Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supporting Information

Mechanistic Insight to Selective Catalytic Reduction of NO by NH_3 over Low-valent Titanium-porphyrin: A DFT Study

Phornphimon Maitarad,[a] Jittima Meeprasert,[b] Liyi Shi,[a] Jumras Limtrakul,[c] Dengsong Zhang[a] and Supawadee Namuangruk[b]**

[a] Research Center of Nano Science and Technology, Shanghai University, Shanghai 200444, P. R. China

[b] National Nanotechnology Center, NSTDA, 111 Thailand Science Park, Pahonyothin Road, Klong Luang, Pathum Thani 12120, Thailand

[c] Vidyasirimedhi Institute of Science and Technology, Rayong 21210, Thailand

Supporting Information Details

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Table S1. Total energies of all reaction steps over the Ti-porphyrin with low and high spin states based on M06L/6-31G(d,p) (C, N, O, H) LANL2DZ (Ti)

Low spin	Total energy (au)	Relative energy (kcal/mol)
singlet		
^{1}Ti-Por	-1046.469415	0.00
^{1}Ti-NH_3	-1103.105530	-54.92
^{1}TS1	-1103.047604	-18.57
^{1}TiH-NH_2	-1103.062580	-27.96
doublet		
NO-^{2}TiH-NH_2	-1232.951737	-37.23
^{2}TS2	-1232.947110	-34.33
^{2}TiH-NH_2NO	-1232.957085	-40.59
^{2}TS3	-1232.926783	-21.57
^{2}TiH-NHNOH	-1233.008607	-72.92
^{2}TS4	-1232.996984	-65.62
^{2}TiH-N_2-H_2O	-1233.013784	-76.16
^{2}TiH-H_2O	-1123.497923	-75.46
^{1}TiH-Por	-1047.042187	-47.40
High Spin		
triplet		
^{3}Ti-Por	-1046.482844	0.00
^{3}Ti-NH_3	-1103.113733	-60.06
^{3}TS1	-1103.057248	-24.62
^{3}TiH-NH_2	-1103.068147	-31.46
quartet		
NO-^{4}TiH-NH_2	-1232.952167	-37.50
^{4}TS2	-1232.937503	-28.30
^{4}TiH-NH_2NO	-1232.941243	-30.64
^{4}TS3	-1232.891061	0.85
^{4}TiH-NHNOH	-1232.922410	-70.10
^{4}TS4	-1232.990522	-61.57
^{4}TiH-N_2-H_2O	-1233.010911	-74.36
^{4}TiH-H_2O	-1123.494560	-73.35
^{3}TiH-Por	-1047.053015	-54.20
Isolated molecule		
$^{1}NH_3$	-56.5486011	
^{2}NO	-129.8743916	
$^{1}H_2O$	-76.4110228	
$^{1}N_2$	-109.5147356	

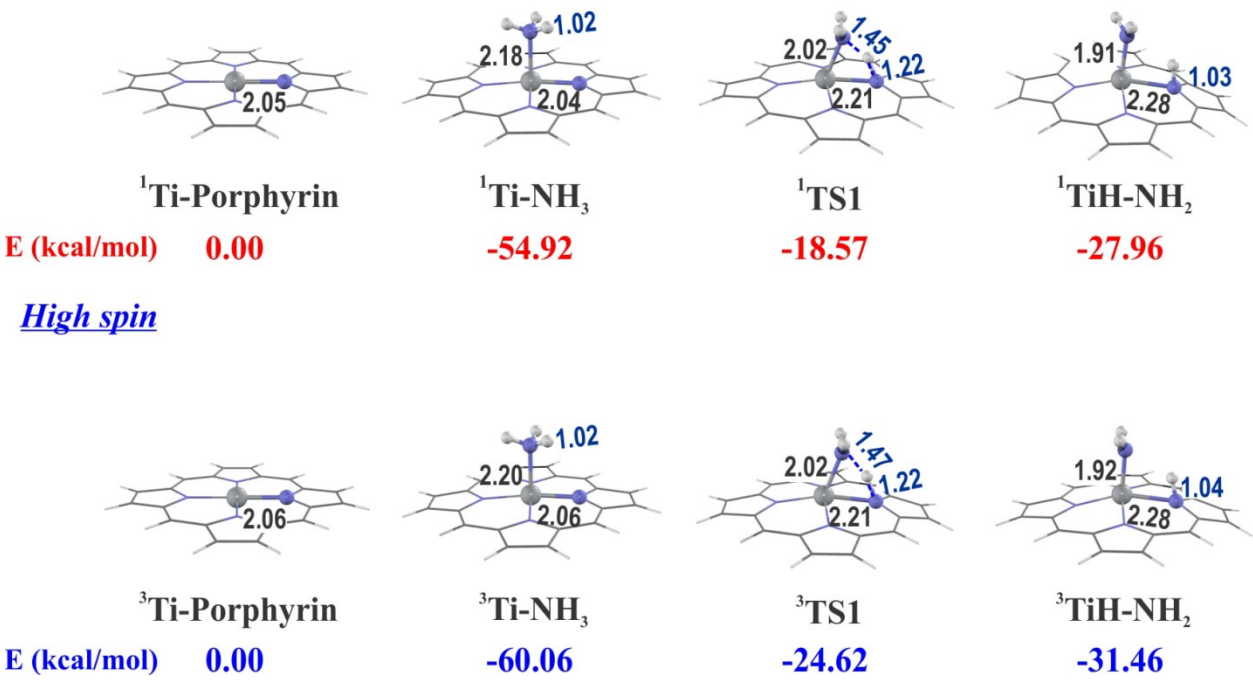
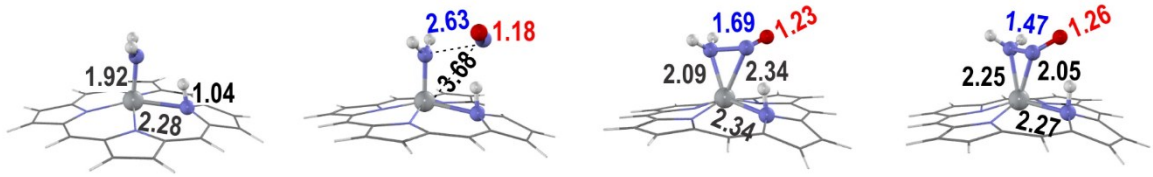


