077	0.061523
N 0	-1.313889	-1.407013	-2.383209
C 0	1.271606	-0.565460	-3.577408
C 0	2.526657	-0.171082	-4.169022
C 0	3.517548	-0.604858	-3.335495
C 0	2.879089	-1.267609	-2.224838

C 0	2.945618	-2.478485	-0.105286
C 0	3.654312	-3.078979	0.997406
C 0	2.717209	-3.596405	1.843826
C 0	1.424744	-3.319702	1.266098
C 0	-1.015762	-3.449112	1.270432
C 0	-2.270264	-3.858139	1.853287
C 0	-3.259583	-3.443298	1.008545
C 0	-2.621170	-2.774689	-0.098007
C 0	-2.688461	-1.571533	-2.221573
C 0	-3.396515	-0.981628	-3.330566
H 0	-2.612946	0.081329	-5.096680
H 0	0.001968	0.239365	-5.068420
H 0	4.637787	-1.773560	-1.161362
H 0	0.251892	-4.217102	2.782593
H 0	-4.381027	-2.253174	-1.151077
H 0	2.620239	0.364670	-5.102188
H 0	4.586029	-0.494690	-3.447464
H 0	4.729309	-3.087097	1.098984
H 0	2.869644	-4.118484	2.776855
H 0	-2.364120	-4.395065	2.785751
H 0	-4.327377	-3.568649	1.111038
H 0	-4.471115	-0.980988	-3.436478
C 0	2.584976	2.076904	-0.140900
O 0	2.450729	0.834763	0.585220
H 0	3.558105	2.495010	0.127853
H 0	2.559174	1.929703	-1.230759
H 0	1.809067	2.808121	0.129303
H 0	1.572189	0.426407	0.390411
O 0	-2.511551	0.592194	0.509613
H 0	-1.623306	0.385269	0.135025
H 0	-2.450439	0.491425	1.477692

18) ^{L}Porph-CH_3OH-W2-TS
Total spin density: 2.0
Absolute energy: -1378.500879 Hartree

C 0	-4.444336	-0.380554	-1.554703
C 0	-3.078018	-0.139282	-1.957230
C 0	-2.676300	0.881805	-2.799942
C 0	2.095596	0.367722	-3.553009
C 0	2.186646	-3.234300	-0.299713
C 0	-2.649963	-3.033798	0.068039
O 0	0.009506	-0.004456	-0.111771
Fe 0	-0.230682	-1.106079	-1.462753
N 0	-0.283463	0.279816	-2.909790

N 0	1.715744	-1.396484	-1.875992
N 0	-0.240952	-2.810852	-0.405777
N 0	-2.239441	-1.107803	-1.413681
C 0	-1.382828	1.062744	-3.257477
C 0	-0.990967	2.076569	-4.207672
C 0	0.344330	1.914093	-4.442566
C 0	0.787720	0.808914	-3.627792
C 0	2.529419	-0.649612	-2.723419
C 0	3.903931	-1.072617	-2.596680
C 0	3.933105	-2.066437	-1.659912
C 0	2.573715	-2.270920	-1.215118
C 0	0.877533	-3.497391	0.060730
C 0	0.474380	-4.558517	0.953094
C 0	-0.887726	-4.518906	1.034332
C 0	-1.331116	-3.425262	0.203918
C 0	-3.069794	-1.944733	-0.673218
C 0	-4.439957	-1.498260	-0.769608
H 0	-5.286423	0.227707	-1.851105
H 0	-3.435715	1.569321	-3.156189
H 0	2.835434	0.874207	-4.162766
H 0	2.963058	-3.850555	0.140640
H 0	-3.401443	-3.597458	0.609131
H 0	0.673477	0.820100	-0.237213
H 0	-1.663422	2.805939	-4.635147
H 0	0.985168	2.486862	-5.096649
H 0	4.727158	-0.652802	-3.155914
H 0	4.784637	-2.627167	-1.302780
H 0	1.156235	-5.237137	1.444305
H 0	-1.544449	-5.153488	1.610672
H 0	-5.276886	-1.985565	-0.291275
C 0	2.711456	1.332489	0.767136
O 0	1.778076	1.618835	-0.273514
H 0	3.395096	2.195541	0.812164
H 0	2.227814	1.232361	1.747284
H 0	3.312546	0.440811	0.547470
O 0	-1.419876	-0.557190	2.146423
H 0	-0.784729	-0.383942	1.405853
H 0	-2.218704	-0.025848	1.972977

19) ^{L}Porph-SH-CH_4

Total spin density: 2.0

Absolute energy: -1626.03278772 Hartree

C 0	1.891220	-3.847305	1.654100
C 0	1.891220	-2.400711	1.654100

C 0	3.030624	-1.611420	1.654100
C 0	1.609085	3.030273	1.658539
C 0	-3.031754	1.609924	1.567947
C 0	-1.613449	-3.032730	1.653854
O 0	-0.006866	-0.020737	-0.150620
Fe 0	0.008514	-0.000870	1.498276
N 0	1.925766	0.588898	1.641678
N 0	-0.589462	1.924026	1.621048
N 0	-1.922592	-0.588486	1.663147
N 0	0.588669	-1.926285	1.657715
C 0	3.045486	-0.224258	1.650635
C 0	4.245651	0.584213	1.670349
C 0	3.845566	1.889771	1.675415
C 0	2.398422	1.887314	1.656219
C 0	0.225006	3.047363	1.637039
C 0	-0.585953	4.246033	1.616104
C 0	-1.889877	3.845322	1.577026
C 0	-1.889557	2.397598	1.582047
C 0	-3.048889	0.227737	1.619293
C 0	-4.245500	-0.584747	1.623260
C 0	-3.848160	-1.890076	1.653381
C 0	-2.401932	-1.896393	1.664185
C 0	-0.223648	-3.046783	1.650467
C 0	0.585083	-4.246490	1.650772
H 0	2.780090	-4.460938	1.655777
H 0	3.988968	-2.119965	1.657822
H 0	2.119690	3.987381	1.672119
H 0	-3.988358	2.119873	1.529282
H 0	-2.120636	-3.991700	1.646011
H 0	5.251205	0.190018	1.682495
H 0	4.457718	2.779480	1.692017
H 0	-0.193176	5.252106	1.629089
H 0	-2.779388	4.457474	1.553467
H 0	-5.251221	-0.191376	1.603073
H 0	-4.463943	-2.777481	1.661331
H 0	0.190781	-5.252090	1.649017
C 0	0.020050	0.205963	-3.862823
H 0	0.183975	-0.785736	-4.294479
H 0	0.002609	0.132950	-2.772247
H 0	-0.934845	0.602966	-4.219543
H 0	0.828766	0.874207	-4.172882
S 0	-0.355545	0.098053	4.063461
H 0	-0.540070	-1.253098	4.294479

20) ^{L}Porph-SH-CH_4-TS
Total spin density: 2.0
Absolute energy: -1625.99009533 Hartree

