Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information to

Reaction Mechanism of Hydrogen Evolution Catalysed by Co and Fe Complexes Containing a Tetra-dentate Phosphine Ligand – A DFT Study

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1. Several possible structures of Co-1.

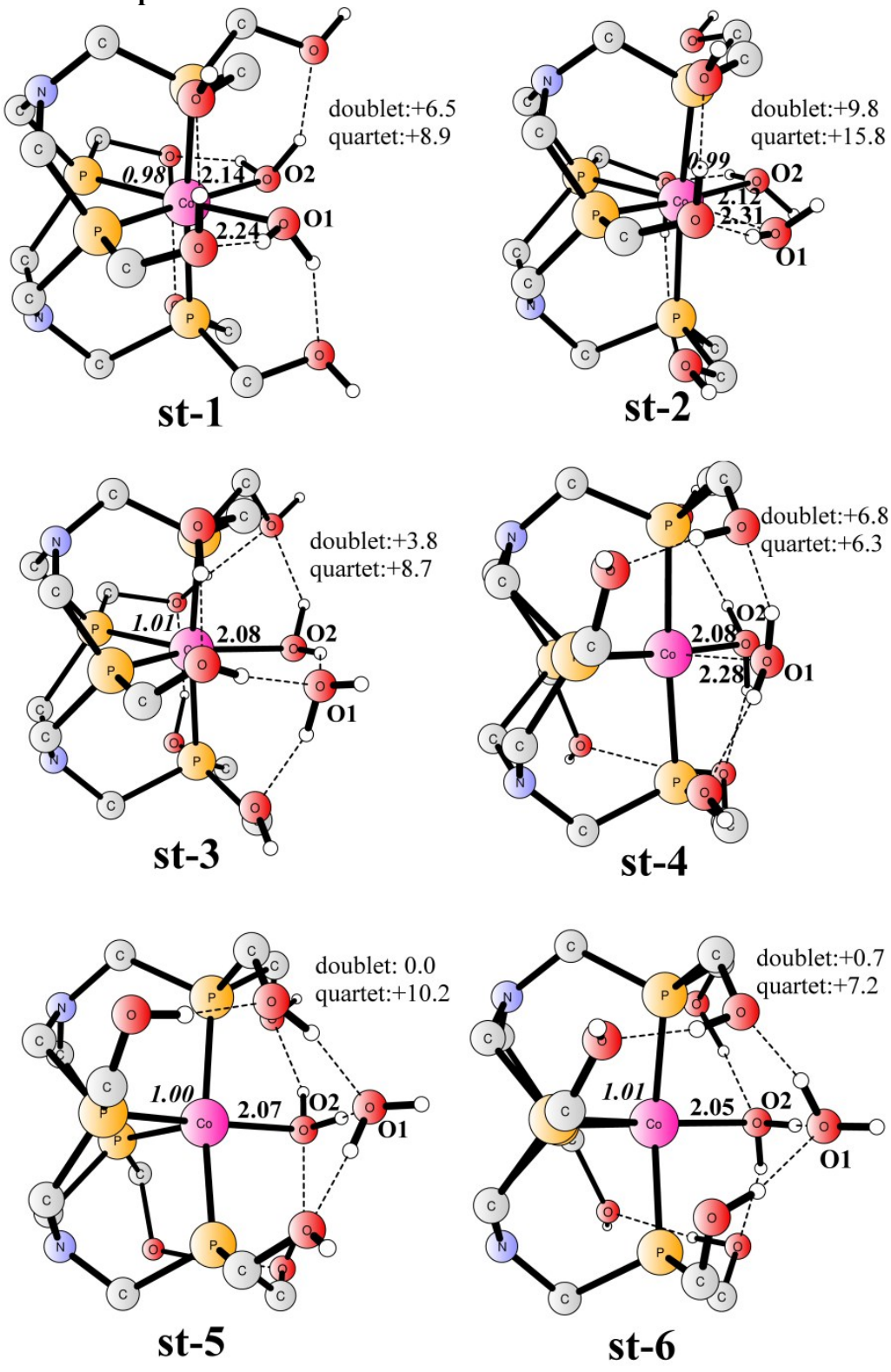


Fig.S1 *Several possible structures of* ***Co-1****. Distances are given in Ångstroms. The spin density on Co is shown in italic. The hydrogen atoms on the* CH_2 *are omitted for clarity.*

2. Optimized structure of Co-2pt.

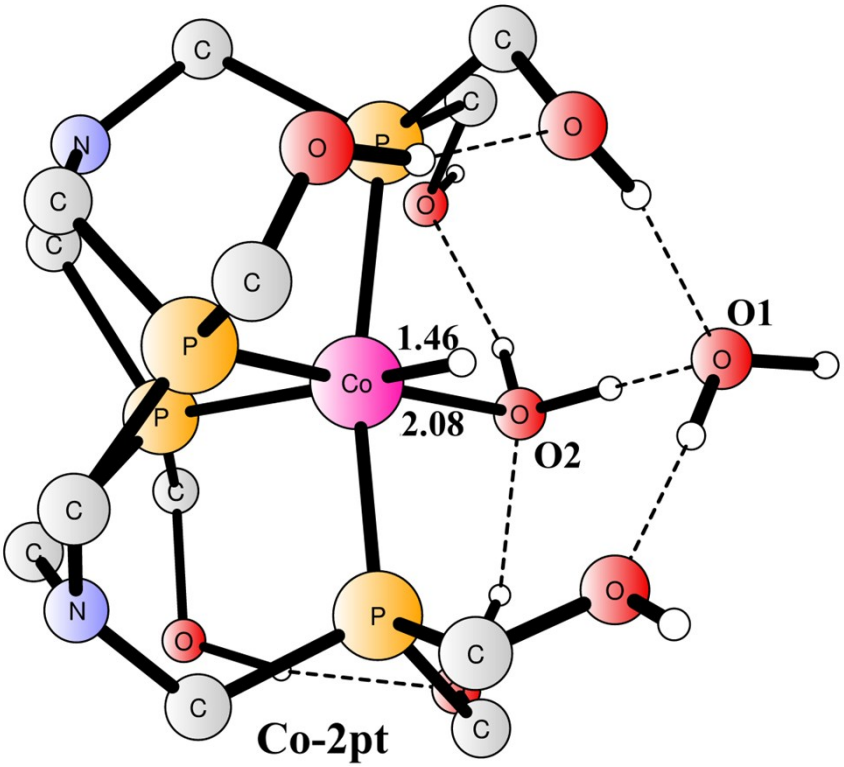


Fig. S2 *Optimized structure of* ***Co-2$_{pt}$***.

3. Optimized structure of Co-3dp.

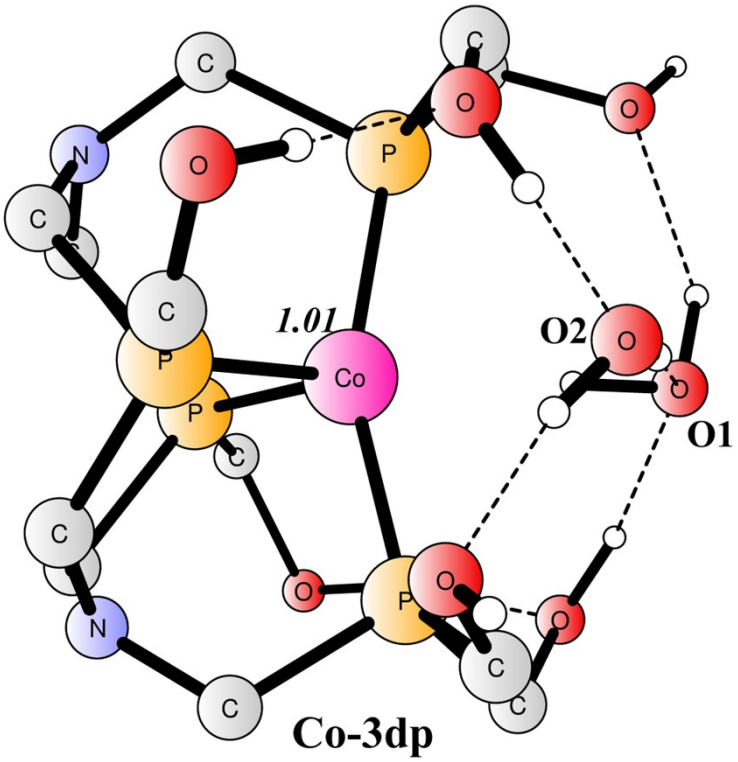


Fig. S3 *Optimized structure of* ***Co-3$_{dp}$***

4. Optimized structure of Co-1dp.

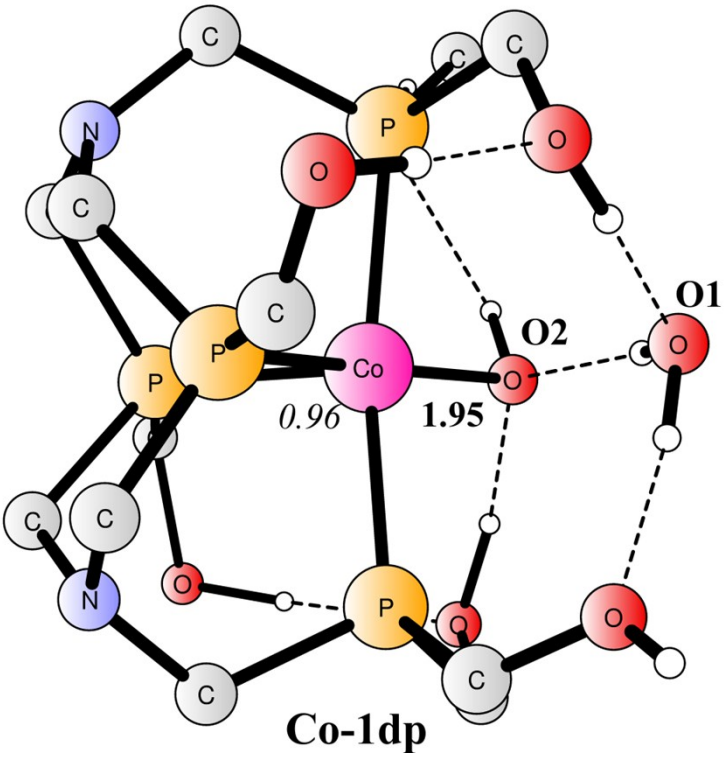
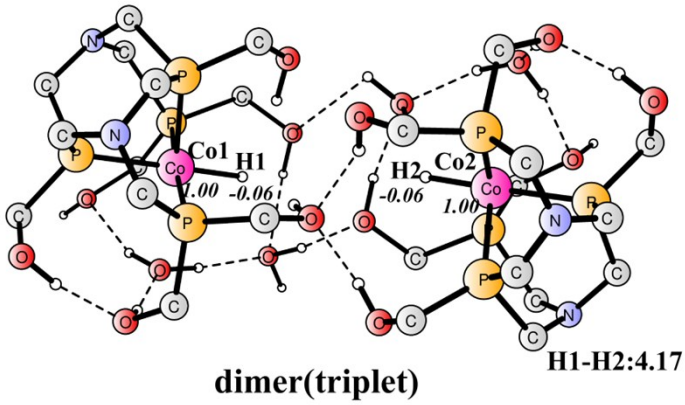
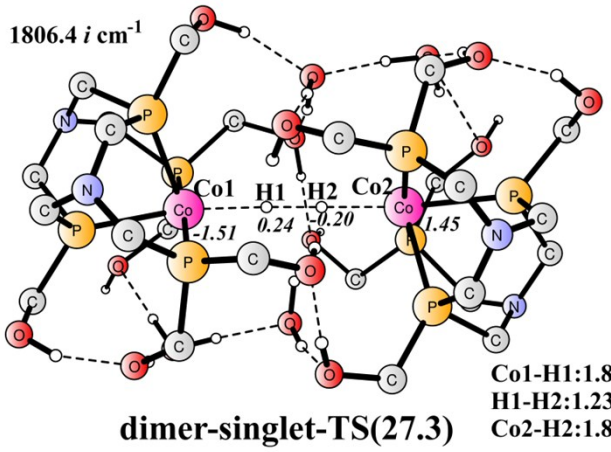


Fig. S4 *Optimized structure of* ***Co-1$_{dp}$***.