Figure S1. Step 1 of NH_3 oxidation over the low and high spin states of Ti-porphyrin.

Low spin

	^{1}TiH-NH$_2$	NO-^{2}TiH-NH$_2$	^{2}TS2	^{2}TiH-NH$_2$NO
E (kcal/mol)	-27.96	-37.23	-34.33	-40.59

High spin



	^{3}TiH-NH$_2$	NO-^{2}TiH-NH$_2$	^{4}TS2	^{4}TiH-NH$_2$NO
E (kcal/mol)	-31.46	-37.50	-28.30	-30.64

Figure S2. Step 2 of NH_2NO intermediate formation over the low and high spin states of Ti-porphyrin

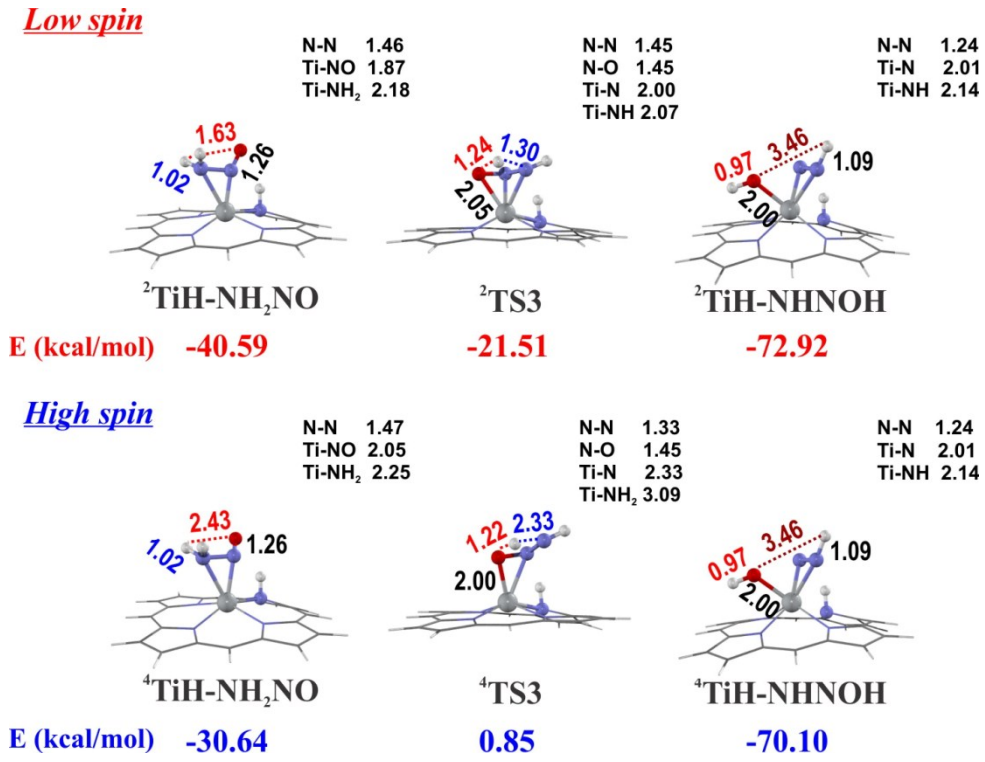


Figure S3. Step 3 of NHNOH intermediate formation over the low and high spin states of Ti-porphyrin