C 0	-1.793732	-1.760666	3.583145
C 0	-1.502319	-0.631180	2.723587
C 0	-1.440567	0.689148	3.146591
C 0	-0.511642	3.477005	-0.720993
C 0	0.001282	-0.530975	-3.418365
C 0	-1.305740	-3.282242	0.357010
O 0	0.975082	-0.236435	0.247757
Fe 0	-0.743118	0.089157	-0.136673
N 0	-0.905106	1.746048	0.983841
N 0	-0.335739	1.243774	-1.736435
N 0	-0.727051	-1.569733	-1.308762
N 0	-1.306091	-1.062943	1.423843
C 0	-1.179138	1.790176	2.341003
C 0	-1.207352	3.164093	2.796738
C 0	-0.969788	3.951843	1.705963
C 0	-0.783600	3.064468	0.578171
C 0	-0.287766	2.630905	-1.795990
C 0	0.063263	3.056580	-3.133545
C 0	0.236649	1.925842	-3.879730
C 0	-0.022507	0.796616	-3.010956
C 0	-0.341019	-1.624908	-2.639420
C 0	-0.355438	-2.999298	-3.100739
C 0	-0.741318	-3.773331	-2.045502
C 0	-0.958252	-2.883347	-0.922668
C 0	-1.454361	-2.436203	1.451492
C 0	-1.766785	-2.876251	2.796097
H 0	-1.989288	-1.692535	4.643356
H 0	-1.631714	0.881241	4.197571
H 0	-0.449158	4.544907	-0.903122
H 0	0.280273	-0.725250	-4.448975
H 0	-1.450226	-4.344238	0.526886
H 0	1.636810	0.624435	0.249756
H 0	-1.398346	3.469696	3.815140
H 0	-0.924927	5.029907	1.654388
H 0	0.161377	4.086304	-3.444870
H 0	0.501434	1.847443	-4.924072
H 0	-0.101288	-3.312164	-4.102936
H 0	-0.863251	-4.846146	-2.010880
H 0	-1.933990	-3.904083	3.083344
C 0	2.652939	1.724030	0.321854
H 0	3.540848	1.135681	0.539703

H 0	2.594482	2.156662	-0.673447
H 0	2.268066	2.332947	1.135620
S 0	-3.064957	0.213303	-0.998276
H 0	-3.526596	-1.006058	-0.540070

21) ^{L}Porph-SH-CH_4-W1

Total spin density: 2.0

Absolute energy: -1702.43636665 Hartree

C 0	1.891312	-3.845200	0.950470
C 0	1.891312	-2.399323	0.950470
C 0	3.031052	-1.609909	0.950470
C 0	1.611755	3.030807	0.906296
C 0	-3.030914	1.611877	0.878815
C 0	-1.612747	-3.030991	0.940964
O 0	-0.003769	-0.034103	-0.870500
Fe 0	0.008759	0.000320	0.785095
N 0	1.924652	0.589920	0.918365
N 0	-0.586349	1.923721	0.904449
N 0	-1.921585	-0.586472	0.958084
N 0	0.589249	-1.924667	0.949936
C 0	3.045380	-0.223587	0.934967
C 0	4.244812	0.584854	0.942078
C 0	3.844925	1.890030	0.929504
C 0	2.398865	1.887817	0.914597
C 0	0.228043	3.047012	0.899612
C 0	-0.581879	4.244629	0.882248
C 0	-1.887115	3.844986	0.867737
C 0	-1.888306	2.398331	0.881210
C 0	-3.048325	0.229431	0.925446
C 0	-4.244308	-0.582687	0.933594
C 0	-3.846527	-1.888290	0.954147
C 0	-2.400864	-1.894485	0.956177
C 0	-0.223373	-3.045288	0.938828
C 0	0.584976	-4.244415	0.941742
H 0	2.780243	-4.458633	0.954926
H 0	3.989456	-2.118027	0.958084
H 0	2.123032	3.986633	0.889984
H 0	-3.987442	2.122696	0.851044
H 0	-2.120117	-3.989822	0.931595
H 0	5.250153	0.190552	0.952652
H 0	4.455704	2.780258	0.922760
H 0	-0.187469	5.249969	0.880295
H 0	-2.776337	4.457886	0.855194
H 0	-5.250153	-0.189346	0.922867

H 0	-4.462051	-2.775833	0.962006
H 0	0.190689	-5.249954	0.937881
O 0	1.115875	2.052841	-2.322632
H 0	0.854523	1.215103	-1.868713
H 0	0.318771	2.427505	-2.740417
C 0	3.826553	4.204483	-2.523178
H 0	3.585175	5.106888	-1.951614
H 0	4.735947	3.750977	-2.116165
H 0	4.003220	4.480881	-3.567093
H 0	2.999649	3.489807	-2.463715
S 0	-0.317886	0.100861	3.334564
H 0	-0.511154	-1.248215	3.567078

22) ^{L}Porph-SH-CH_4-W1-TS
Total spin density: 2.0
Absolute energy: -1702.38291292 Hartree

C 0	-2.696106	-0.165085	-3.676804
C 0	-1.358612	-0.291168	-3.133926
C 0	-0.207458	0.172500	-3.749405
C 0	3.587769	-1.061432	-0.975357
C 0	0.515152	-2.717529	2.399506
C 0	-3.251312	-1.777512	-0.510239
O 0	-0.031326	0.317642	0.153839
Fe 0	0.158615	-1.285202	-0.674667
N 0	1.434509	-0.584229	-2.070892
N 0	1.738251	-1.783127	0.474106
N 0	-1.116531	-2.110077	0.660217
N 0	-1.405121	-0.940521	-1.906509
C 0	1.088486	0.019547	-3.270111
C 0	2.282150	0.433212	-3.978210
C 0	3.352783	0.061432	-3.213303
C 0	2.824600	-0.570877	-2.024063
C 0	3.081329	-1.614716	0.195190
C 0	3.884125	-2.077698	1.307037
C 0	3.016296	-2.525238	2.262344
C 0	1.678833	-2.345291	1.735672
C 0	-0.776749	-2.607574	1.905319
C 0	-1.970886	-3.017212	2.619049
C 0	-3.031219	-2.760956	1.798233
C 0	-2.490524	-2.190491	0.579819
C 0	-2.750107	-1.198456	-1.663849
C 0	-3.551392	-0.728195	-2.774902
H 0	-2.931732	0.295609	-4.625107
H 0	-0.323883	0.669189	-4.707382

H	0	4.666367	-0.985657	-1.065186
H	0	0.629822	-3.143387	3.391281
H	0	-4.327072	-1.903519	-0.442734
H	0	0.832550	0.791763	0.221405
H	0	2.286240	0.924759	-4.940200
H	0	4.403992	0.194748	-3.423187
H	0	4.963440	-2.052933	1.339539
H	0	3.244141	-2.943451	3.231888
H	0	-1.978897	-3.441177	3.612595
H	0	-4.081268	-2.932312	1.985046
H	0	-4.626221	-0.817154	-2.836945
C	0	-0.036896	3.593842	-0.021790
H	0	-0.703659	2.736954	0.068146
H	0	0.037079	4.209595	0.875397
H	0	-0.151627	4.168335	-0.941055
O	0	2.098679	2.288345	-0.263931
H	0	2.041489	2.077805	-1.228683
H	0	1.120636	3.034119	-0.073990
S	0	0.275055	-3.392929	-1.986435
H	0	-0.999405	-3.867935	-1.740845