5. Optimized structure of dimer, dimer-singlet-TS and dimer-triplet-TS.





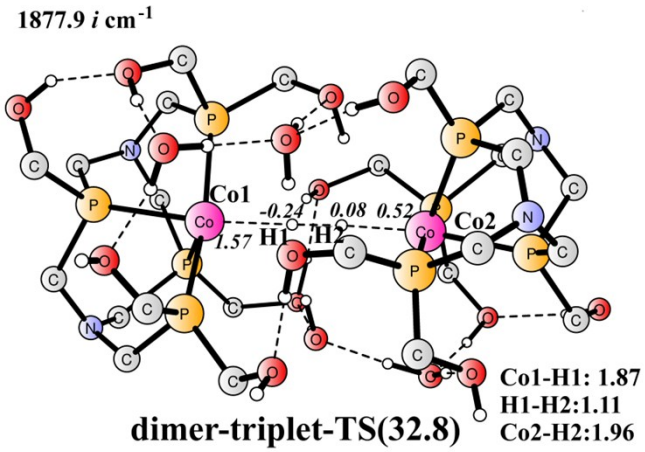


Fig S5. Optimized structure of ***dimer***, ***dimer-singlet-TS*** *and* ***dimer-triplet-TS.*** Distances are given in angstrom, spin densities are shown in italic, and energies are given relative to the triplet reactant complex.

6. Optimized structure of Co-1'dp.

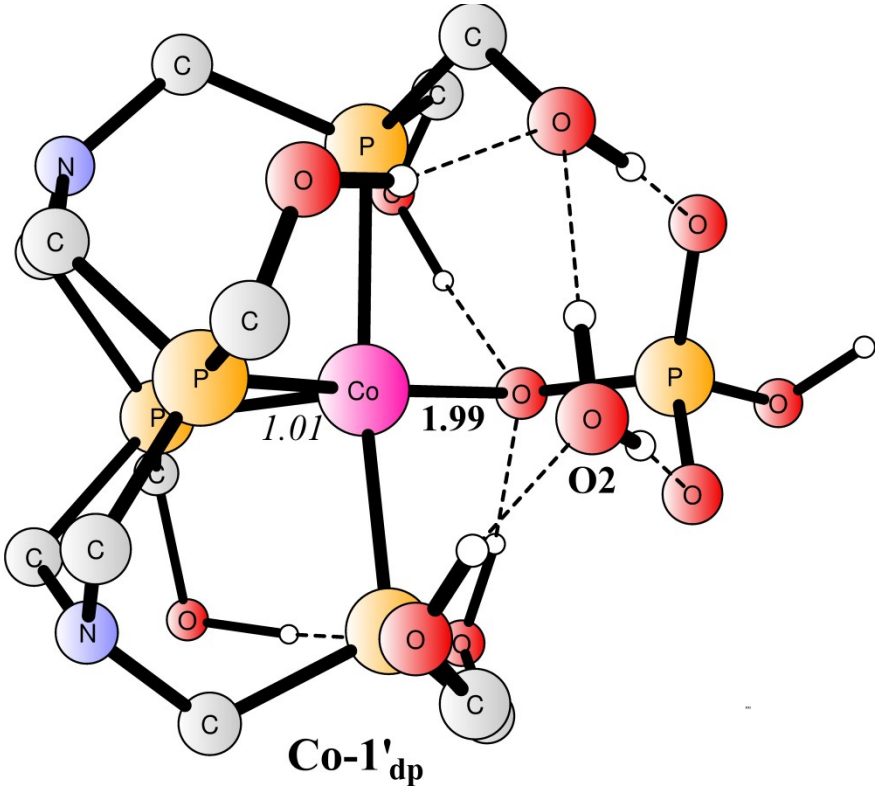


Fig. S6 Optimized structure of ***Co-1'$_{dp}$***.

7. Optimized structure of Co^{III}-hydride(Co^{III}-H-HPO_4-H_2O).

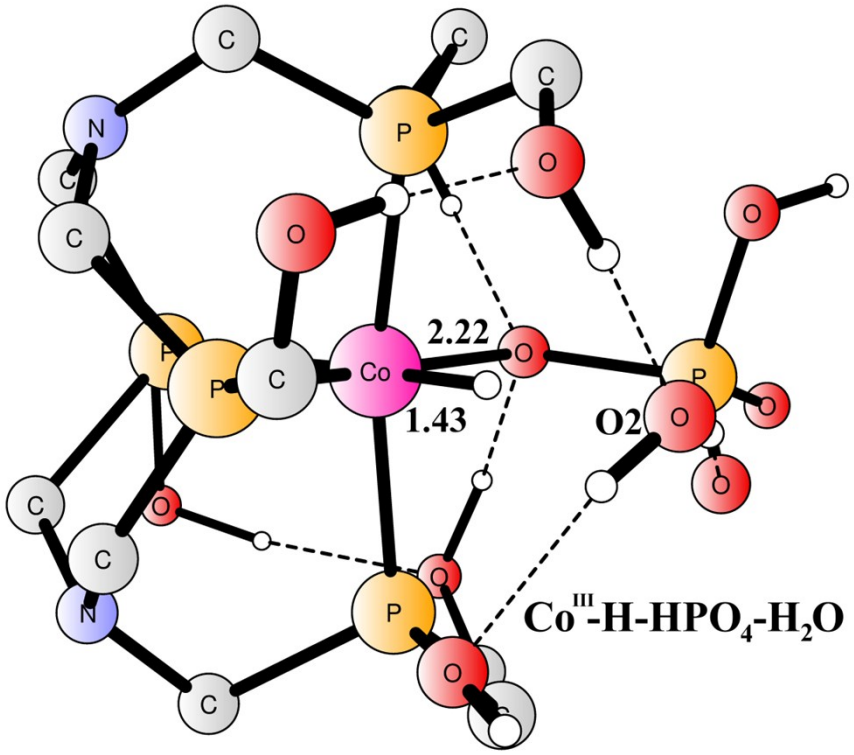


Fig. S7 Optimized structure of ***Co^{III}-H-HPO_4-H_2O.***

8. Optimized structure of Co-3'dp.

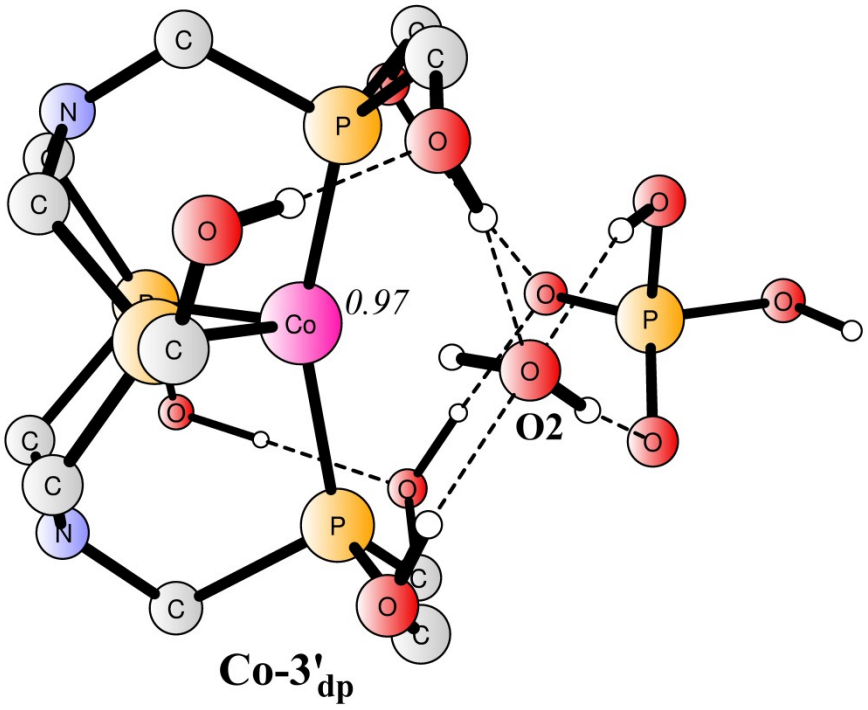


Fig. S8 Optimized structure of ***Co-3'$_{dp}$***.