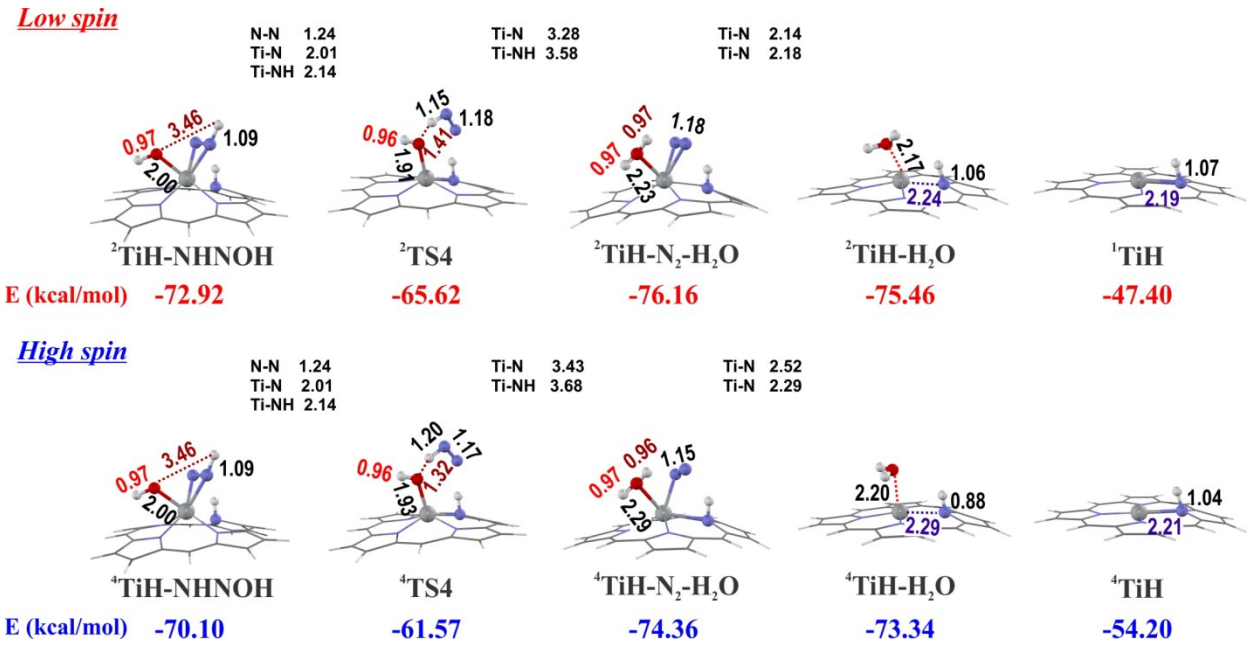


Figure S4. Step 4 of NHNOH decomposition to nitrogen and water molecules over the low and high spin states of Ti-porphyrin.