23) ^{L}Porph-SH-CH_4-W2

Total spin density: 2.0

Absolute energy: -1702.43464064 Hartree

C	0	-3.597305	-1.652634	2.015976
C	0	-2.949554	-1.165070	0.818924
C	0	-3.589294	-0.496933	-0.209579
C	0	-0.258087	0.548889	-3.582108
C	0	3.184937	-1.435211	-0.794388
C	0	-0.152359	-2.515533	2.561874
O	0	0.072174	0.599472	0.307953
Fe	0	-0.175385	-0.852722	-0.449997
N	0	-1.629425	-0.149841	-1.660492
N	0	1.181671	-0.522842	-1.897415
N	0	1.220581	-1.812622	0.641983
N	0	-1.588989	-1.455811	0.865036
C	0	-2.978409	-0.036682	-1.366516
C	0	-3.668442	0.624573	-2.452515
C	0	-2.734207	0.910797	-3.405609
C	0	-1.462372	0.433060	-2.909317
C	0	0.970413	0.106415	-3.109772
C	0	2.218979	0.231583	-3.829437
C	0	3.188141	-0.325134	-3.044205
C	0	2.537186	-0.794922	-1.841034

C 0	2.575424	-1.901900	0.359009
C 0	3.266220	-2.556061	1.447876
C 0	2.327805	-2.854675	2.393768
C 0	1.055862	-2.388168	1.889679
C 0	-1.378800	-2.090225	2.086212
C 0	-2.631668	-2.223053	2.794037
H 0	-4.654068	-1.560822	2.219421
H 0	-4.656738	-0.331955	-0.109604
H 0	-0.274368	1.026917	-4.555725
H 0	4.256363	-1.579102	-0.885117
H 0	-0.129486	-2.975235	3.543427
H 0	-4.728745	0.829315	-2.469666
H 0	-2.875870	1.398376	-4.358887
H 0	2.322510	0.684875	-4.804291
H 0	4.244797	-0.419022	-3.246948
H 0	4.328583	-2.748886	1.472260
H 0	2.467667	-3.337418	3.349503
H 0	-2.739120	-2.687393	3.763184
C 0	2.041779	3.447708	-0.949448
H 0	2.589142	3.060013	-1.813660
H 0	1.424805	2.652069	-0.523209
H 0	1.404312	4.278732	-1.265427
H 0	2.753189	3.802444	-0.198257
O 0	0.230316	0.753815	3.093414
H 0	0.346680	0.746109	2.113556
H 0	-0.555923	1.296844	3.288696
S 0	-0.882736	-3.092346	-1.503738
H 0	-0.537155	-3.924300	-0.455139

24) ^{L}Porph-SH-CH_4-W2-TS
Total spin density: 2.0
Absolute energy: -1702.39661078 Hartree

C 0	1.868393	-3.860779	0.883300
C 0	1.868393	-2.412567	0.883300
C 0	3.008209	-1.621155	0.883300
C 0	1.632294	3.036972	0.970596
C 0	-3.002243	1.613983	0.673538
C 0	-1.636276	-3.034607	0.877670
O 0	-0.042557	-0.134186	-1.019608
Fe 0	0.010406	0.000290	0.780075
N 0	1.926941	0.595474	0.877625
N 0	-0.559128	1.932846	0.806320
N 0	-1.927475	-0.595245	0.839539
N 0	0.567032	-1.939056	0.891403

C 0	3.037262	-0.231781	0.891449
C 0	4.245636	0.561447	0.958221
C 0	3.861252	1.872269	1.000595
C 0	2.415924	1.888336	0.951813
C 0	0.249008	3.060349	0.891434
C 0	-0.564606	4.255783	0.859146
C 0	-1.864426	3.851105	0.748734
C 0	-1.860260	2.403442	0.726761
C 0	-3.038010	0.230621	0.742813
C 0	-4.246841	-0.568542	0.723190
C 0	-3.865234	-1.875946	0.795761
C 0	-2.418762	-1.893875	0.853363
C 0	-0.245056	-3.056076	0.887787
C 0	0.561157	-4.258270	0.887390
H 0	2.756348	-4.475952	0.881700
H 0	3.965057	-2.133469	0.891525
H 0	2.145920	3.990433	1.037781
H 0	-3.954239	2.129532	0.599503
H 0	-2.148056	-3.990509	0.860703
H 0	5.246582	0.155884	0.979980
H 0	4.484711	2.752213	1.061951
H 0	-0.178970	5.263260	0.914307
H 0	-2.753784	4.462112	0.699081
H 0	-5.246597	-0.165359	0.656326
H 0	-4.488937	-2.757477	0.793457
H 0	0.165482	-5.263245	0.886490
H 0	0.310928	0.742889	-1.617065
C 0	0.762970	1.783463	-2.480591
H 0	0.702316	1.295502	-3.451385
H 0	0.038315	2.576752	-2.310989
H 0	1.768784	1.979828	-2.116074
O 0	-1.088882	-2.298126	-2.271790
H 0	-0.282791	-2.821518	-2.436813
H 0	-0.803375	-1.437317	-1.861923
S 0	-0.297913	0.142639	3.210190
H 0	-0.675842	-1.164459	3.451370

2) The coordinates of the optimized structures (Optimized with LANL2DZ(6-31+G*))

25) ^{L}Porph-CH_4
Total spin density: 2.0
Absolute energy: Hartree

C	0	-4.467270	-1.788437	-0.031830
C	0	-3.577255	-1.107300	-0.938889
C	0	-3.892380	0.070313	-1.598511
C	0	-0.082200	1.257019	-4.334290
C	0	2.263596	-2.675339	-2.771652
C	0	-1.545059	-3.860031	-0.032898
O	0	-0.093292	-0.310059	-0.764435
Fe	0	-0.709656	-1.159149	-1.978683
N	0	-1.787704	0.315430	-2.839447
N	0	0.755249	-0.818512	-3.324722
N	0	0.150085	-2.933044	-1.548096
N	0	-2.390656	-1.796051	-1.059586
C	0	-3.053741	0.726669	-2.485748
C	0	-3.401733	1.943436	-3.176422
C	0	-2.328461	2.278244	-3.945877
C	0	-1.326965	1.265000	-3.724503
C	0	0.883148	0.280594	-4.144730
C	0	2.168274	0.276947	-4.798370
C	0	2.828842	-0.830368	-4.358398
C	0	1.946182	-1.501175	-3.436508
C	0	1.419662	-3.339050	-1.895020
C	0	1.757904	-4.569641	-1.224228
C	0	0.685455	-4.903580	-0.453247
C	0	-0.306198	-3.876495	-0.654388
C	0	-2.513412	-2.887909	-0.229065
C	0	-3.805969	-2.894714	0.409592
H	0	-5.465012	-1.451508	0.220749
H	0	-4.868149	0.507904	-1.409729
H	0	0.151703	2.072189	-5.012466
H	0	3.242538	-3.108627	-2.953873
H	0	-1.775375	-4.669556	0.653290
H	0	-4.348557	2.459335	-3.075333
H	0	-2.210159	3.126511	-4.608597
H	0	2.503632	1.029556	-5.501129
H	0	3.819855	-1.176590	-4.624435
H	0	2.696655	-5.096664	-1.341553
H	0	0.559814	-5.762238	0.194580
H	0	-4.147324	-3.655807	1.100250
C	0	2.322495	2.138062	1.047455
H	0	2.991577	2.624817	0.330444
H	0	1.648804	1.458267	0.518372
H	0	1.737106	2.899750	1.572479
H	0	2.917084	1.573776	1.773178

26) ^{L}Porph-CH_4-TS
Total spin density: 2.0
Absolute energy: -1227.54555741 Hartree