9. Optimized structure of Co-2'$_{pt}$.

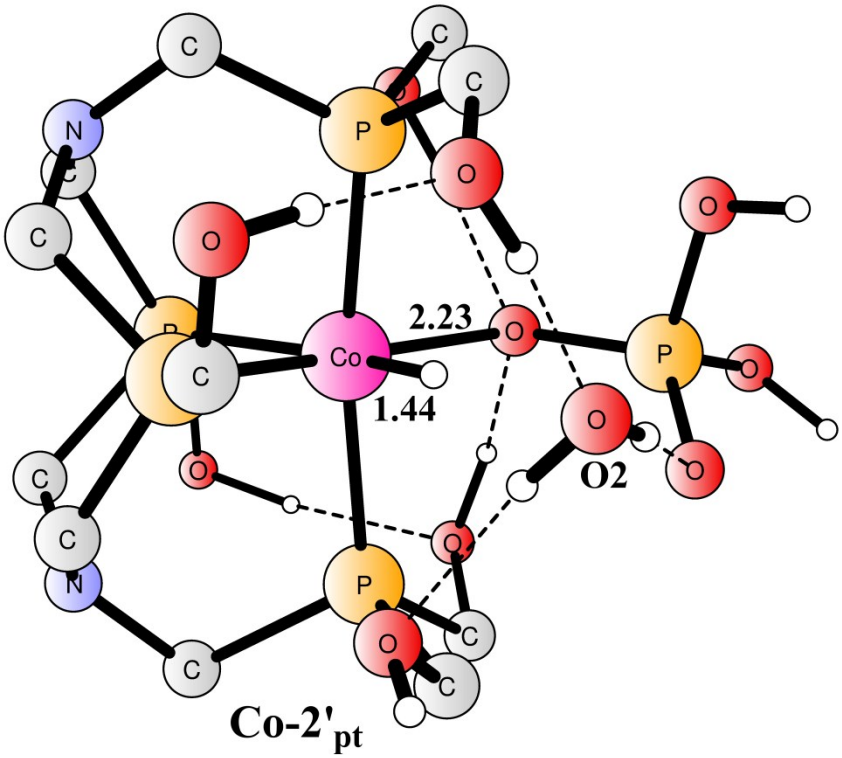


Fig. S9 Optimized structure of ***Co-2'$_{pt}$.***

10. Optimized structure of Co-TS'-w(waterbridge).

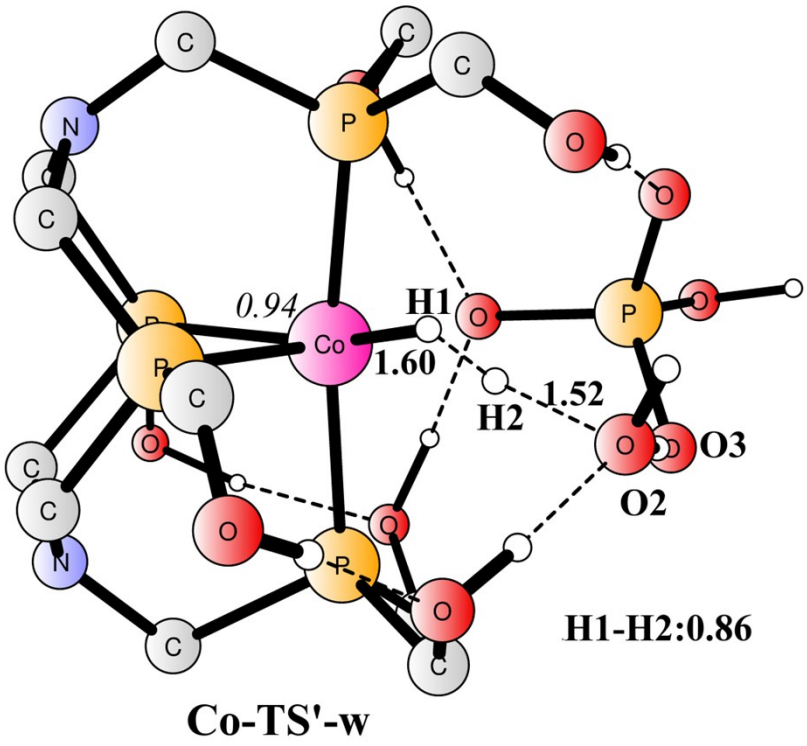


Fig. S10 Optimized structure of ***Co-TS'-w.***

11. Optimized structure of Fe-1.

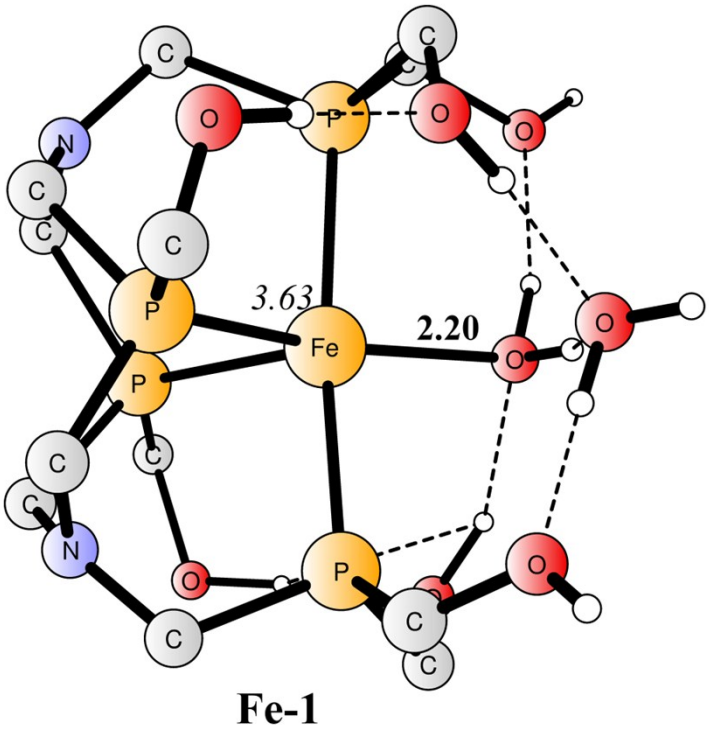


Fig. S11 Optimized structure of ***Fe-1.***

12. Optimized structure of Fe-1'.

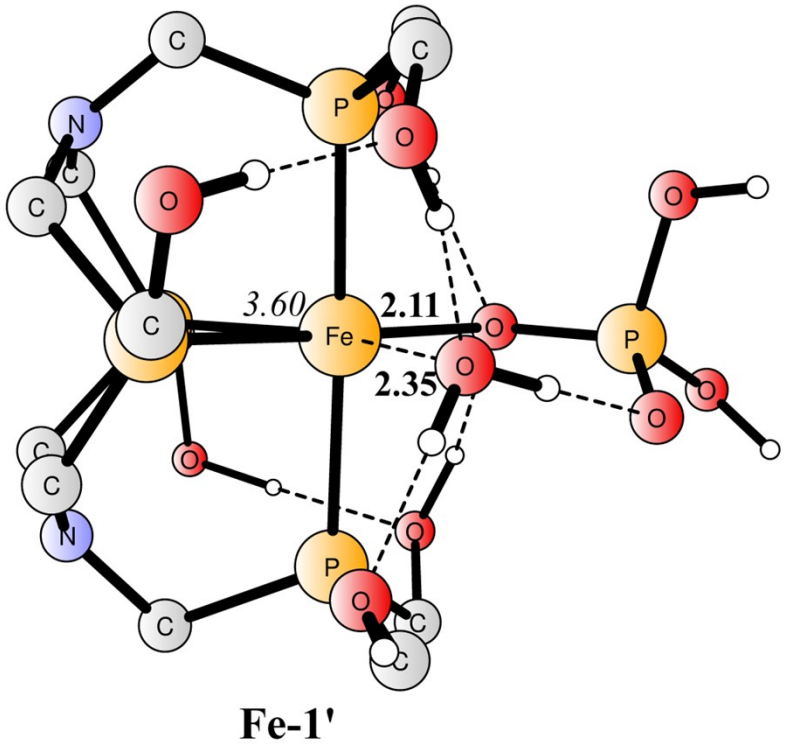
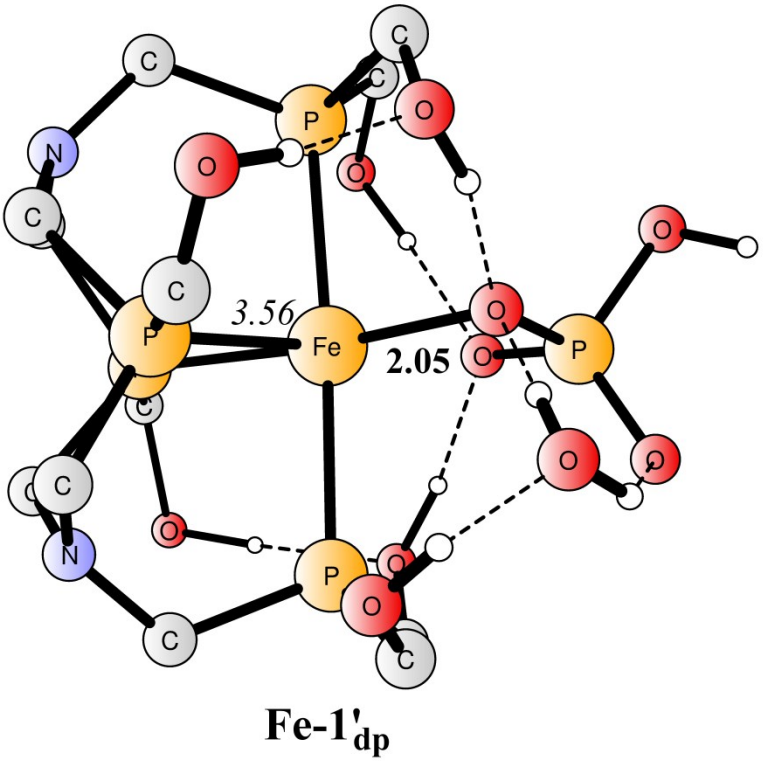


*Fig. S12 Optimized structure of **Fe-1'**.*

13. Optimized structure of Fe-1'$_{dp}$.



Fe-1'$_{dp}$

Fig. S13 Optimized structure of ***Fe-1'$_{dp}$***.