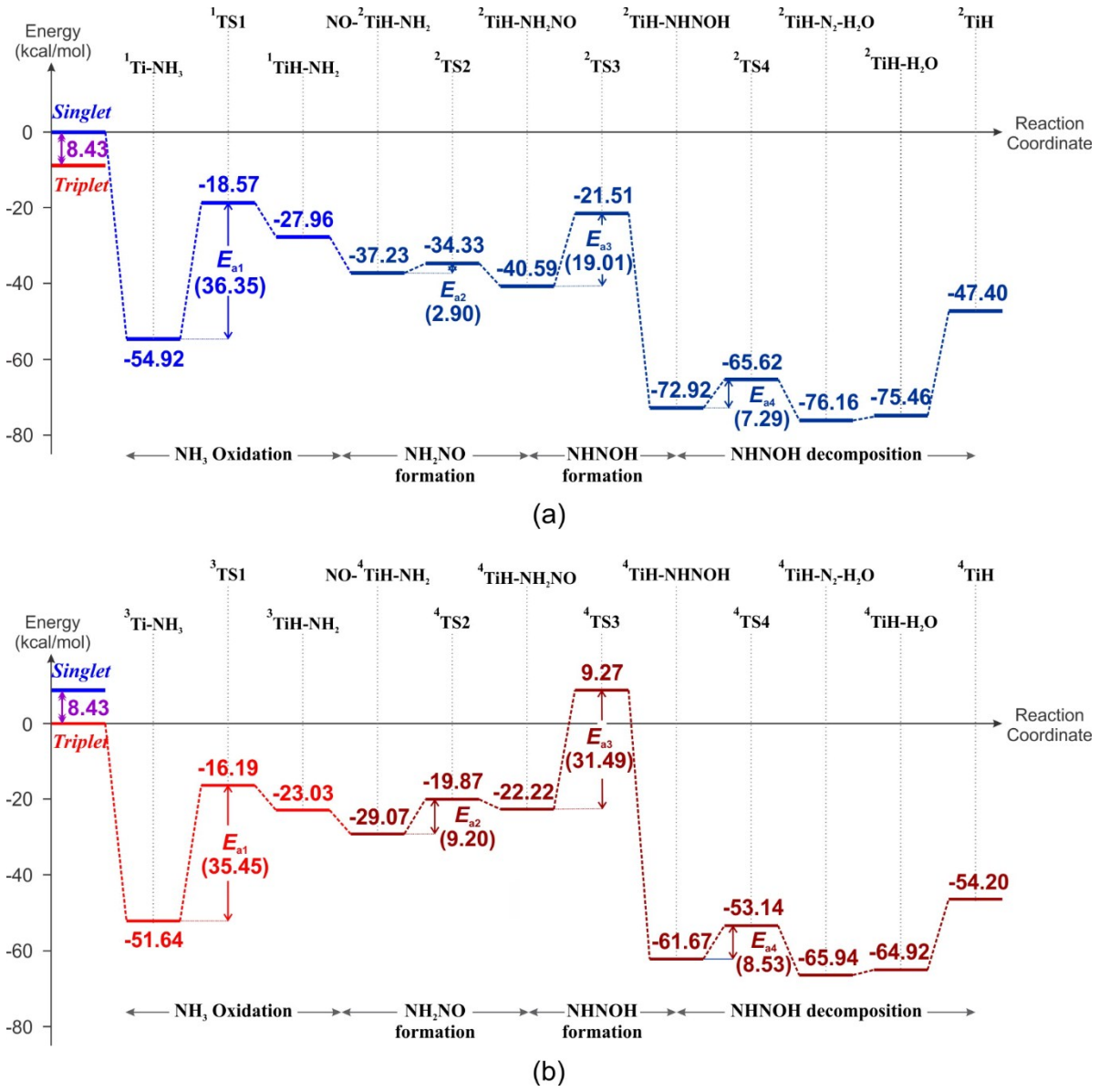


Figure S5. Full reaction pathway of NH_3-SCR of NO over the low spin state (a) and high spin state (b) of Ti-porphyrin catalyst.

Catalyst Regeneration

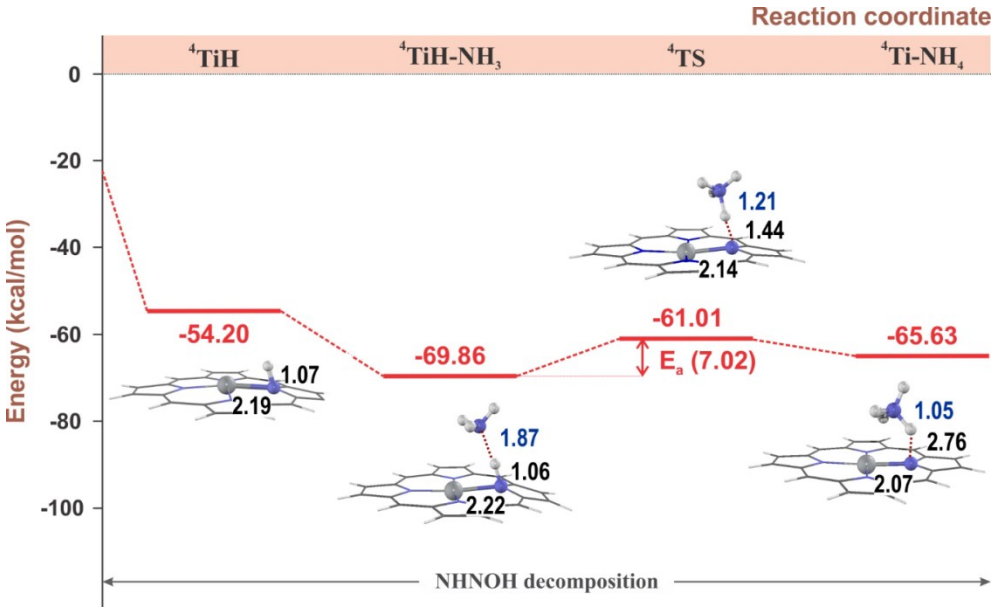


Figure S6. Catalyst regeneration step by NH_3 reducing agent over the Brønsted site of TiH-porphyrin calculated at the high spin state.