C 0	-3.508957	-1.456589	-2.716263
C 0	-2.083328	-1.497879	-2.496368
C 0	-1.135300	-1.326400	-3.494949
C 0	3.222000	-2.010040	-1.500488
C 0	1.141800	-2.275772	2.864761
C 0	-3.229600	-2.085876	0.802048
O 0	0.003372	0.026642	-0.041687
Fe 0	0.002838	-1.688965	-0.297760
N 0	0.869095	-1.688461	-2.121246
N 0	1.806732	-2.100327	0.504593
N 0	-0.867935	-2.137070	1.463531
N 0	-1.808517	-1.763458	-1.174179
C 0	0.237549	-1.439026	-3.319000
C 0	1.199539	-1.370865	-4.392044
C 0	2.424271	-1.595871	-3.836807
C 0	2.209946	-1.784470	-2.423080
C 0	3.028168	-2.142334	-0.132629
C 0	4.091568	-2.314423	0.825775
C 0	3.506714	-2.356964	2.056671
C 0	2.085587	-2.227280	1.847229
C 0	-0.232895	-2.253357	2.678131
C 0	-1.199341	-2.398132	3.740875
C 0	-2.430222	-2.370468	3.157364
C 0	-2.213806	-2.196487	1.740921
C 0	-3.032852	-1.870895	-0.554871
C 0	-4.098785	-1.695938	-1.511398
H 0	-3.980316	-1.273300	-3.673981
H 0	-1.496689	-1.126175	-4.499481
H 0	4.240860	-2.064377	-1.872772
H 0	1.508163	-2.377487	3.882156
H 0	-4.253616	-2.147949	1.158371
H 0	0.952591	-1.190247	-5.431046
H 0	3.390350	-1.633789	-4.324921
H 0	5.142487	-2.388229	0.574432
H 0	3.978912	-2.477051	3.023972
H 0	-0.951248	-2.514023	4.788773
H 0	-3.402405	-2.455963	3.626984
H 0	-5.154358	-1.746689	-1.274307
H 0	0.897324	0.589859	-0.395050
C 0	1.954529	1.498825	-0.774734
H 0	1.575882	2.445663	-0.393539

H 0	2.818710	1.094086	-0.251068
H 0	1.975418	1.404160	-1.858887

27) ^{L}Porph-CH_4-W1

Total spin density: 2.0

Absolute energy: -1304.02728810 Hartree

C 0	-2.928833	0.290833	-4.066269
C 0	-1.586900	-0.037811	-3.657867
C 0	-0.447205	0.523438	-4.211365
C 0	3.363159	-1.444183	-1.973251
C 0	0.385391	-4.114380	0.748154
C 0	-3.426331	-2.124100	-1.469238
O 0	-0.057587	-0.416626	-0.437943
Fe 0	-0.035355	-1.590744	-1.539886
N 0	1.197113	-0.704880	-2.862762
N 0	1.541275	-2.617569	-0.818893
N 0	-1.259964	-2.897461	-0.608810
N 0	-1.603729	-0.983383	-2.655685
C 0	0.847794	0.207047	-3.836227
C 0	2.024719	0.789291	-4.429291
C 0	3.097137	0.236100	-3.798615
C 0	2.575058	-0.684570	-2.821579
C 0	2.873856	-2.345703	-1.042343
C 0	3.705109	-3.143570	-0.177612
C 0	2.866776	-3.897522	0.586624
C 0	1.524033	-3.557770	0.189240
C 0	-0.910767	-3.802368	0.370255
C 0	-2.086884	-4.395386	0.953796
C 0	-3.160355	-3.832870	0.330948
C 0	-2.638138	-2.897781	-0.632600
C 0	-2.937057	-1.236359	-2.413696
C 0	-3.767853	-0.453796	-3.292908
H 0	-3.178268	0.999298	-4.846390
H 0	-0.578598	1.262390	-4.996002
H 0	4.439667	-1.322708	-2.041351
H 0	0.518005	-4.847565	1.538010
H 0	-4.503983	-2.224808	-1.382080
H 0	2.012787	1.526840	-5.222031
H 0	4.150528	0.425308	-3.962250
H 0	4.787506	-3.116348	-0.169525
H 0	3.116684	-4.620667	1.352951
H 0	-2.074829	-5.144684	1.735580
H 0	-4.213700	-4.023727	0.494492
H 0	-4.850235	-0.484543	-3.305634

O 0	1.917633	1.561249	0.212585
H 0	1.289368	0.862747	-0.065048
H 0	1.413620	2.110291	0.830963
C 0	5.483109	2.260132	0.452179
H 0	5.719040	2.283752	1.521362
H 0	6.121140	1.517502	-0.039246
H 0	5.678650	3.246170	0.017639
H 0	4.430389	1.996460	0.312897

28) ^{L}Porph-CH_4-W1-TS

Total spin density: 2.0

Absolute energy: -1303.96355233 Hartree

C 0	1.848068	-3.843369	2.659012
C 0	1.848068	-2.399506	2.659012
C 0	2.996613	-1.620712	2.659012
C 0	1.623642	3.015717	2.961029
C 0	-2.993317	1.631012	2.504044
C 0	-1.639282	-3.009171	2.660446
O 0	0.069794	0.031998	0.718353
Fe 0	0.004379	0.011124	2.487259
N 0	1.915649	0.583893	2.782578
N 0	-0.563736	1.923782	2.735931
N 0	-1.921539	-0.573654	2.602493
N 0	0.558960	-1.918182	2.687576
C 0	3.023407	-0.233078	2.733017
C 0	4.230453	0.551849	2.818512
C 0	3.844925	1.857056	2.931595
C 0	2.403259	1.867081	2.902939
C 0	0.239609	3.035690	2.873123
C 0	-0.557907	4.237259	2.876785
C 0	-1.853943	3.847168	2.718796
C 0	-1.848343	2.406693	2.632477
C 0	-3.022903	0.243591	2.508041
C 0	-4.233902	-0.542908	2.461900
C 0	-3.854691	-1.849228	2.531509
C 0	-2.412460	-1.858154	2.608154
C 0	-0.251160	-3.029663	2.686707
C 0	0.543228	-4.234909	2.683228
H 0	2.737885	-4.460846	2.647995
H 0	3.951660	-2.137833	2.633835
H 0	2.136658	3.968307	3.055069
H 0	-3.943405	2.152039	2.429031
H 0	-2.156600	-3.964188	2.657684
H 0	0.595261	0.809235	0.431274

H 0	5.234039	0.144272	2.811279
H 0	4.466919	2.738144	3.031754
H 0	-0.161911	5.239960	2.979614
H 0	-2.742859	4.463974	2.670242
H 0	-5.234039	-0.132858	2.393845
H 0	-4.478165	-2.734818	2.529861
H 0	0.139816	-5.239960	2.693344
C 0	2.259155	-0.100418	-2.079391
H 0	1.574646	-0.813324	-1.618805
H 0	1.930328	0.262344	-3.055069
H 0	3.302856	-0.418747	-2.067398
O 0	2.087616	1.863144	-0.479980
H 0	2.811768	1.622635	0.134171
H 0	2.180222	0.902893	-1.356293