14. Optimized structure of Fe-2'.

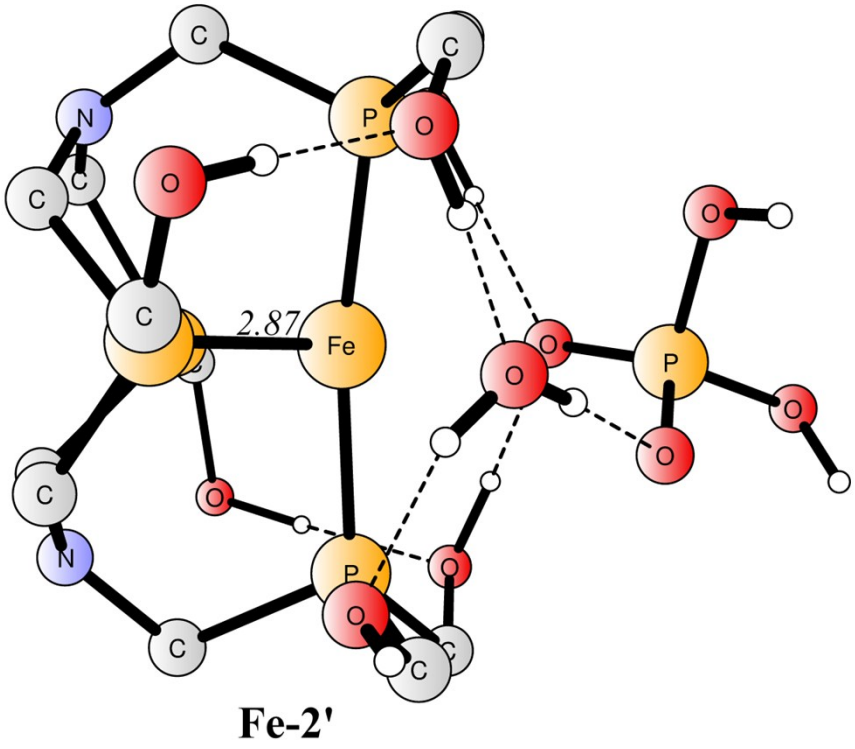


*Fig. S14 Optimized structure of **Fe-2'**.*

15. Optimized structure of Fe-3' $_{dp}$.

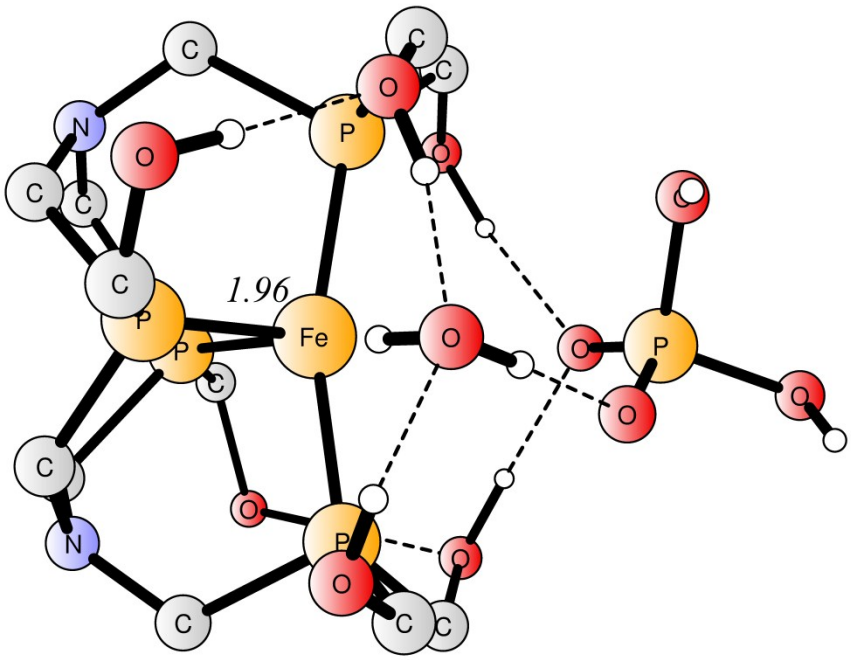


Fig. S15 Optimized structure of ***Fe-3$_{dp}$'.***

16. Optimized structure of Fe-2'$_{pt}$.

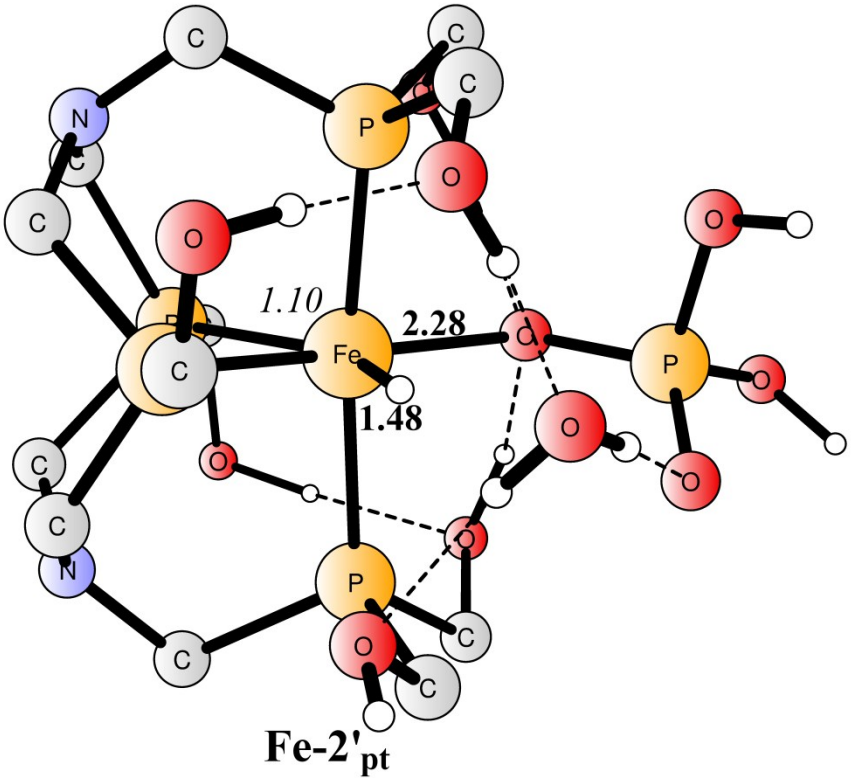


Fig. S16 Optimized structure of ***Fe-2$_{pt}$'.***

17. Optimized structure of Fe-3'.

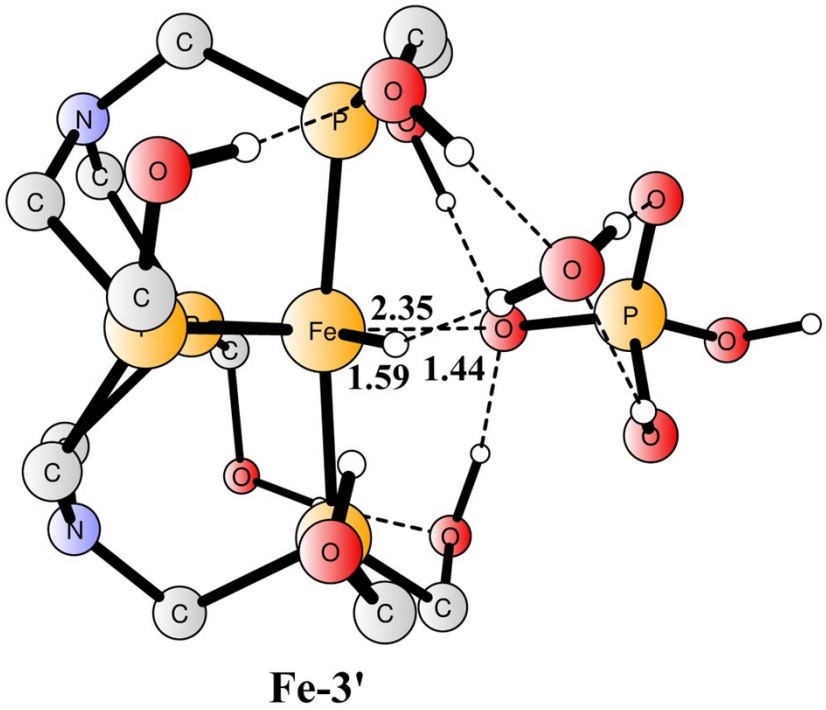


*Fig. S17 Optimized structure of **Fe-3'**.*

18. Distortion/interaction analysis for Co-1', Fe-1' and Co-1'$_{dp}$, Fe-1'$_{dp}$.

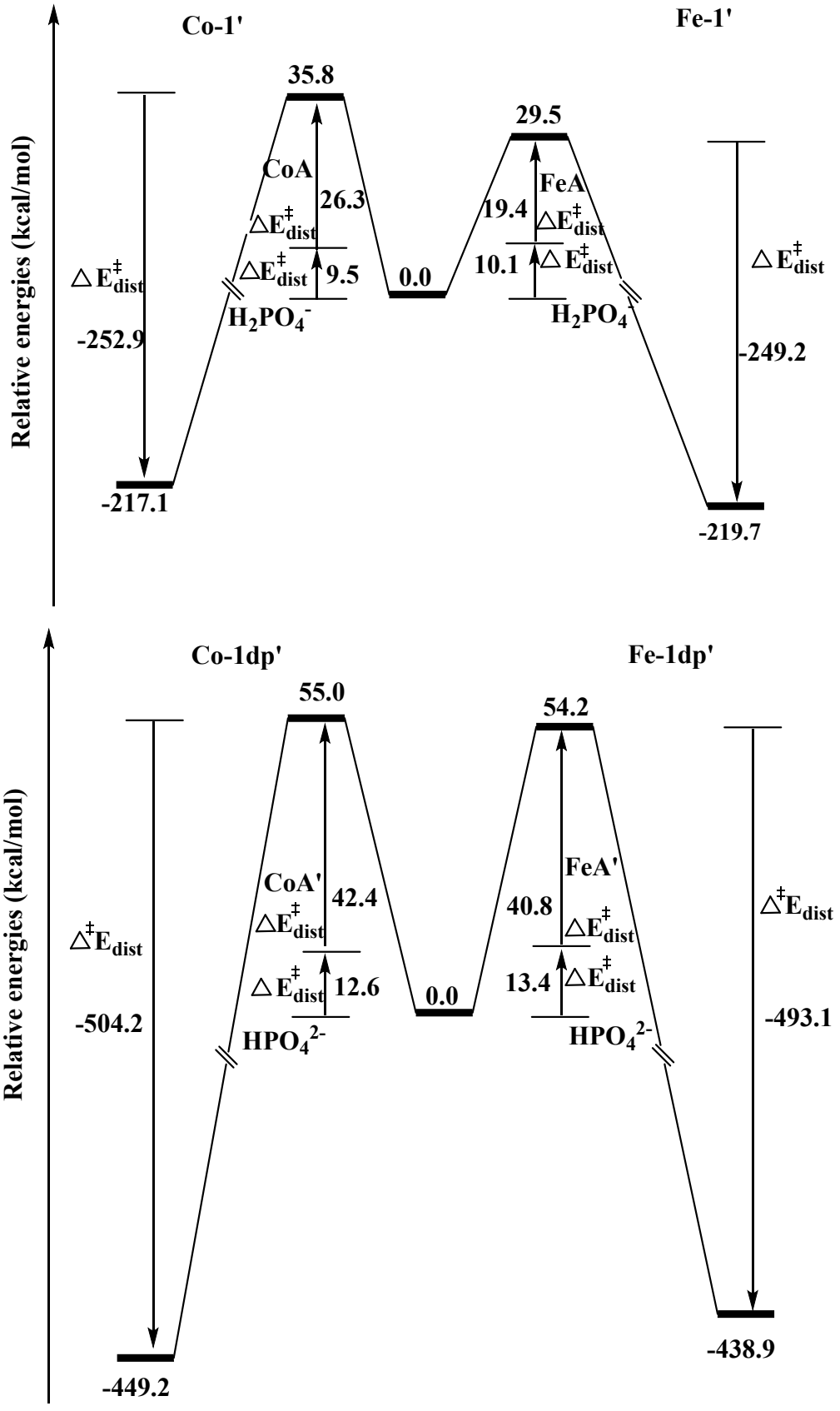


Fig. S18. Distortion/Interaction analysis for Co-1', Fe-1' and Co-1'dp, Fe-1'dp.

19. Comparison of calculated and experimental standard hydrogen electrode potential (In V at pH=7)

Method	Experiment	Calculation	Error
B3LYP-D3	-0.414	-0.344	0.070
B3LYP*-D3	-0.414	-0.440	-0.026
M06-D3	-0.414	-0.501	-0.088
M06L-D3	-0.414	-0.489	-0.075

20. Cartesian coordinates for optimized structures.

Co-1：E(opt)= -2700.0657243 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.062151	0.245027	-0.311086
2	15	0	-2.171913	-0.467069	-0.900417
3	15	0	0.889829	-1.906866	0.006488
4	15	0	-0.583907	0.032099	1.877431
5	15	0	1.879376	1.323041	0.198512
6	6	0	-0.494178	-3.106856	0.489279
7	1	0	-0.760972	-3.701269	-0.389628
8	1	0	-0.107077	-3.804703	1.241269
9	6	0	-2.680262	-2.020987	0.054070
10	1	0	-3.620703	-1.807957	0.573533
11	1	0	-2.875789	-2.816620	-0.671192
12	6	0	-1.530676	-1.607778	2.158568
13	1	0	-1.001529	-2.152115	2.947883
14	1	0	-2.513724	-1.319809	2.543375
15	7	0	-1.698535	-2.468899	1.012141
16	6	0	2.016726	-1.884262	1.544773
17	1	0	1.654627	-2.631860	2.258704
18	1	0	3.003460	-2.198234	1.195982
19	6	0	0.972398	-0.163600	2.947274
20	1	0	1.179702	0.796401	3.432386
21	1	0	0.725826	-0.874809	3.744346
22	6	0	2.872213	0.425635	1.536104
23	1	0	3.743002	-0.014965	1.042368
24	1	0	3.242070	1.167582	2.253845
25	6	0	-1.648515	1.274838	2.795319
26	1	0	-1.168300	2.262113	2.744368
27	1	0	-1.675502	0.970427	3.848415
28	6	0	1.712904	3.054509	0.855936
29	1	0	2.706122	3.518213	0.925628
30	1	0	1.285776	3.003095	1.866289
31	6	0	3.059900	1.543610	-1.245779
32	1	0	2.800026	2.481433	-1.753462
33	1	0	4.077060	1.645155	-0.854355
34	6	0	2.029508	-2.766442	-1.228281
35	1	0	2.125049	-3.822278	-0.954246
36	1	0	1.565661	-2.712162	-2.222311
37	6	0	-2.316328	-0.951430	-2.702607

38	1	0	-3.115831	-1.692299	-2.823975
39	1	0	-2.584101	-0.062046	-3.288089
40	6	0	-3.517977	0.843547	-0.748339
41	1	0	-4.043300	0.942459	-1.707104
42	1	0	-4.244329	0.509833	-0.003139
43	7	0	2.147575	-0.610982	2.236623
44	8	0	-2.999973	2.081924	-0.299222
45	1	0	-2.385770	2.464257	-0.957390
46	8	0	-1.048782	-1.482860	-3.119986
47	1	0	-1.137305	-1.897277	-3.992169
48	8	0	0.863047	3.789255	-0.033251
49	1	0	0.883927	4.727062	0.208393
50	8	0	3.040785	0.438611	-2.125944
51	1	0	2.168615	0.451701	-2.557696
52	8	0	-2.953385	1.257274	2.290430
53	1	0	-2.985205	1.827805	1.497210
54	8	0	3.302362	-2.182703	-1.159756
55	1	0	3.307248	-1.319609	-1.618844
56	8	0	0.313738	0.631964	-2.314336
57	1	0	-0.301197	3.332388	-1.310536
58	1	0	-0.087928	-0.105105	-2.841419
59	8	0	-0.913241	2.971847	-1.994288
60	1	0	-0.143573	1.489529	-2.504403
61	1	0	-1.072686	3.681811	-2.633362