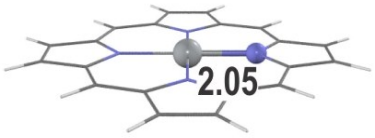
Ti-porphyrin catalyst in NH_3-SCR can generate the Brønsted acid site namely TiH after production of H_2O and N_2 molecules. This TiH species could be then regenerated to Ti-porphyrin. In literature, it is found that during NH_3-SCR process, NH_3 molecule can adsorb on the Brønsted acid site to produce NH_4^+ species. [1-3] Thus, in the present work, we have provided a possibility of catalyst regeneration by NH_3 oxidation process; TiH + NH_3 → Ti-porphyrin + NH_4^+, as shown in Figure S6. The reaction started with the NH_3 adsorption on the Brønsted acid site of TiH with the adsorption energy -15.66 kcal/mol. Then the NH_3 oxidation process occurred by requiring energy of only 7.02 kcal/mol to form the NH_4^+ species. Finally, the catalyst is regenerated to Ti-porphyrin which it could continually become Lewis site for new reaction.

References

1. G. Busca, L. Lietti, G. Ramis and F. Berti, *Appl. Catal., B*, 1998, 18, 1-36.
2. M. Calatayud, B. Mguig and C. Minot, *Surf. Sci. Rep.,* 2004, 55, 169-236.
3. R. Yuan, G. Fu, X. Xu and H. Wan, *Phys. Chem. Chem. Phys.,* 2011, 13, 453–460.

Table S2. Cartesian coordinates of Ti-porphyrin and the transition states of NH_3-SCR of NO reaction in low and high spin states of Ti-porphyrin.

^{1}Ti-Por (Ti-porphyrin at singlet state)



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C	4.263148	-0.676562	0.000185
C	4.263147	0.676577	0.000185
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N	2.045302	0.000005	0.000103
C	2.885221	-1.112742	0.000128
C	-0.692808	-4.209656	-0.000063
C	0.692821	-4.209647	-0.000045
C	1.116886	-2.867421	-0.000049
N	-0.000008	-2.033191	-0.000187
C	-1.116887	-2.867436	-0.000097
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C	-4.263141	-0.676577	0.000000
C	-2.885212	-1.112751	0.000006
N	-2.045294	-0.000005	0.000019
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C	-2.451318	-2.418012	-0.000054
C	-2.451328	2.418003	-0.000053
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H	-5.116283	-1.346804	-0.000013
H	-5.116286	1.346787	-0.000014
H	-1.355462	5.068643	-0.000041
H	1.355452	5.068631	0.000013
H	5.116291	1.346801	0.000211
H	5.116294	-1.346784	0.000210
H	1.355469	-5.068628	-0.000002
H	-1.355444	-5.068646	-0.000038
H	-3.216282	-3.192436	-0.000057
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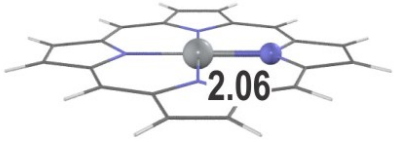
H	3.216262	3.192443	0.000087
Ti	0.000012	0.000000	0.000023

^{3}Ti-Por (Ti-porphyrin at triplet state)



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N	-2.056111	0.001212	-0.000241
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C	1.114456	2.881585	-0.000787
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N	2.056076	-0.001212	-0.000315
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H	1.345715	-5.105910	0.000186
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H	-1.345747	5.105853	0.000244
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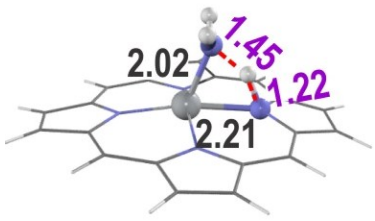
H	3.205156	3.201343	-0.000271
H	3.201360	-3.205139	-0.000272
H	-3.201273	3.205185	-0.000127
H	-3.205068	-3.201389	-0.000119
Ti	-0.000036	0.000000	-0.000226

^{1}TS1 (first transition state at singlet state)



C	4.216125	0.841725	-0.364067
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C	2.861130	1.242495	-0.121443
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C	0.525780	4.216844	-0.059379
C	0.989692	2.889560	-0.082836
N	-0.095506	2.014320	-0.155821
C	-1.234578	2.815308	-0.180321
C	-4.269465	-0.817382	-0.166658
C	-4.319684	0.532974	-0.271253
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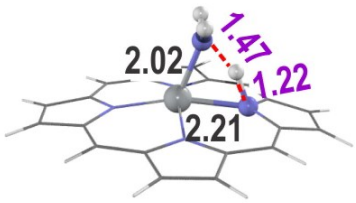
H	3.292679	-3.077281	-0.379488
H	-3.339187	3.099289	-0.321608
H	3.067867	3.328431	-0.138993