29) ^{L}Porph-CH_4-W2

Total spin density: 2.0

Absolute energy: -1304.02710863 Hartree

C 0	-1.677338	-3.738647	-2.961395
C 0	-0.430573	-3.205994	-2.473618
C 0	0.613632	-2.804184	-3.290237
C 0	4.171951	-1.237091	-0.410553
C 0	1.463013	-2.230881	3.472961
C 0	-2.107147	-3.765259	0.592865
O 0	0.307953	-0.770279	0.042770
Fe 0	0.930191	-2.255905	0.083800
N 0	2.160034	-2.117264	-1.510651
N 0	2.510941	-1.880646	1.279938
N 0	-0.076736	-2.930405	1.692200
N 0	-0.429031	-3.163177	-1.095596
C 0	1.820251	-2.298218	-2.834000
C 0	2.903412	-1.895325	-3.694153
C 0	3.904968	-1.452744	-2.883041
C 0	3.432068	-1.586319	-1.528870
C 0	3.737000	-1.380417	0.896896
C 0	4.524506	-1.032944	2.052338
C 0	3.762100	-1.314087	3.146072
C 0	2.509933	-1.832458	2.657166
C 0	0.259903	-2.742400	3.015884
C 0	-0.817825	-3.160507	3.876083
C 0	-1.823624	-3.589722	3.065002
C 0	-1.359268	-3.436142	1.710419
C 0	-1.664978	-3.638596	-0.713669
C 0	-2.444580	-4.005966	-1.867996

H	0	-1.917114	-3.882523	-4.007584
H	0	0.477753	-2.893448	-4.363770
H	0	5.164764	-0.827362	-0.569656
H	0	1.595123	-2.135757	4.546402
H	0	-3.111908	-4.143677	0.751328
H	0	2.884628	-1.953033	-4.775360
H	0	4.880066	-1.071167	-3.159286
H	0	5.528839	-0.629807	2.013580
H	0	4.009674	-1.190125	4.192978
H	0	-0.792282	-3.118896	4.957794
H	0	-2.798920	-3.971054	3.339722
H	0	-3.446747	-4.413925	-1.827835
C	0	1.353439	2.821869	0.581207
H	0	2.338638	2.944626	1.042618
H	0	1.133118	1.756760	0.465073
H	0	1.349365	3.306503	-0.400467
H	0	0.595642	3.288132	1.219193
O	0	-2.323212	-0.051651	0.962936
H	0	-1.437195	-0.342728	0.663803
H	0	-2.339951	0.901825	0.794769

30) ^{L}Porph-CH_4-W2-TS
Total spin density: 2.0
Absolute energy: -1303.98041726 Hartree

C	0	-1.840317	-1.289261	-4.094070
C	0	-0.656097	-1.303223	-3.270157
C	0	0.615540	-0.992813	-3.729553
C	0	3.702057	-1.741547	-0.077835
C	0	-0.048355	-2.521713	2.884262
C	0	-3.079956	-2.277054	-0.880508
O	0	0.024872	0.033676	-0.037994
Fe	0	0.267227	-1.653442	-0.401810
N	0	1.839111	-1.436310	-1.646378
N	0	1.563705	-2.088257	1.079559
N	0	-1.247803	-2.309128	0.752228
N	0	-0.966034	-1.699631	-1.988708
C	0	1.777283	-1.078796	-2.974762
C	0	3.102676	-0.862869	-3.501587
C	0	3.975143	-1.105576	-2.482681
C	0	3.180618	-1.452835	-1.330612
C	0	2.940400	-2.024414	1.047165
C	0	3.488052	-2.260941	2.359497
C	0	2.429810	-2.448807	3.198044
C	0	1.237625	-2.342896	2.394058

C 0	-1.200989	-2.524231	2.111694
C 0	-2.520874	-2.803940	2.622421
C 0	-3.371368	-2.762787	1.556900
C 0	-2.572067	-2.445145	0.399658
C 0	-2.326370	-1.915741	-1.987305
C 0	-2.876312	-1.677643	-3.299179
H 0	-1.858322	-1.019653	-5.142792
H 0	0.714400	-0.696136	-4.769623
H 0	4.781967	-1.722427	0.036300
H 0	-0.157486	-2.710190	3.948212
H 0	-4.148743	-2.408569	-1.019897
H 0	3.321030	-0.578461	-4.523529
H 0	5.056992	-1.057281	-2.493820
H 0	4.545471	-2.274400	2.593185
H 0	2.439346	-2.651352	4.261917
H 0	-2.748993	-3.015228	3.659912
H 0	-4.441589	-2.927400	1.540558
H 0	-3.921738	-1.789200	-3.558487
H 0	0.936798	0.687271	0.110062
C 0	1.929840	1.663925	0.344100
H 0	1.339478	2.498642	0.718430
H 0	2.575363	1.183334	1.077393
H 0	2.367447	1.805313	-0.642914
O 0	-2.093414	1.096390	1.539551
H 0	-2.462326	0.330215	2.003815
H 0	-1.387192	0.720627	0.969955

31) ^{L}Porph-SH-CH_4

Total spin density: 2.0

Absolute energy: -1626.34631431 Hartree

C 0	-2.409088	-1.866959	-3.436523
C 0	-1.170120	-1.847504	-2.695007
C 0	0.092178	-1.937515	-3.270004
C 0	3.357803	-1.759293	0.296082
C 0	-0.203568	-1.290192	3.537003
C 0	-3.473572	-1.561111	-0.019592
O 0	-0.017410	0.112198	-0.009659
Fe 0	-0.047928	-1.503067	0.116135
N 0	1.431290	-1.806396	-1.220932
N 0	1.307205	-1.551544	1.622300
N 0	-1.541794	-1.510544	1.491974
N 0	-1.420532	-1.735031	-1.351288
C 0	1.299561	-1.918533	-2.579178
C 0	2.597641	-2.029007	-3.202866

C 0	3.517242	-1.981888	-2.197800
C 0	2.775085	-1.840942	-0.966736
C 0	2.672791	-1.618622	1.495407
C 0	3.301712	-1.511261	2.791489
C 0	2.298553	-1.366318	3.701630
C 0	1.058472	-1.393295	2.960800
C 0	-1.408875	-1.359314	2.854538
C 0	-2.709595	-1.272141	3.474716
C 0	-3.631180	-1.355300	2.474945
C 0	-2.896606	-1.488770	1.239441
C 0	-2.782013	-1.674011	-1.224350
C 0	-3.412979	-1.758148	-2.520996
H 0	-2.483749	-1.953461	-4.513351
H 0	0.140182	-2.029785	-4.351303
H 0	4.442154	-1.801147	0.345352
H 0	-0.248917	-1.161285	4.614502
H 0	-4.557938	-1.523590	-0.072098
H 0	2.765335	-2.131165	-4.267792
H 0	4.596527	-2.036774	-2.266434
H 0	4.370316	-1.542496	2.963684
H 0	2.372818	-1.256073	4.776276
H 0	-2.877914	-1.159576	4.538452
H 0	-4.711075	-1.323257	2.549332
H 0	-4.482269	-1.736633	-2.690582
C 0	0.318161	3.812103	-0.217087
H 0	-0.437225	4.217484	-0.898270
H 0	0.208649	2.725876	-0.151093
H 0	0.186523	4.256378	0.775009
H 0	1.315842	4.058929	-0.594772
S 0	-0.237091	-4.008133	0.686600
H 0	-1.490662	-4.208435	0.220428

32) ^{L}Porph-SH-CH_4-TS

Total spin density: 2.0

Absolute energy: -1626.30289965 Hartree

C 0	-2.735458	-1.192383	-3.192230
C 0	-1.468552	-1.265793	-2.499374
C 0	-0.269226	-1.655777	-3.088348
C 0	3.171936	-1.632523	0.315369
C 0	-0.005630	0.267853	3.435043
C 0	-3.531921	-0.159256	0.156708
O 0	0.055511	0.959763	-0.261047
Fe 0	-0.137451	-0.737045	0.178543
N 0	1.201874	-1.460510	-1.131897