Co-2：E(opt)= -2700.3700613 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.021088	0.273384	0.175870
2	15	0	2.043770	-0.039462	1.187914
3	15	0	-0.603165	-1.938320	0.048899
4	15	0	0.836977	-0.082874	-1.947304
5	15	0	-2.015275	1.065228	-0.444417
6	6	0	0.950638	-2.995190	-0.170193
7	1	0	1.178272	-3.458290	0.795770
8	1	0	0.739836	-3.807338	-0.877845
9	6	0	2.884389	-1.556519	0.381509
10	1	0	3.823662	-1.212834	-0.064573
11	1	0	3.135246	-2.255191	1.187328
12	6	0	1.994697	-1.593290	-1.911938
13	1	0	1.655049	-2.322938	-2.656962
14	1	0	2.979477	-1.228115	-2.219021

15	7	0	2.125571	-2.262566	-0.627265
16	6	0	-1.600783	-2.217499	-1.544240
17	1	0	-1.126949	-3.007684	-2.138796
18	1	0	-2.583022	-2.574620	-1.222287
19	6	0	-0.589637	-0.586508	-3.086897
20	1	0	-0.850886	0.279300	-3.706363
21	1	0	-0.248851	-1.376025	-3.768769
22	6	0	-2.671302	-0.025088	-1.873227
23	1	0	-3.579141	-0.512025	-1.503169
24	1	0	-2.970389	0.636092	-2.695732
25	6	0	1.876264	1.120338	-2.937590
26	1	0	1.283500	2.028040	-3.129386
27	1	0	2.141217	0.685887	-3.908259
28	6	0	-2.147614	2.760337	-1.206816
29	1	0	-3.193272	3.006045	-1.438789
30	1	0	-1.572414	2.758739	-2.142582
31	6	0	-3.402076	1.124952	0.822833
32	1	0	-3.441183	2.151558	1.213297
33	1	0	-4.362618	0.913837	0.340198
34	6	0	-1.675656	-2.860948	1.287644
35	1	0	-1.616819	-3.938279	1.094699
36	1	0	-1.260493	-2.670700	2.287684
37	6	0	2.120362	-0.448070	3.007831
38	1	0	3.034701	-1.004526	3.254492
39	1	0	2.119612	0.489085	3.581322
40	6	0	3.258827	1.393404	1.066868
41	1	0	3.526544	1.734275	2.076560
42	1	0	4.178227	1.068482	0.572351
43	7	0	-1.783168	-1.045360	-2.390951
44	8	0	2.724143	2.457289	0.289225
45	1	0	1.890218	2.757349	0.708332
46	8	0	0.947356	-1.228227	3.288238
47	1	0	0.993692	-1.551115	4.199948
48	8	0	-1.606906	3.697045	-0.262997
49	1	0	-1.721926	4.596480	-0.599065
50	8	0	-3.214716	0.180300	1.856140
51	1	0	-2.415013	0.452509	2.373750
52	8	0	3.072816	1.373630	-2.238509
53	1	0	2.875424	1.915620	-1.445909
54	8	0	-3.018245	-2.470750	1.148903
55	1	0	-3.132087	-1.553967	1.485497
56	8	0	-0.930147	0.914221	3.064959
57	1	0	-0.347143	3.314669	0.939171
58	1	0	-0.345650	0.133700	3.119568

59	8	0	0.325509	3.089315	1.622805
60	1	0	-0.433911	1.614342	2.599275
61	1	0	0.359170	3.845093	2.226079

Co-3$_{dp}$: E(opt)= -2700.5069384 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.013684	0.140800	0.159236
2	15	0	1.868295	0.023974	1.203004
3	15	0	-0.581842	-1.938716	-0.015355
4	15	0	0.905120	-0.099890	-1.850267
5	15	0	-1.844081	1.073569	-0.504649
6	6	0	0.970837	-3.006919	-0.199403
7	1	0	1.137141	-3.518468	0.755976
8	1	0	0.812918	-3.781417	-0.963733
9	6	0	2.810682	-1.515681	0.541280
10	1	0	3.803746	-1.198251	0.200520
11	1	0	2.952088	-2.199440	1.386693
12	6	0	2.126572	-1.551845	-1.816054
13	1	0	1.876256	-2.270021	-2.608072
14	1	0	3.117690	-1.137975	-2.029404
15	7	0	2.183131	-2.260568	-0.540706
16	6	0	-1.561391	-2.210560	-1.617402
17	1	0	-1.122332	-3.031127	-2.201473
18	1	0	-2.567594	-2.509432	-1.307534
19	6	0	-0.419405	-0.616224	-3.099484
20	1	0	-0.621935	0.235802	-3.760769
21	1	0	-0.041895	-1.432310	-3.730843
22	6	0	-2.514557	0.043211	-1.983462
23	1	0	-3.466797	-0.393459	-1.662195
24	1	0	-2.734270	0.718723	-2.821970
25	6	0	1.911933	1.166471	-2.798548
26	1	0	1.274647	2.052671	-2.955641
27	1	0	2.182194	0.774468	-3.787851
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29	1	0	-3.108854	2.897263	-1.638526
30	1	0	-1.397367	2.831220	-2.143723
31	6	0	-3.318744	1.137744	0.669299
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33	1	0	-4.247207	0.940241	0.119646
34	6	0	-1.652695	-2.897524	1.192788
35	1	0	-1.624599	-3.969144	0.956918

36	1	0	-1.212320	-2.757105	2.191721
37	6	0	1.885577	-0.346040	3.041902
38	1	0	2.820741	-0.841048	3.344151
39	1	0	1.804204	0.606359	3.583475
40	6	0	3.201252	1.383257	1.216945
41	1	0	3.394709	1.694086	2.254059
42	1	0	4.138202	0.996402	0.804411
43	7	0	-1.674103	-1.036910	-2.485397
44	8	0	2.842639	2.506543	0.418561
45	1	0	1.993234	2.861290	0.760157
46	8	0	0.751400	-1.187306	3.313404
47	1	0	0.752580	-1.409604	4.254944
48	8	0	-1.766022	3.778225	-0.301795
49	1	0	-1.865708	4.647487	-0.709925
50	8	0	-3.232849	0.195877	1.724663
51	1	0	-2.495581	0.487548	2.322184
52	8	0	3.110470	1.461417	-2.118469
53	1	0	2.906953	1.937144	-1.281442
54	8	0	-2.997521	-2.482881	1.110393
55	1	0	-3.067348	-1.535377	1.371668
56	8	0	-1.144490	0.988334	3.224889
57	1	0	0.220196	2.117835	1.018271
58	1	0	-0.561972	0.211033	3.130803
59	8	0	0.282367	2.964838	1.554893
60	1	0	-0.679803	1.718101	2.768147
61	1	0	-0.371092	3.517449	1.086152

Co-2$_{pt}$: E(opt)= -2700.6538929 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.065022	0.263101	-0.186437
2	15	0	-2.164207	-0.314712	-0.839570
3	15	0	0.847578	-1.847988	-0.246493
4	15	0	-0.508492	-0.283238	1.920817
5	15	0	1.865530	1.260372	0.360092
6	6	0	-0.517329	-3.118776	0.078670
7	1	0	-0.810584	-3.557013	-0.879835
8	1	0	-0.099271	-3.927341	0.690388
9	6	0	-2.706069	-1.965733	-0.096609
10	1	0	-3.611653	-1.798032	0.495324
11	1	0	-2.966369	-2.644653	-0.914660
12	6	0	-1.474931	-1.924330	2.005517

13	1	0	-0.920897	-2.594586	2.671814
14	1	0	-2.435817	-1.694815	2.475617
15	7	0	-1.702747	-2.586689	0.741794
16	6	0	2.060731	-2.064081	1.206854
17	1	0	1.744925	-2.929934	1.799017
18	1	0	3.026440	-2.297160	0.751194
19	6	0	1.066099	-0.615587	2.915656
20	1	0	1.279606	0.257442	3.541206
21	1	0	0.856017	-1.450936	3.593991
22	6	0	2.905276	0.227977	1.551318
23	1	0	3.786928	-0.110052	0.998196
24	1	0	3.258504	0.866608	2.369468
25	6	0	-1.560682	0.903259	2.905889
26	1	0	-1.037409	1.866152	2.980576
27	1	0	-1.673098	0.499728	3.919212
28	6	0	1.692445	2.917385	1.181703
29	1	0	2.692612	3.331621	1.368339
30	1	0	1.188796	2.781919	2.148172
31	6	0	3.005478	1.678527	-1.073447
32	1	0	2.705189	2.662122	-1.454784
33	1	0	4.025064	1.765168	-0.684477
34	6	0	1.896657	-2.469953	-1.692882
35	1	0	1.896941	-3.564706	-1.661377
36	1	0	1.405216	-2.156127	-2.622847
37	6	0	-2.298320	-0.596286	-2.684533
38	1	0	-3.159002	-1.245296	-2.887591
39	1	0	-2.477976	0.368920	-3.176398
40	6	0	-3.546923	0.958988	-0.612891
41	1	0	-4.072904	1.069964	-1.570540
42	1	0	-4.257012	0.560336	0.115221
43	7	0	2.219739	-0.925118	2.098965
44	8	0	-3.093744	2.197723	-0.116211
45	1	0	-2.467697	2.612634	-0.740974
46	8	0	-1.075580	-1.191002	-3.146047
47	1	0	-1.188018	-1.504190	-4.056919
48	8	0	0.940538	3.762866	0.306846
49	1	0	0.992599	4.674616	0.629082
50	8	0	3.006182	0.693984	-2.085376
51	1	0	2.123885	0.737408	-2.494504
52	8	0	-2.824764	0.993870	2.310608
53	1	0	-2.811812	1.679172	1.610901
54	8	0	3.215285	-2.027288	-1.561636
55	1	0	3.285663	-1.093644	-1.845602
56	8	0	0.294349	0.845453	-2.149163

57	1	0	-0.325281	3.456112	-1.042846
58	1	0	-0.090626	0.160915	-2.748610
59	8	0	-0.918144	3.183722	-1.777751
60	1	0	-0.177581	1.714154	-2.253691
61	1	0	-0.994603	3.939327	-2.378490
62	1	0	-0.647813	1.563606	0.120576

Co-3：E(opt)= -27 00.9564996 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.033939	0.268880	-0.022960
2	15	0	1.995697	0.378456	1.017776
3	15	0	-0.653908	-1.656631	0.890344
4	15	0	0.789131	-1.075948	-1.698269
5	15	0	-1.922492	0.750163	-0.902160
6	6	0	0.837568	-2.776743	1.206675
7	1	0	1.059896	-2.737288	2.278063
8	1	0	0.561985	-3.811506	0.966907
9	6	0	2.828594	-1.334538	1.014722
10	1	0	3.758728	-1.255256	0.443097
11	1	0	3.093425	-1.582896	2.048702
12	6	0	1.906884	-2.433504	-0.987327
13	1	0	1.526189	-3.414707	-1.295753
14	1	0	2.898039	-2.301468	-1.431896
15	7	0	2.040207	-2.420711	0.464196
16	6	0	-1.709114	-2.609278	-0.376143
17	1	0	-1.287590	-3.612957	-0.505933
18	1	0	-2.697183	-2.708633	0.081847
19	6	0	-0.653181	-1.985079	-2.509017
20	1	0	-0.878179	-1.504843	-3.467762
21	1	0	-0.365558	-3.020847	-2.728710
22	6	0	-2.676550	-0.794075	-1.720185
23	1	0	-3.618753	-1.003808	-1.202714
24	1	0	-2.923939	-0.559232	-2.762375
25	6	0	1.849518	-0.342280	-3.048296
26	1	0	1.240847	0.371179	-3.623709
27	1	0	2.197262	-1.119904	-3.737413
28	6	0	-1.885614	1.959546	-2.314894
29	1	0	-2.893289	2.076430	-2.738387
30	1	0	-1.222040	1.552065	-3.089463
31	6	0	-3.284549	1.501372	0.157235
32	1	0	-3.233826	2.588750	0.012963