N	0.532982	-0.150286	2.113804
H	0.512753	0.669904	2.711261
H	0.336812	-0.972444	2.673737
H	1.629924	-0.037171	1.177478

^{3}TS1 (first transition state at triplet state)



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C	-2.896497	-1.133996	-0.173381
C	0.713127	-4.209001	-0.148480
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C	-0.664374	4.215693	-0.163865
C	0.712963	4.209026	-0.148440
C	1.129698	2.852089	-0.129362
N	0.014224	2.025981	-0.118490
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C	2.471064	-2.418034	-0.153427
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H	-3.180203	3.212060	-0.267822
H	3.220492	-3.201906	-0.224455
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N	-0.560256	-0.000118	2.171296
H	-0.551166	-0.825801	2.760342
H	-0.551411	0.825497	2.760444
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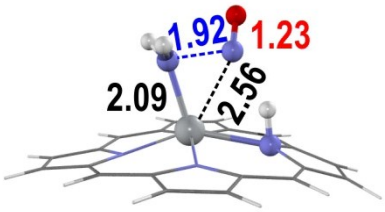
^{2}TS2 (second transition state at doublet state)



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C	-3.091546	0.181088	-0.500563
C	-0.979618	-4.057211	-0.449164
C	-2.244328	-3.516345	-0.437153
C	-2.096604	-2.107371	-0.379674

N	-0.754502	-1.773372	-0.341284
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C	4.234229	-0.974012	-0.618974
C	3.694518	-2.223069	-0.710508
C	2.270534	-2.085425	-0.564316
N	1.958497	-0.750024	-0.405439
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C	1.073600	4.194645	-0.093166
C	2.333726	3.640055	-0.059769
C	2.172513	2.230240	-0.116695
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H	0.806268	5.243704	-0.099374
H	-4.002013	3.295988	-1.224127
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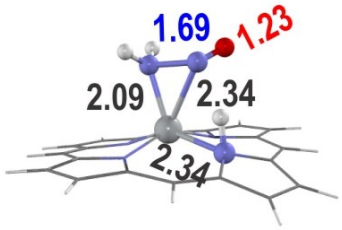
H	-3.192642	-4.037065	-0.481113
H	-0.700412	-5.101633	-0.503954
H	4.211338	-3.163244	-0.857664
H	5.278866	-0.694689	-0.677150
Ti	0.183996	-0.032687	0.289276
H	4.232504	1.751372	-0.258098
H	-1.589550	4.304378	-0.475131
H	1.710119	-4.119685	-0.636065
H	-4.142148	-1.619218	-0.660143
N	0.796671	-0.275315	2.273849
H	1.034478	-1.168670	2.700142
H	1.224178	0.489055	2.787924
H	-1.824624	0.858538	0.895899
N	-0.874744	-0.073570	2.377389
O	-1.435516	-1.117641	2.691408

^{4}TS2 (second transition state at quartet state)



C	-4.069863	1.118737	-0.923080
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C	-2.186447	2.298633	-0.443720
N	-1.910292	0.919740	-0.130666
C	-3.091546	0.181088	-0.500563
C	-0.979618	-4.057211	-0.449164
C	-2.244328	-3.516345	-0.437153
C	-2.096604	-2.107371	-0.379674
N	-0.754502	-1.773372	-0.341284
C	-0.061504	-2.973076	-0.416632
C	4.234229	-0.974012	-0.618974
C	3.694518	-2.223069	-0.710508
C	2.270534	-2.085425	-0.564316
N	1.958497	-0.750024	-0.405439
C	3.148843	-0.053686	-0.416989
C	1.073600	4.194645	-0.093166
C	2.333726	3.640055	-0.059769
C	2.172513	2.230240	-0.116695
N	0.819637	1.911692	-0.129325
C	0.147862	3.125424	-0.149622
C	1.335490	-3.104825	-0.532700
C	3.236487	1.316288	-0.243727
C	-1.242610	3.284176	-0.332024
C	-3.159722	-1.187828	-0.486178
H	3.287684	4.151363	-0.030374

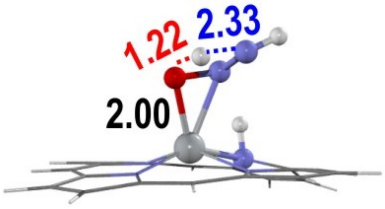
H	0.806268	5.243704	-0.099374
H	-4.002013	3.295988	-1.224127
H	-5.051864	0.841089	-1.284886
H	-3.192642	-4.037065	-0.481113
H	-0.700412	-5.101633	-0.503954
H	4.211338	-3.163244	-0.857664
H	5.278866	-0.694689	-0.677150
Ti	0.183996	-0.032687	0.289276
H	4.232504	1.751372	-0.258098
H	-1.589550	4.304378	-0.475131
H	1.710119	-4.119685	-0.636065
H	-4.142148	-1.619218	-0.660143
N	0.796671	-0.275315	2.273849
H	1.034478	-1.168670	2.700142
H	1.224178	0.489055	2.787924
H	-1.824624	0.858538	0.895899
N	-0.874744	-0.073570	2.377389
O	-1.435516	-1.117641	2.691408