N 0	1.304840	-0.694397	1.590912
N 0	-1.518509	-0.121338	1.546783
N 0	-1.622864	-0.913528	-1.185867
C 0	0.963409	-1.759644	-2.448410
C 0	2.165955	-2.256760	-3.076782
C 0	3.130600	-2.275955	-2.113281
C 0	2.515442	-1.777878	-0.905167
C 0	2.609131	-1.109695	1.474000
C 0	3.317902	-0.890533	2.712875
C 0	2.427811	-0.324524	3.576523
C 0	1.171432	-0.216141	2.870712
C 0	-1.255493	0.292892	2.827667
C 0	-2.472366	0.746307	3.466217
C 0	-3.471619	0.605515	2.551819
C 0	-2.863388	0.077026	1.350479
C 0	-2.945831	-0.605881	-1.028030
C 0	-3.656815	-0.784271	-2.274277
H 0	-2.883392	-1.424179	-4.239685
H 0	-0.301102	-1.923691	-4.140945
H 0	4.215942	-1.930237	0.358078
H 0	0.051910	0.625244	4.459503
H 0	-4.598419	0.047104	0.134415
H 0	2.242264	-2.560150	-4.113647
H 0	4.162216	-2.594559	-2.197281
H 0	4.358749	-1.136993	2.882339
H 0	2.588120	-0.015976	4.602142
H 0	-2.535446	1.118484	4.481277
H 0	-4.523056	0.841278	2.660416
H 0	-4.716600	-0.609756	-2.413086
S 0	-0.647705	-2.905000	1.161667
H 0	-1.972916	-2.936386	0.895111
H 0	1.111511	1.287277	-0.480423
C 0	2.365372	1.851440	-0.789169
H 0	2.096863	2.888336	-0.986069
H 0	2.946700	1.687790	0.116638
H 0	2.691956	1.284332	-1.659088

33) ^{L}Porph-SH-CH_4-W1
Total spin density: 2.0
Absolute energy: -1702.77909809 Hartree

C 0	-2.823074	-0.308243	-3.555756
C 0	-1.510178	-0.420853	-2.967300
C 0	-0.319763	-0.193985	-3.648911
C 0	3.321655	-0.894958	-0.541473

C	0	0.141556	-1.909073	2.960785
C	0	-3.500458	-1.251007	-0.156494
O	0	-0.155365	0.631668	0.116837
Fe	0	-0.088760	-0.933014	-0.321533
N	0	1.237885	-0.625046	-1.805496
N	0	1.430588	-1.358765	0.947311
N	0	-1.411453	-1.539429	1.097702
N	0	-1.609024	-0.783875	-1.648407
C	0	0.955627	-0.287979	-3.102921
C	0	2.176285	-0.053879	-3.837646
C	0	3.201508	-0.253174	-2.962524
C	0	2.601471	-0.606857	-1.698166
C	0	2.773500	-1.237625	0.686646
C	0	3.541107	-1.511063	1.878479
C	0	2.644653	-1.786407	2.866104
C	0	1.330841	-1.687027	2.274506
C	0	-1.129364	-1.853149	2.408676
C	0	-2.351563	-2.102295	3.134415
C	0	-3.377319	-1.920776	2.256500
C	0	-2.785553	-1.556320	0.991684
C	0	-2.948608	-0.892670	-1.384857
C	0	-3.718903	-0.600723	-2.570206
H	0	-3.017181	-0.039993	-4.586731
H	0	-0.392258	0.084061	-4.696457
H	0	4.404037	-0.834167	-0.603287
H	0	0.215515	-2.159271	4.015060
H	0	-4.583923	-1.296326	-0.093857
H	0	2.224625	0.226593	-4.882339
H	0	4.266464	-0.167908	-3.137680
H	0	4.621918	-1.483932	1.935242
H	0	2.836838	-2.036530	3.901917
H	0	-2.400696	-2.377136	4.180664
H	0	-4.441422	-2.014435	2.434235
H	0	-4.800110	-0.622467	-2.625412
O	0	1.807236	2.688110	0.255325
H	0	1.155136	1.959274	0.180313
H	0	1.283829	3.460480	0.514709
C	0	5.425781	3.274567	0.285049
H	0	5.675858	3.703369	1.261169
H	0	5.987030	2.343719	0.148193
H	0	5.705704	3.982239	-0.502426
H	0	4.351974	3.070923	0.236053
S	0	-0.069183	-3.462067	-0.658707
H	0	-1.333237	-3.586395	-1.122818

34) ^{L}Porph-SH-CH_4-W1-TS
Total spin density: 2.0
Absolute energy: -1702.72203865 Hartree

C 0	1.844727	-3.862213	1.659714
C 0	1.844727	-2.415833	1.659714
C 0	2.988876	-1.627167	1.659714
C 0	1.629532	3.014893	1.873932
C 0	-2.984253	1.626648	1.440765
C 0	-1.642654	-3.015991	1.570847
O 0	0.013657	-0.003998	-0.222961
Fe 0	-0.001740	0.003784	1.586227
N 0	1.927231	0.585358	1.741119
N 0	-0.559448	1.946976	1.643250
N 0	-1.940400	-0.588318	1.537338
N 0	0.556595	-1.939438	1.662964
C 0	3.026321	-0.235596	1.720932
C 0	4.238541	0.546677	1.809921
C 0	3.857147	1.853363	1.899307
C 0	2.413864	1.867218	1.850220
C 0	0.239639	3.049393	1.762039
C 0	-0.553772	4.256317	1.736435
C 0	-1.851471	3.861877	1.595596
C 0	-1.840103	2.417175	1.544113
C 0	-3.028152	0.235336	1.434311
C 0	-4.243698	-0.544342	1.340378
C 0	-3.868484	-1.853745	1.387146
C 0	-2.426559	-1.862000	1.506165
C 0	-0.256622	-3.049255	1.642776
C 0	0.540833	-4.255142	1.655777
H 0	2.734300	-4.479935	1.663071
H 0	3.944382	-2.144592	1.647766
H 0	2.145111	3.967209	1.960510
H 0	-3.934677	2.148453	1.367386
H 0	-2.161209	-3.970444	1.542282
H 0	0.497482	0.785675	-0.534912
H 0	5.240631	0.135910	1.818085
H 0	4.481842	2.733444	1.988464
H 0	-0.157547	5.261276	1.810989
H 0	-2.740509	4.477219	1.534653
H 0	-5.240646	-0.130814	1.251511
H 0	-4.492996	-2.737457	1.343552
H 0	0.140121	-5.261276	1.651779
C 0	1.496536	-0.058868	-3.301346

H 0	0.789749	-0.650528	-2.718567
H 0	1.056351	0.429794	-4.172852
H 0	2.430817	-0.576492	-3.525558
O 0	2.061935	1.770996	-1.634171
H 0	2.754120	1.293030	-1.132874
H 0	1.780000	0.885071	-2.553467
S 0	0.098572	-0.170593	4.012970
H 0	-0.738739	-1.220230	4.172836