33	1	0	-4.258450	1.157712	-0.208593
34	6	0	-1.742696	-1.803842	2.418902
35	1	0	-1.700436	-2.837480	2.781473
36	1	0	-1.311503	-1.152218	3.189987
37	6	0	2.010144	0.828205	2.830189
38	1	0	2.934448	0.472994	3.305885
39	1	0	1.974611	1.922647	2.918168
40	6	0	3.291717	1.599808	0.378683
41	1	0	3.632802	2.219012	1.220488
42	1	0	4.152380	1.035198	0.011052
43	7	0	-1.860223	-1.994789	-1.688277
44	8	0	2.832330	2.395136	-0.694609
45	1	0	2.043133	2.894324	-0.399707
46	8	0	0.852213	0.224291	3.424070
47	1	0	0.888996	0.350641	4.383513
48	8	0	-1.401384	3.208880	-1.809702
49	1	0	-1.442476	3.869406	-2.514575
50	8	0	-3.175864	1.151106	1.518491
51	1	0	-2.368641	1.602653	1.881426
52	8	0	2.982355	0.246138	-2.452235
53	1	0	2.739292	1.095101	-2.026301
54	8	0	-3.076551	-1.507513	2.103159
55	1	0	-3.174078	-0.535892	1.975113
56	8	0	-0.889422	2.225252	2.343202
57	1	0	-0.142251	3.475416	-0.436949
58	1	0	-0.363652	1.482008	2.691265
59	8	0	0.466724	3.688151	0.302682
60	1	0	-0.349378	2.675542	1.662175
61	1	0	0.400484	4.641487	0.451872
62	1	0	0.466516	1.475442	-0.744355

Co-TS：E(opt)= -2700.9165886 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.009126	-0.111185	0.415092
2	15	0	-2.174476	0.671355	0.466741
3	15	0	0.664478	1.423706	-1.114681
4	15	0	-0.481237	-1.376614	-1.540102
5	15	0	2.088156	-0.922078	0.591134
6	6	0	-0.768305	1.978215	-2.213811
7	1	0	-1.154569	2.919714	-1.812838
8	1	0	-0.365654	2.183857	-3.213296

9	6	0	-2.837811	1.106101	-1.243762
10	1	0	-3.663888	0.424938	-1.469812
11	1	0	-3.246877	2.121926	-1.210993
12	6	0	-1.517519	-0.319059	-2.747970
13	1	0	-0.973623	-0.253040	-3.697281
14	1	0	-2.443439	-0.872538	-2.931239
15	7	0	-1.863649	1.026578	-2.316806
16	6	0	1.844355	0.641904	-2.397257
17	1	0	1.401573	0.777206	-3.389750
18	1	0	2.762626	1.233328	-2.346858
19	6	0	1.108997	-1.707618	-2.512008
20	1	0	1.459863	-2.719225	-2.282429
21	1	0	0.891508	-1.681428	-3.586779
22	6	0	2.998949	-1.027492	-1.055407
23	1	0	3.818401	-0.302531	-1.028810
24	1	0	3.446482	-2.024214	-1.146246
25	6	0	-1.481930	-2.952904	-1.419942
26	1	0	-0.893414	-3.710025	-0.881825
27	1	0	-1.717044	-3.351232	-2.412828
28	6	0	2.150305	-2.699626	1.137035
29	1	0	3.208607	-3.001244	1.192952
30	1	0	1.668222	-3.306076	0.353748
31	6	0	3.201398	-0.087072	1.850716
32	1	0	3.043012	-0.629796	2.792183
33	1	0	4.247509	-0.213704	1.550221
34	6	0	1.637166	2.959290	-0.633903
35	1	0	1.618295	3.658852	-1.477865
36	1	0	1.119984	3.428648	0.212158
37	6	0	-2.428816	2.227400	1.448994
38	1	0	-3.422144	2.640368	1.224882
39	1	0	-2.386172	1.945500	2.508124
40	6	0	-3.483449	-0.456397	1.241409
41	1	0	-4.040341	0.146957	1.972383
42	1	0	-4.171914	-0.759614	0.448363
43	7	0	2.182343	-0.758310	-2.224940
44	8	0	-2.940925	-1.613126	1.819797
45	1	0	-2.338643	-1.279386	2.547143
46	8	0	-1.387641	3.149214	1.096086
47	1	0	-1.573461	4.000824	1.516334
48	8	0	1.494279	-2.793456	2.385458
49	1	0	1.594821	-3.689525	2.733730
50	8	0	2.928840	1.287408	1.982290
51	1	0	1.969838	1.356137	2.272109
52	8	0	-2.698266	-2.631836	-0.783197

53	1	0	-2.572822	-2.530009	0.184298
54	8	0	2.969433	2.613653	-0.370878
55	1	0	3.030503	2.221106	0.533872
56	8	0	0.375766	1.231746	2.327805
57	1	0	-0.536184	-0.979615	1.962197
58	1	0	-0.035569	2.077697	2.089871
59	8	0	-1.244719	-0.266927	3.315018
60	1	0	-0.357219	0.611761	2.920943
61	1	0	-1.004474	-0.605071	4.187349
62	1	0	-0.336238	-1.451846	1.320735

Co-1$_{dp}$: E(opt)= -2699.7717091 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.015673	0.185480	-0.417962
2	15	0	-2.176580	-0.380233	-0.868989
3	15	0	0.635483	-1.905377	0.438266
4	15	0	-0.543553	0.546966	1.739400
5	15	0	2.044319	1.119021	-0.108077
6	6	0	-0.877923	-2.810157	1.112891
7	1	0	-1.227950	-3.506601	0.345736
8	1	0	-0.588096	-3.402778	1.989677
9	6	0	-2.901537	-1.546614	0.428292
10	1	0	-3.772021	-1.058881	0.880152
11	1	0	-3.252605	-2.448441	-0.083210
12	6	0	-1.657479	-0.855371	2.405236
13	1	0	-1.165416	-1.279230	3.287631
14	1	0	-2.582723	-0.368627	2.727560
15	7	0	-1.982558	-1.925129	1.484597
16	6	0	1.756820	-1.706225	1.958553
17	1	0	1.285613	-2.189419	2.822185
18	1	0	2.684232	-2.238503	1.733848
19	6	0	0.982975	0.440466	2.860096
20	1	0	1.326016	1.458920	3.073883
21	1	0	0.659040	0.008177	3.814856
22	6	0	2.934663	0.381564	1.385276
23	1	0	3.688459	-0.308893	0.997039
24	1	0	3.463255	1.185387	1.913256
25	6	0	-1.465613	2.067824	2.338625
26	1	0	-0.927060	2.961168	1.988882
27	1	0	-1.444151	2.070966	3.435280
28	6	0	2.181581	2.945499	0.224081

29	1	0	3.244403	3.226251	0.261203
30	1	0	1.739176	3.153948	1.209179
31	6	0	3.195059	0.875757	-1.569006
32	1	0	3.061665	1.745611	-2.227135
33	1	0	4.234319	0.867333	-1.221122
34	6	0	1.660739	-3.085845	-0.602919
35	1	0	1.691875	-4.073185	-0.129012
36	1	0	1.167037	-3.186307	-1.578483
37	6	0	-2.374184	-1.339677	-2.448450
38	1	0	-3.389681	-1.758389	-2.495928
39	1	0	-2.244747	-0.648332	-3.291896
40	6	0	-3.384124	1.041235	-1.152943
41	1	0	-3.653757	1.049740	-2.218195
42	1	0	-4.297185	0.855206	-0.578701
43	7	0	2.087237	-0.332705	2.325796
44	8	0	-2.856037	2.282816	-0.745783
45	1	0	-2.044822	2.465772	-1.299968
46	8	0	-1.375732	-2.362049	-2.440351
47	1	0	-1.514533	-2.942104	-3.202148
48	8	0	1.497606	3.625150	-0.823673
49	1	0	1.668373	4.575031	-0.767523
50	8	0	2.912096	-0.336711	-2.226464
51	1	0	1.924564	-0.268767	-2.442956
52	8	0	-2.799640	2.018158	1.918311
53	1	0	-2.834782	2.279444	0.966905
54	8	0	2.973431	-2.590529	-0.678637
55	1	0	3.009666	-1.835876	-1.313299
56	8	0	0.390513	0.033911	-2.321545
57	1	0	0.040401	2.975398	-1.827217
58	1	0	-0.004093	-0.782658	-2.661378
59	8	0	-0.697016	2.506582	-2.257318
60	1	0	-0.316728	1.640496	-2.540606

Co-dimer-triplet： E(opt)= -5401.91002838 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	3.580189	0.049100	0.101281
2	15	0	3.233078	1.839104	-1.161895
3	15	0	5.841940	0.118555	-0.001383
4	15	0	3.806270	-1.377617	-1.706682
5	15	0	3.564573	-1.546432	1.626651
6	6	0	6.393243	0.821579	-1.666773

7	1	0	6.707956	1.858002	-1.510462
8	1	0	7.272117	0.262053	-2.009198
9	6	0	4.408864	1.871764	-2.655456
10	1	0	3.806864	1.851849	-3.570721
11	1	0	4.946386	2.825684	-2.637920
12	6	0	4.846173	-0.519445	-3.052909
13	1	0	5.684128	-1.172568	-3.324527
14	1	0	4.209455	-0.417609	-3.938005
15	7	0	5.373626	0.793550	-2.707596
16	6	0	6.560393	-1.641429	-0.008993
17	1	0	7.192907	-1.757356	-0.896241
18	1	0	7.198081	-1.704911	0.876933
19	6	0	4.822658	-2.897828	-1.200029
20	1	0	4.132985	-3.739177	-1.068763
21	1	0	5.506354	-3.167633	-2.014307
22	6	0	4.878451	-2.867244	1.279256
23	1	0	5.605627	-2.837026	2.096914
24	1	0	4.398916	-3.853146	1.309115
25	6	0	2.355760	-2.063428	-2.668198
26	1	0	1.900565	-2.866690	-2.068905
27	1	0	2.697436	-2.506612	-3.610046
28	6	0	1.987363	-2.552745	1.673227
29	1	0	1.991233	-3.190660	2.563817
30	1	0	1.983452	-3.213222	0.792223
31	6	0	3.759385	-1.041628	3.422859
32	1	0	2.752329	-0.795484	3.788415
33	1	0	4.124097	-1.900096	3.998217
34	6	0	6.930154	0.936245	1.307394
35	1	0	7.911623	1.127552	0.858838
36	1	0	6.476349	1.903383	1.558618
37	6	0	3.491778	3.527029	-0.414359
38	1	0	3.536417	4.279578	-1.212907
39	1	0	2.644770	3.757839	0.244813
40	6	0	1.585083	2.088223	-2.013782
41	1	0	1.565367	3.113418	-2.416466
42	1	0	1.576135	1.384828	-2.850457
43	7	0	5.594170	-2.724997	0.022588
44	8	0	0.417815	1.819053	-1.244385
45	1	0	0.500529	2.140263	-0.317248
46	8	0	4.726870	3.463621	0.312006
47	1	0	5.001970	4.361009	0.550900
48	8	0	0.832707	-1.739653	1.736971
49	1	0	0.774714	-1.248224	0.894311
50	8	0	4.659565	0.025922	3.598308