^{2}TS3 (third transition state at doublet state)

C	-3.935334	-1.710253	-0.743752
C	-4.293197	-0.391357	-0.652227
C	-3.162260	0.372415	-0.254933
N	-2.081092	-0.547896	0.019471
C	-2.564622	-1.847384	-0.399434
C	1.719998	-3.847224	-0.427872
C	0.394157	-4.200764	-0.463205
C	-0.354682	-2.999325	-0.372648
N	0.488220	-1.908061	-0.292259
C	1.767606	-2.428465	-0.332346
C	3.911701	1.761088	-0.647183
C	4.271200	0.451261	-0.576988
C	3.068149	-0.309116	-0.372346
N	1.988793	0.546164	-0.298561
C	2.483474	1.823212	-0.476890
C	-1.764772	3.889525	-0.324497
C	-0.439371	4.239537	-0.413930
C	0.311275	3.032832	-0.373776
N	-0.536981	1.947076	-0.254817
C	-1.814332	2.475437	-0.225864
C	2.957697	-1.684028	-0.347261
C	1.710878	2.966654	-0.482345
C	-3.011868	1.732093	-0.240477
C	-1.759559	-2.948481	-0.466285
H	-0.012457	5.227753	-0.525651
H	-2.631728	4.537442	-0.349340
H	-5.245568	0.043518	-0.928299
H	-4.550273	-2.527727	-1.097986
H	-0.034763	-5.190706	-0.551705
H	2.588815	-4.490915	-0.474271
H	5.259662	0.022840	-0.682914
H	4.546203	2.621831	-0.816730
Ti	0.137862	0.064116	0.443437
H	2.229020	3.913620	-0.604680
H	-3.922850	2.312715	-0.366235
H	3.879374	-2.255838	-0.410779
H	-2.254400	-3.891934	-0.683706
N	-0.490509	0.662718	2.325680
H	0.780624	0.533950	2.589701
H	-1.385697	0.940611	2.729532
H	-1.999114	-0.629849	1.038560
N	-0.285611	-0.763637	2.209367

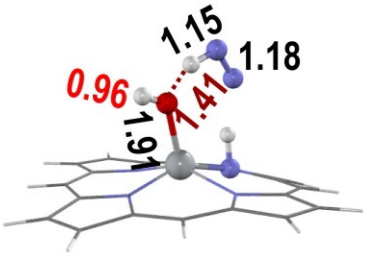
O	1.145450	-0.549794	2.122785

^{4}TS3 (third transition state at quartet state)



C	3.688164	2.199300	-0.800636
C	4.157004	0.909040	-0.841487
C	3.114483	0.023500	-0.460837
N	1.972647	0.824425	-0.095524
C	2.335746	2.191536	-0.383005
C	-2.100747	3.799483	-0.034481
C	-0.813648	4.276002	-0.073434
C	0.048671	3.151704	-0.136606
N	-0.697212	1.979407	-0.126788
C	-2.025415	2.378968	-0.098209
C	-3.820199	-1.967101	-0.702329
C	-4.284656	-0.688994	-0.590125
C	-3.145661	0.162771	-0.381459
N	-2.001699	-0.602788	-0.376056
C	-2.392382	-1.917474	-0.565808
C	2.034235	-3.615504	-0.513869
C	0.737459	-4.076955	-0.555778
C	-0.111599	-2.941420	-0.505568
N	0.654220	-1.786871	-0.407821
C	1.971235	-2.202163	-0.430274
C	-3.147185	1.538294	-0.211703
C	-1.514998	-2.985168	-0.594232
C	3.095701	-1.347373	-0.479572
C	1.443171	3.229662	-0.289434
H	0.395920	-5.101719	-0.629159
H	2.948803	-4.193452	-0.558342
H	5.126787	0.581207	-1.193206
H	4.218995	3.091469	-1.108129
H	-0.483340	5.307138	-0.071039
H	-3.022239	4.366322	0.001267
H	-5.310877	-0.347291	-0.639258
H	-4.393720	-2.871498	-0.863306
Ti	-0.174716	-0.001390	0.268654
H	-1.950644	-3.972780	-0.721541
H	4.052474	-1.835175	-0.648922
H	-4.113653	2.034817	-0.213046
H	1.853563	4.229018	-0.410986
N	0.907962	-1.485814	2.756809
H	-0.414854	-1.438975	2.602185
H	1.813494	-1.692418	3.173056
H	1.869634	0.747361	0.927487
N	0.747622	-0.214337	2.382968
O	-0.680955	-0.322530	2.175063