35) ^{L}Porph-SH-CH_4-W2

Total spin density: 2.0

Absolute energy: -1702.77890832 Hartree

C 0	1.876282	-3.845276	1.431442
C 0	1.876282	-2.402008	1.431442
C 0	3.016434	-1.613556	1.431442
C 0	1.610443	3.016479	1.479980
C 0	-3.015854	1.612457	1.257690
C 0	-1.611328	-3.017807	1.300385
O 0	0.057800	-0.023788	-0.391403
Fe 0	-0.000977	0.006470	1.234665
N 0	1.929916	0.585846	1.448669
N 0	-0.586655	1.933319	1.360382
N 0	-1.932037	-0.585846	1.299744
N 0	0.582794	-1.927780	1.419678
C 0	3.036926	-0.222565	1.453278
C 0	4.239441	0.575058	1.503525
C 0	3.844376	1.878937	1.530426
C 0	2.401382	1.875671	1.487700
C 0	0.219193	3.037827	1.415802
C 0	-0.576721	4.241943	1.405670
C 0	-1.880066	3.846451	1.339340
C 0	-1.871826	2.403458	1.311722
C 0	-3.038300	0.223679	1.246674
C 0	-4.239929	-0.574295	1.185318
C 0	-3.843262	-1.877945	1.194122
C 0	-2.401428	-1.870850	1.262573
C 0	-0.227859	-3.041733	1.378052
C 0	0.573822	-4.241241	1.400620
H 0	2.767487	-4.460098	1.446487
H 0	3.974640	-2.124878	1.430466
H 0	2.119720	3.975082	1.519379
H 0	-3.972610	2.125320	1.219131
H 0	-2.122772	-3.974289	1.251251
H 0	5.245087	0.174057	1.521957

H 0	4.458496	2.769760	1.573395
H 0	-0.177139	5.247574	1.445419
H 0	-2.771774	4.460236	1.314056
H 0	-5.245102	-0.174484	1.138367
H 0	-4.454010	-2.770874	1.151794
H 0	0.175018	-5.247574	1.380600
C 0	-0.008026	2.595764	-3.121719
H 0	-0.357178	3.553741	-2.723083
H 0	0.011963	1.851517	-2.320313
H 0	0.998642	2.719604	-3.534058
H 0	-0.686813	2.266022	-3.915024
O 0	-1.018860	-2.046494	-2.091248
H 0	-0.653107	-1.355225	-1.499359
H 0	-0.780273	-1.760315	-2.985077
S 0	0.154541	-0.242691	3.765793
H 0	-0.819107	-1.168716	3.915024

36) ^{L}Porph-SH-CH_4-W2-TS

Total spin density: 2.0

Absolute energy: -1702.73870311 Hartree

C 0	-3.523178	0.287750	-2.571640
C 0	-2.103043	0.119583	-2.362991
C 0	-1.124329	0.433792	-3.302094
C 0	3.196304	-0.709518	-1.444473
C 0	1.038361	-1.807449	2.746887
C 0	-3.301559	-1.051346	0.757660
O 0	-0.088776	0.915497	0.384567
Fe 0	-0.038498	-0.724258	-0.299300
N 0	0.867523	-0.210464	-2.018570
N 0	1.765350	-1.165558	0.488831
N 0	-0.960342	-1.364319	1.399719
N 0	-1.863510	-0.405975	-1.120895
C 0	0.249222	0.266006	-3.145386
C 0	1.222626	0.527176	-4.180389
C 0	2.438690	0.183380	-3.668198
C 0	2.201935	-0.274734	-2.319534
C 0	2.991592	-1.108582	-0.129105
C 0	4.035873	-1.490128	0.792221
C 0	3.426285	-1.767853	1.979218
C 0	2.008759	-1.573349	1.776398
C 0	-0.337524	-1.729568	2.565674
C 0	-1.319534	-2.036072	3.583130
C 0	-2.543213	-1.844681	3.018341
C 0	-2.309723	-1.410751	1.658890

C	0	-3.088470	-0.568649	-0.534424
C	0	-4.137390	-0.144272	-1.432526
H	0	-3.974900	0.681519	-3.473663
H	0	-1.464981	0.831314	-4.254181
H	0	4.217789	-0.715164	-1.814331
H	0	1.389435	-2.112778	3.728653
H	0	-4.331329	-1.121872	1.096024
H	0	0.990433	0.911652	-5.165726
H	0	3.409683	0.229813	-4.145325
H	0	5.090591	-1.530090	0.550110
H	0	3.878387	-2.086823	2.910049
H	0	-1.085144	-2.352615	4.591827
H	0	-3.520523	-1.967407	3.468170
H	0	-5.195877	-0.172714	-1.205978
H	0	0.882370	1.533752	0.312485
C	0	1.935120	2.410263	0.289047
H	0	1.454407	3.349380	0.560394
H	0	2.618774	2.011429	1.037598
H	0	2.297531	2.360809	-0.736740
O	0	-2.159210	2.817200	0.444870
H	0	-2.693817	2.608444	-0.335556
H	0	-1.451233	2.133011	0.448776
S	0	-0.101822	-3.079666	-0.837372
H	0	-1.441986	-3.254500	-0.801147

2) The coordinates of the optimized structures (Optimized with CEP-121G(6-31+G*))

37) ^{L}Porph-SH
Total spin density: 2.0
Absolute energy: -1585.74744341 Hartree

C	0	-1.775284	0.109161	-3.906418
C	0	-0.677109	0.248611	-2.979630
C	0	0.650162	0.411163	-3.349900
C	0	3.286667	0.708572	0.694916
C	0	-0.750748	0.439148	3.348068
C	0	-3.376800	0.030518	-0.696259
O	0	-0.236938	2.155777	-0.091019
Fe	0	-0.060806	0.532974	0.005081
N	0	1.634674	0.520462	-1.105865
N	0	1.048065	0.560165	1.685074
N	0	-1.727951	0.262848	1.107635

N 0	-1.139267	0.202881	-1.682983
C 0	1.725143	0.522156	-2.474900
C 0	3.104782	0.638474	-2.887161
C 0	3.849655	0.707428	-1.749023
C 0	2.922500	0.641541	-0.643387
C 0	2.409042	0.675674	1.776154
C 0	2.819153	0.747131	3.158844
C 0	1.681747	0.672897	3.906067
C 0	0.584641	0.555038	2.974823
C 0	-1.824478	0.306549	2.475128
C 0	-3.203049	0.187851	2.887192
C 0	-3.941940	0.076111	1.747269
C 0	-3.010254	0.125046	0.645111
C 0	-2.506927	0.065765	-1.775970
C 0	-2.909042	-0.008072	-3.160721
H 0	-1.673340	0.101059	-4.984497
H 0	0.870453	0.433502	-4.413269
H 0	4.345688	0.801651	0.918015
H 0	-0.972672	0.452286	4.411316
H 0	-4.435577	-0.076981	-0.914368
H 0	3.441757	0.656281	-3.916168
H 0	4.924194	0.796646	-1.649048
H 0	3.844208	0.838898	3.495667
H 0	1.578186	0.690750	4.983841
H 0	-3.543640	0.190689	3.915070
H 0	-5.014587	-0.031921	1.644958
H 0	-3.930054	-0.129135	-3.500748
S 0	0.191696	-2.006927	-0.272446
H 0	-1.121841	-2.325058	-0.247116