51	1	0	4.232067	0.864588	3.278140
52	8	0	1.440321	-1.030398	-2.973794
53	1	0	0.887796	-0.877738	-2.179064
54	8	0	7.109036	0.087145	2.404041
55	1	0	6.286686	0.071167	2.944032
56	8	0	3.599979	2.232602	2.600488
57	1	0	1.415167	1.062202	1.202819
58	1	0	4.116838	2.621851	1.872102
59	8	0	1.076547	1.949434	1.449381
60	1	0	2.665474	2.257841	2.313426
61	1	0	0.295386	1.788354	2.017529
62	1	0	2.086707	-0.015884	0.216222
63	27	0	-3.598152	0.103298	-0.137359
64	15	0	-4.152863	2.211916	0.478798
65	15	0	-5.711946	-0.700359	0.081849
66	15	0	-3.438216	-0.642712	2.071315
67	15	0	-2.882762	-1.825983	-1.005498
68	6	0	-6.658970	0.248571	1.412609
69	1	0	-7.290672	0.994930	0.922053
70	1	0	-7.324595	-0.451575	1.931559
71	6	0	-5.323609	2.222259	1.971624
72	1	0	-4.796915	2.687530	2.811860
73	1	0	-6.182253	2.860858	1.737148
74	6	0	-4.863383	0.085795	3.111922
75	1	0	-5.412413	-0.743939	3.572206
76	1	0	-4.423780	0.674784	3.923581
77	7	0	-5.809567	0.921735	2.387441
78	6	0	-5.710061	-2.465855	0.803028
79	1	0	-6.268150	-2.455037	1.745397
80	1	0	-6.258944	-3.083655	0.087732
81	6	0	-3.671396	-2.518444	2.173393
82	1	0	-2.684584	-2.989572	2.225786
83	1	0	-4.204139	-2.774813	3.096780
84	6	0	-3.658626	-3.340271	-0.174629
85	1	0	-4.336824	-3.801405	-0.898937
86	1	0	-2.868228	-4.068068	0.043451
87	6	0	-1.843911	-0.190014	2.927155
88	1	0	-1.109013	-0.986910	2.759898
89	1	0	-1.969401	-0.044743	4.003846
90	6	0	-1.081538	-2.166684	-0.674427
91	1	0	-0.711801	-2.917631	-1.383035
92	1	0	-0.995185	-2.582690	0.336457
93	6	0	-3.009528	-2.117949	-2.855721
94	1	0	-2.105812	-1.687168	-3.310934

95	1	0	-3.002568	-3.195465	-3.053372
96	6	0	-6.870759	-0.935445	-1.385096
97	1	0	-7.892518	-1.048768	-1.005492
98	1	0	-6.832992	-0.025038	-1.995967
99	6	0	-5.058434	3.264072	-0.768661
100	1	0	-5.565288	4.090168	-0.253413
101	1	0	-4.318526	3.687681	-1.461237
102	6	0	-2.828471	3.437402	1.009536
103	1	0	-3.243203	4.454799	0.930783
104	1	0	-2.618020	3.241527	2.063130
105	7	0	-4.408004	-3.063744	1.037909
106	8	0	-1.610843	3.300088	0.314278
107	1	0	-1.777692	3.375146	-0.642730
108	8	0	-5.998050	2.424868	-1.455808
109	1	0	-6.600311	2.977885	-1.974658
110	8	0	-0.252732	-1.011053	-0.787209
111	1	0	-0.808163	-0.207646	-0.665957
112	8	0	-4.187068	-1.575706	-3.412023
113	1	0	-4.122576	-0.595723	-3.314717
114	8	0	-1.397404	1.057048	2.378538
115	1	0	-1.590860	1.045770	1.418383
116	8	0	-6.528042	-2.104023	-2.079667
117	1	0	-5.751904	-1.936025	-2.659365
118	8	0	-3.964346	0.935484	-2.625703
119	1	0	-1.041570	2.263137	-2.062825
120	1	0	-4.772568	1.434629	-2.403427
121	8	0	-1.864921	2.700164	-2.398920
122	1	0	-3.206303	1.558992	-2.610209
123	1	0	-1.609677	3.217662	-3.174154
124	1	0	-2.174292	0.631355	-0.297212

Co-dimer-singlet-ts：E(opt)= -5401.8529 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	2.435895	0.004036	0.062080
2	15	0	2.622531	-0.102852	2.395575
3	15	0	4.887702	-0.162054	-0.097199
4	15	0	3.008698	2.407174	0.023897
5	15	0	2.458369	-0.460887	-2.209292
6	6	0	5.699257	0.663918	1.391233
7	1	0	5.951540	-0.127895	2.102265
8	1	0	6.641049	1.116893	1.056874

9	6	0	3.940746	1.140961	3.011425
10	1	0	3.387232	1.982126	3.443816
11	1	0	4.472728	0.646937	3.834201
12	6	0	4.443670	2.761057	1.245509
13	1	0	5.299823	3.143517	0.679072
14	1	0	4.115623	3.569785	1.906494
15	7	0	4.890191	1.656557	2.064057
16	6	0	5.474211	0.937274	-1.542018
17	1	0	6.176309	1.682592	-1.152886
18	1	0	6.041409	0.268411	-2.196336
19	6	0	3.804535	2.738296	-1.664274
20	1	0	3.011050	3.117719	-2.315482
21	1	0	4.540665	3.544503	-1.541749
22	6	0	3.621886	0.746470	-3.119767
23	1	0	4.276438	0.143868	-3.759396
24	1	0	3.001045	1.363242	-3.777912
25	6	0	2.074602	4.037147	0.273965
26	1	0	2.518965	4.801241	-0.379664
27	1	0	2.227573	4.357578	1.307327
28	6	0	0.936418	-0.390884	-3.296697
29	1	0	1.105205	-0.989591	-4.197164
30	1	0	0.761214	0.638631	-3.614155
31	6	0	3.018964	-2.164128	-2.823732
32	1	0	2.142274	-2.822337	-2.758156
33	1	0	3.253933	-2.031990	-3.887323
34	6	0	6.098526	-1.641079	-0.285677
35	1	0	6.951972	-1.405160	0.358603
36	1	0	5.596430	-2.525607	0.117059
37	6	0	3.238551	-1.725527	3.093885
38	1	0	3.629640	-1.552454	4.106727
39	1	0	2.388686	-2.417028	3.152941
40	6	0	1.405431	0.290478	3.778440
41	1	0	1.974412	0.478683	4.696527
42	1	0	0.869667	1.196889	3.494535
43	7	0	4.440360	1.605592	-2.301372
44	8	0	0.438947	-0.750633	4.005801
45	1	0	0.669124	-1.239120	4.807043
46	8	0	4.252820	-2.239480	2.228747
47	1	0	4.651097	-3.023388	2.636208
48	8	0	-0.206392	-0.965609	-2.657764
49	1	0	-0.525217	-0.416735	-1.919349
50	8	0	4.128569	-2.714948	-2.185536
51	1	0	3.811400	-3.124449	-1.330817
52	8	0	0.669405	3.962793	0.084745

53	1	0	0.493703	3.547398	-0.785481
54	8	0	6.575725	-1.812543	-1.581187
55	1	0	5.864580	-2.258992	-2.082569
56	8	0	3.044159	-3.558178	0.018396
57	1	0	0.302563	-2.191747	-1.375317
58	1	0	3.303368	-3.002308	0.773254
59	8	0	0.444274	-2.861485	-0.680241
60	1	0	2.098766	-3.394160	-0.174453
61	1	0	0.328776	-2.401084	0.179689
62	1	0	0.591545	-0.013859	0.032529
63	27	0	-2.491973	-0.008120	0.018169
64	15	0	-2.563182	-1.535315	1.722704
65	15	0	-4.883670	0.372378	0.198572
66	15	0	-3.282263	-1.696952	-1.537375
67	15	0	-2.453288	1.783936	-1.389945
68	6	0	-5.767605	-1.166815	0.832619
69	1	0	-5.939621	-1.025618	1.903172
70	1	0	-6.748470	-1.209448	0.342598
71	6	0	-4.068224	-2.710120	1.624368
72	1	0	-3.676110	-3.714622	1.437000
73	1	0	-4.538085	-2.714722	2.613197
74	6	0	-4.696884	-2.716483	-0.738313
75	1	0	-5.587025	-2.623636	-1.370685
76	1	0	-4.363375	-3.756617	-0.780029
77	7	0	-5.062469	-2.410946	0.629255
78	6	0	-5.628077	0.546999	-1.546245
79	1	0	-6.384232	-0.233301	-1.681010
80	1	0	-6.142411	1.512772	-1.546042
81	6	0	-4.145415	-0.813865	-2.969030
82	1	0	-3.420347	-0.709090	-3.783123
83	1	0	-4.956202	-1.452376	-3.342519
84	6	0	-3.811297	1.632084	-2.730583
85	1	0	-4.410069	2.547898	-2.678466
86	1	0	-3.308294	1.628745	-3.703933
87	6	0	-2.426106	-3.163780	-2.346319
88	1	0	-1.621049	-2.811885	-2.996869
89	1	0	-3.163627	-3.691429	-2.962417
90	6	0	-1.026103	2.162615	-2.531807
91	1	0	-1.180757	3.141421	-2.997862
92	1	0	-1.025105	1.417018	-3.334892
93	6	0	-2.685412	3.510780	-0.659796
94	1	0	-1.709481	3.847280	-0.288460
95	1	0	-2.965285	4.169080	-1.491580
96	6	0	-5.889613	1.706357	1.125051

97	1	0	-6.818455	1.214574	1.434289
98	1	0	-5.331704	1.979961	2.027509
99	6	0	-2.770745	-0.859007	3.449797
100	1	0	-2.950235	-1.693956	4.140899
101	1	0	-1.860600	-0.334503	3.760184
102	6	0	-1.262773	-2.854316	1.980322
103	1	0	-1.465604	-3.381765	2.924049
104	1	0	-1.400408	-3.570522	1.166797
105	7	0	-4.691756	0.497726	-2.648204
106	8	0	0.074726	-2.392136	1.915230
107	1	0	0.216476	-1.750470	2.642346
108	8	0	-3.902524	0.023283	3.402169
109	1	0	-4.174036	0.242621	4.305682
110	8	0	0.251308	2.225968	-1.887889
111	1	0	0.382391	1.467924	-1.288725
112	8	0	-3.671860	3.595324	0.325458
113	1	0	-3.333435	3.180500	1.170598
114	8	0	-1.981595	-4.045432	-1.333752
115	1	0	-1.066812	-3.796715	-1.092169
116	8	0	-6.228955	2.796541	0.326175
117	1	0	-5.425063	3.349405	0.242267
118	8	0	-2.739964	2.399004	2.445973
119	1	0	-0.030419	1.290891	1.241133
120	1	0	-3.168621	1.569444	2.723626
121	8	0	-0.141306	2.063519	1.818578
122	1	0	-1.784028	2.214691	2.304876
123	1	0	0.091977	2.835194	1.247907
124	1	0	-0.639994	-0.032958	0.023417

Co-dimer-triplet-ts：E(opt)= -5401.8529 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	2.414082	0.016855	0.066874
2	15	0	2.615010	-0.085133	2.406104
3	15	0	4.894477	-0.169802	-0.094003
4	15	0	3.006137	2.405683	-0.002487
5	15	0	2.449350	-0.482062	-2.209987
6	6	0	5.700305	0.677322	1.385983
7	1	0	5.957697	-0.105565	2.105138
8	1	0	6.639364	1.135116	1.050190
9	6	0	3.939076	1.161281	3.005725
10	1	0	3.388270	2.005523	3.435755