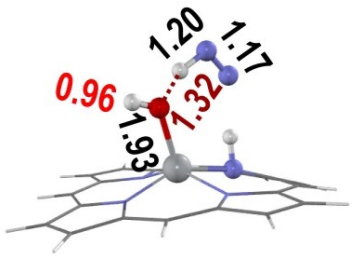
^{2}TS4 (fourth transition state at doublet state)



C	4.073104	0.687331	-1.064028
C	4.074118	-0.680144	-1.064445
C	2.792475	-1.135153	-0.647194
N	1.990925	0.001829	-0.320678
C	2.790779	1.140180	-0.646530
C	-0.788481	4.206557	-0.276355
C	0.577674	4.216011	-0.373998
C	1.004630	2.856890	-0.386565

N	-0.089023	2.017854	-0.284656
C	-1.199765	2.839999	-0.240989
C	-4.364883	-0.684786	-0.437788
C	-4.365896	0.678643	-0.437648
C	-2.999778	1.106602	-0.300733
N	-2.181931	-0.001460	-0.211210
C	-2.998092	-1.110720	-0.301002
C	0.584166	-4.214506	-0.375543
C	-0.781988	-4.207218	-0.277660
C	-1.195403	-2.841344	-0.241852
N	-0.085957	-2.017413	-0.285465
C	1.009005	-2.854709	-0.387762
C	-2.536050	2.412611	-0.261217
C	-2.532375	-2.416015	-0.261782
C	2.331179	-2.430227	-0.574209
C	2.327494	2.434506	-0.573002
H	-1.453529	-5.056215	-0.257292
H	1.244303	-5.069501	-0.448722
H	4.874349	-1.336286	-1.381295
H	4.872332	1.344869	-1.380527
H	1.236473	5.072070	-0.446735
H	-1.461365	5.054494	-0.255800
H	-5.215346	1.344254	-0.526468
H	-5.213316	-1.351671	-0.526792
Ti	-0.190489	0.000014	0.243830
H	-3.280589	-3.203405	-0.303895
H	3.067666	-3.212105	-0.740373
H	-3.285483	3.198848	-0.303205
H	3.062793	3.217585	-0.738789
N	1.480215	-0.002723	3.414023
H	0.376129	-0.002516	3.091483
H	1.906885	0.001290	0.768710
N	2.202220	-0.000819	2.486608
O	-0.628901	-0.000556	2.106756
H	-1.535956	-0.005478	2.422853

^{4}TS4 (fourth transition state at quartet state)



C	-4.073748	-0.683270	-1.064099
C	-4.073600	0.684213	-1.064083
C	-2.791541	1.137964	-0.646784
N	-1.990903	0.000239	-0.320819
C	-2.791788	-1.137311	-0.646810
C	0.784655	-4.206947	-0.276888
C	-0.581488	-4.215197	-0.374578
C	-1.007272	-2.855680	-0.386991
N	0.087116	-2.017618	-0.284924
C	1.197149	-2.840754	-0.241359
C	4.365345	0.681282	-0.438115
C	4.365185	-0.682161	-0.438157
C	2.998705	-1.108943	-0.301142
N	2.181853	-0.000187	-0.211404
C	2.998968	1.108375	-0.301076
C	-0.580572	4.215359	-0.374511
C	0.785566	4.206825	-0.276779
C	1.197774	2.840543	-0.241240
N	0.087569	2.017637	-0.284832
C	-1.006638	2.855933	-0.386936
C	2.533807	-2.414548	-0.261628
C	2.534345	2.414079	-0.261508
C	-2.329174	2.432655	-0.573367

C	-2.329713	-2.432110	-0.573414	H	3.283228	3.200836	-0.303575
H	1.457883	5.055211	-0.256329	H	-3.065023	3.215203	-0.739197
H	-1.239943	5.070962	-0.447455	H	3.282530	-3.201455	-0.303739
H	-4.873282	1.341160	-1.380655	H	-3.065740	-3.214489	-0.739247
H	-4.873579	-1.340033	-1.380675	N	-1.479624	-0.000098	3.413780
H	-1.241041	-5.070662	-0.447501	H	-0.375539	-0.000178	3.091647
H	1.456794	-5.055474	-0.256462	H	-1.906464	0.000215	0.768639
H	5.214040	-1.348506	-0.527173	N	-2.201308	0.000104	2.486085
H	5.214360	1.347430	-0.527081	O	0.629518	-0.000213	2.106584
Ti	0.190465	-0.000030	0.243878	H	1.536689	-0.000242	2.422388