38) ^{L}Porph-SH-CH_4-TS

Total spin density: 2.0

Absolute energy: -1626.22506561 Hartree

C 0	-3.199402	-1.219833	-2.721054
C 0	-1.821808	-1.228470	-2.283768
C 0	-0.731613	-1.464371	-3.116669
C 0	3.287430	-1.362015	-0.422379
C 0	0.629807	-0.009491	3.391647
C 0	-3.415024	-0.498184	0.792450
O 0	-0.063522	0.977081	-0.173065
Fe 0	-0.045807	-0.776657	0.137283
N 0	1.066879	-1.271103	-1.455826
N 0	1.630676	-0.706848	1.256393
N 0	-1.181839	-0.384018	1.785019

N 0	-1.745529	-0.983139	-0.938843
C 0	0.604950	-1.496200	-2.728180
C 0	1.699585	-1.829102	-3.610321
C 0	2.830170	-1.824875	-2.848495
C 0	2.421600	-1.477463	-1.507721
C 0	2.917923	-0.985413	0.863708
C 0	3.831711	-0.795242	1.965088
C 0	3.082275	-0.383881	3.026840
C 0	1.709610	-0.341049	2.578247
C 0	-0.711487	-0.047180	3.028839
C 0	-1.813812	0.248245	3.918533
C 0	-2.955856	0.090454	3.194016
C 0	-2.550400	-0.290634	1.858856
C 0	-3.034256	-0.805954	-0.513763
C 0	-3.955338	-0.959335	-1.617050
H 0	-3.527420	-1.390381	-3.738998
H 0	-0.944427	-1.658890	-4.164368
H 0	4.340408	-1.560974	-0.601395
H 0	0.855865	0.273285	4.416122
H 0	-4.478485	-0.385864	0.984726
H 0	1.598236	-2.047745	-4.666200
H 0	3.848587	-2.035873	-3.150253
H 0	4.901871	-0.953766	1.915482
H 0	3.411484	-0.139877	4.029297
H 0	-1.708954	0.535156	4.957565
H 0	-3.981720	0.223938	3.514359
H 0	-5.031967	-0.869720	-1.541595
S 0	-0.196838	-3.036270	0.984238
H 0	-1.542175	-3.170731	0.978729
H 0	0.889481	1.423294	-0.570251
C 0	2.009903	2.117600	-1.074066
H 0	1.630264	3.137283	-1.120224
H 0	2.776215	1.942368	-0.320709
H 0	2.190948	1.646393	-2.038635

39) ^{L}Porph-SH-CH_4-W1-TS

Total spin density: 2.0

Absolute energy: -1702.64337238 Hartree

C 0	-2.823715	1.011963	-3.468018
C 0	-1.532486	0.507736	-3.055191
C 0	-0.327927	0.822098	-3.673370
C 0	3.201340	-1.660324	-1.476654
C 0	-0.007568	-3.226105	1.786209
C 0	-3.581329	-1.020340	-0.608139

O 0	0.023148	0.211578	0.135254
Fe 0	-0.168396	-1.235168	-0.963455
N 0	1.173767	-0.562866	-2.309448
N 0	1.315094	-2.236984	-0.029312
N 0	-1.538788	-1.993347	0.323013
N 0	-1.668671	-0.326675	-1.972946
C 0	0.923553	0.308060	-3.341324
C 0	2.141357	0.593094	-4.065002
C 0	3.132416	-0.128403	-3.466600
C 0	2.520538	-0.840836	-2.369980
C 0	2.637222	-2.300323	-0.373398
C 0	3.371628	-3.107544	0.572754
C 0	2.467667	-3.531387	1.501251
C 0	1.187775	-2.985596	1.109741
C 0	-1.269150	-2.763428	1.421982
C 0	-2.486450	-3.050583	2.149155
C 0	-3.496704	-2.437271	1.470337
C 0	-2.886368	-1.778946	0.336166
C 0	-3.013336	-0.345108	-1.679993
C 0	-3.743591	0.477386	-2.618164
H 0	-2.986679	1.684235	-4.301331
H 0	-0.370209	1.505966	-4.516830
H 0	4.267883	-1.791351	-1.636383
H 0	0.050873	-3.841980	2.679611
H 0	-4.657089	-0.934967	-0.481384
H 0	0.970428	0.424118	0.237885
H 0	2.210831	1.248825	-4.924179
H 0	4.181656	-0.180252	-3.729416
H 0	4.434372	-3.308929	0.523193
H 0	2.635071	-4.156128	2.369858
H 0	-2.543182	-3.641983	3.054657
H 0	-4.554184	-2.420074	1.703200
H 0	-4.816727	0.622879	-2.607803
C 0	0.926849	3.474213	0.698044
H 0	0.029633	2.854416	0.684494
H 0	1.214691	3.818512	1.693466
H 0	0.930054	4.269928	-0.048874
O 0	2.677429	1.790039	-0.037674
H 0	2.477570	1.805115	-0.996140
H 0	1.835297	2.691818	0.389786
S 0	-0.541534	-3.022873	-2.554443
H 0	-1.861328	-3.222717	-2.339081

40) ^{L}Porph-SH-CH_4-W2-TS

Total spin density: 2.0
Absolute energy: -1702.66090672 Hartree

C 0	-3.470474	-2.557281	0.737076
C 0	-2.317932	-2.161255	-0.038605
C 0	-2.169266	-2.389221	-1.404205
C 0	2.155487	-0.700516	-2.769608
C 0	2.815994	1.052948	1.693253
C 0	-1.326736	-0.967789	3.145508
O 0	-0.515259	0.854187	-0.081253
Fe 0	0.342728	-0.706848	0.142853
N 0	0.045486	-1.378479	-1.724854
N 0	2.128845	0.027481	-0.432541
N 0	0.698364	-0.123611	2.061127
N 0	-1.392303	-1.544600	0.761978
C 0	-1.068329	-2.037582	-2.180237
C 0	-0.923141	-2.365372	-3.579391
C 0	0.304291	-1.911087	-3.961273
C 0	0.896713	-1.298721	-2.795853
C 0	2.721512	-0.067810	-1.669556
C 0	3.996460	0.609360	-1.670120
C 0	4.163437	1.126892	-0.420471
C 0	2.998703	0.750107	0.346909
C 0	1.759262	0.631500	2.492035
C 0	1.629761	0.919922	3.903870
C 0	0.473709	0.333878	4.319778
C 0	-0.108658	-0.303528	3.159958
C 0	-1.929688	-1.533096	2.021057
C 0	-3.226898	-2.167908	2.021942
S 0	1.619125	-2.628677	0.814789
H 0	-4.340118	-3.065704	0.339569
H 0	-2.982544	-2.903000	-1.909286
H 0	2.731583	-0.711060	-3.690628
H 0	3.588593	1.648422	2.171692
H 0	-1.872864	-1.027756	4.082565
H 0	-1.665695	-2.883194	-4.173645
H 0	0.776276	-1.977036	-4.933655
H 0	4.661011	0.676285	-2.522461
H 0	4.995819	1.702759	-0.035446
H 0	2.339081	1.497452	4.483505
H 0	0.035233	0.334030	5.309875
H 0	-3.857452	-2.286774	2.894196
H 0	0.841110	-3.047638	1.838135
H 0	-0.303558	1.437302	-1.051544
C 0	-0.185532	2.235443	-2.161240

H	0	-1.037735	2.904495	-2.048615
H	0	0.788498	2.707200	-2.035889
H	0	-0.255585	1.541900	-2.998032
O	0	-3.182877	1.532700	0.512894
H	0	-3.633652	0.677887	0.579742
H	0	-2.241730	1.301056	0.337265