11	1	0	4.475664	0.672224	3.828491
12	6	0	4.434203	2.768212	1.225594
13	1	0	5.290433	3.153021	0.660583
14	1	0	4.098212	3.577579	1.881842
15	7	0	4.883496	1.670428	2.050270
16	6	0	5.480448	0.913344	-1.550743
17	1	0	6.183979	1.663064	-1.172342
18	1	0	6.045757	0.237547	-2.199490
19	6	0	3.814213	2.714958	-1.689764
20	1	0	3.026626	3.095219	-2.347862
21	1	0	4.554474	3.517743	-1.568794
22	6	0	3.623120	0.713083	-3.126545
23	1	0	4.275061	0.101879	-3.760590
24	1	0	3.006614	1.328140	-3.790541
25	6	0	2.085360	4.049059	0.211734
26	1	0	2.532258	4.794763	-0.460918
27	1	0	2.240925	4.394159	1.236690
28	6	0	0.940596	-0.430794	-3.317084
29	1	0	1.114030	-1.041415	-4.208475
30	1	0	0.761809	0.593832	-3.649301
31	6	0	3.024468	-2.188141	-2.804494
32	1	0	2.153100	-2.853348	-2.737874
33	1	0	3.265766	-2.066551	-3.867915
34	6	0	6.116424	-1.642150	-0.262762
35	1	0	6.970824	-1.393896	0.375608
36	1	0	5.620140	-2.524089	0.153568
37	6	0	3.238152	-1.702810	3.112069
38	1	0	3.635606	-1.522005	4.121140
39	1	0	2.389335	-2.394724	3.182255
40	6	0	1.412107	0.308717	3.802390
41	1	0	1.985950	0.478934	4.721010
42	1	0	0.884542	1.225170	3.535523
43	7	0	4.445576	1.575157	-2.315653
44	8	0	0.434921	-0.726784	4.019484
45	1	0	0.655753	-1.218155	4.821538
46	8	0	4.247378	-2.223211	2.245257
47	1	0	4.647638	-3.004161	2.656335
48	8	0	-0.206441	-1.001389	-2.676154
49	1	0	-0.526657	-0.447253	-1.943068
50	8	0	4.134789	-2.723217	-2.153287
51	1	0	3.816086	-3.128542	-1.297545
52	8	0	0.678144	3.979229	0.026178
53	1	0	0.498176	3.545477	-0.833714
54	8	0	6.592504	-1.831769	-1.557001

55	1	0	5.878577	-2.278668	-2.053411
56	8	0	3.044962	-3.563883	0.051514
57	1	0	0.308607	-2.213496	-1.381759
58	1	0	3.301784	-2.993417	0.796598
59	8	0	0.441965	-2.870487	-0.672855
60	1	0	2.101288	-3.402400	-0.148166
61	1	0	0.334984	-2.390617	0.176956
62	1	0	0.456515	-0.003413	0.035619
63	27	0	-2.521297	-0.010766	0.018494
64	15	0	-2.573679	-1.522583	1.715221
65	15	0	-4.873284	0.378798	0.213291
66	15	0	-3.286576	-1.695617	-1.519843
67	15	0	-2.467328	1.757581	-1.399408
68	6	0	-5.763295	-1.153584	0.858963
69	1	0	-5.926767	-1.008984	1.930254
70	1	0	-6.747397	-1.187047	0.375039
71	6	0	-4.069646	-2.704122	1.641507
72	1	0	-3.677781	-3.708192	1.451624
73	1	0	-4.532063	-2.708638	2.633797
74	6	0	-4.706534	-2.709298	-0.715294
75	1	0	-5.595402	-2.611009	-1.348199
76	1	0	-4.377761	-3.750768	-0.758026
77	7	0	-5.070233	-2.403485	0.651955
78	6	0	-5.631052	0.542013	-1.530927
79	1	0	-6.387397	-0.240337	-1.649859
80	1	0	-6.145944	1.507396	-1.530448
81	6	0	-4.156140	-0.824562	-2.955872
82	1	0	-3.434854	-0.722021	-3.773408
83	1	0	-4.964034	-1.471177	-3.321138
84	6	0	-3.827231	1.620405	-2.734085
85	1	0	-4.424045	2.537126	-2.678382
86	1	0	-3.331544	1.615796	-3.711146
87	6	0	-2.433171	-3.170589	-2.317065
88	1	0	-1.627962	-2.826155	-2.970875
89	1	0	-3.173820	-3.700045	-2.927975
90	6	0	-1.039264	2.106304	-2.549558
91	1	0	-1.204287	3.071222	-3.040731
92	1	0	-1.038183	1.340464	-3.333195
93	6	0	-2.669862	3.493187	-0.681483
94	1	0	-1.687339	3.819041	-0.319633
95	1	0	-2.946035	4.146972	-1.517910
96	6	0	-5.863495	1.726724	1.136298
97	1	0	-6.790918	1.241220	1.459478
98	1	0	-5.295055	2.006153	2.030175

99	6	0	-2.764112	-0.828074	3.436703
100	1	0	-2.938196	-1.658333	4.134645
101	1	0	-1.848795	-0.305348	3.734465
102	6	0	-1.260191	-2.826988	1.978546
103	1	0	-1.462773	-3.349031	2.925513
104	1	0	-1.391556	-3.549506	1.169888
105	7	0	-4.708371	0.486110	-2.642374
106	8	0	0.071692	-2.353598	1.914147
107	1	0	0.214327	-1.719173	2.647974
108	8	0	-3.893214	0.057402	3.396041
109	1	0	-4.154207	0.283538	4.301065
110	8	0	0.238049	2.198675	-1.913563
111	1	0	0.396045	1.445696	-1.314015
112	8	0	-3.647691	3.600829	0.310122
113	1	0	-3.302768	3.186738	1.152555
114	8	0	-1.991025	-4.043303	-1.296550
115	1	0	-1.071843	-3.799871	-1.064514
116	8	0	-6.205338	2.809428	0.329257
117	1	0	-5.400911	3.360518	0.236637
118	8	0	-2.684289	2.389006	2.403431
119	1	0	0.135190	1.327664	1.245950
120	1	0	-3.125415	1.574510	2.704007
121	8	0	-0.083884	2.097170	1.796211
122	1	0	-1.730228	2.194097	2.259935
123	1	0	0.122517	2.873002	1.220702
124	1	0	-0.649118	-0.051813	0.008190

Co-1'：E(opt)= -3267.5831641 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.053903	-0.106935	0.098285
2	15	0	-0.599655	1.756104	1.298588
3	15	0	2.058157	-0.200697	0.962787
4	15	0	1.062895	1.289530	-1.554936
5	15	0	0.324876	-2.005910	-1.095190
6	6	0	2.641537	1.502390	1.530188
7	1	0	2.417810	1.598904	2.596724
8	1	0	3.732355	1.532607	1.416313
9	6	0	0.765535	3.056903	1.333099
10	1	0	0.423053	3.913183	0.743879
11	1	0	0.889125	3.393017	2.369171
12	6	0	2.141365	2.575335	-0.639166

13	1	0	3.190291	2.420265	-0.913849
14	1	0	1.831758	3.547545	-1.031918
15	7	0	2.043700	2.615718	0.814333
16	6	0	3.350869	-0.626539	-0.378933
17	1	0	4.062307	0.203710	-0.431093
18	1	0	3.876802	-1.507313	-0.000762
19	6	0	2.352565	0.241080	-2.453592
20	1	0	1.894018	-0.110048	-3.382600
21	1	0	3.196792	0.888057	-2.724039
22	6	0	2.070361	-2.125408	-1.795984
23	1	0	2.598522	-2.919310	-1.258172
24	1	0	1.991942	-2.429050	-2.845439
25	6	0	0.342863	2.392618	-2.901807
26	1	0	-0.387623	1.803502	-3.470769
27	1	0	1.147720	2.681162	-3.587202
28	6	0	-0.770969	-2.063563	-2.617434
29	1	0	-1.732484	-2.502386	-2.330996
30	1	0	-0.304720	-2.705286	-3.371575
31	6	0	-0.016505	-3.622103	-0.207580
32	1	0	-1.092705	-3.810831	-0.301102
33	1	0	0.521547	-4.436087	-0.703940
34	6	0	2.580603	-1.390086	2.329790
35	1	0	3.501280	-0.994287	2.774495
36	1	0	1.805603	-1.384724	3.106923
37	6	0	-1.048017	1.515566	3.086316
38	1	0	-1.106482	2.486475	3.595259
39	1	0	-2.028469	1.025177	3.126813
40	6	0	-2.124591	2.644086	0.659399
41	1	0	-2.997429	2.197644	1.153010
42	1	0	-2.077992	3.701397	0.937505
43	7	0	2.851923	-0.907348	-1.705707
44	8	0	-2.227341	2.572240	-0.750008
45	1	0	-2.290608	1.618073	-0.969962
46	8	0	-0.019204	0.690545	3.663650
47	1	0	-0.129995	0.679593	4.625273
48	8	0	-0.914624	-0.772055	-3.176945
49	1	0	-1.475881	-0.288463	-2.544926
50	8	0	0.389424	-3.596087	1.148723
51	1	0	-0.164604	-2.925938	1.615920
52	8	0	-0.185833	3.569118	-2.340516
53	1	0	-1.008723	3.343636	-1.861636
54	8	0	2.857440	-2.661785	1.813716
55	1	0	2.010033	-3.121928	1.615967
56	8	0	-0.884391	-1.480964	2.138621

57	1	0	-0.484299	-0.905884	2.816656
58	1	0	-1.844290	-1.237133	2.093218
59	8	0	-1.996131	-0.132231	-0.673615
60	15	0	-3.219327	-0.737149	0.047603
61	8	0	-3.184316	-2.297893	-0.390273
62	8	0	-3.310397	-0.569056	1.540039
63	8	0	-4.500983	-0.104141	-0.695986
64	1	0	-3.874593	-2.823703	0.040381
65	1	0	-5.211087	0.125705	-0.079426

Co-1_{dp}'： E(opt)= -3267.1800018 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.060838	-0.014203	-0.029786
2	15	0	-0.602325	-1.923109	1.044325
3	15	0	-1.130188	1.272219	1.348359
4	15	0	-1.929362	0.078056	-1.325328
5	15	0	0.988124	1.841250	-1.015520
6	6	0	-2.652526	0.378529	2.018738
7	1	0	-2.368878	-0.053034	2.982827
8	1	0	-3.440703	1.123526	2.187835
9	6	0	-2.474142	-1.957320	1.293278
10	1	0	-2.901684	-2.654198	0.566228
11	1	0	-2.671019	-2.354295	2.296127
12	6	0	-3.437281	-0.291350	-0.221576
13	1	0	-4.091225	0.588835	-0.210461
14	1	0	-3.976136	-1.109128	-0.708238
15	7	0	-3.158159	-0.677688	1.153967
16	6	0	-1.899033	2.756988	0.412197
17	1	0	-2.981327	2.723968	0.582813
18	1	0	-1.505638	3.653398	0.901783
19	6	0	-2.280521	1.851564	-1.854393
20	1	0	-1.921138	1.976146	-2.880138
21	1	0	-3.366796	2.013146	-1.862934
22	6	0	-0.279226	3.197668	-1.354531
23	1	0	0.011426	4.086169	-0.783288
24	1	0	-0.234776	3.458687	-2.417157
25	6	0	-2.319948	-0.995513	-2.815581
26	1	0	-1.467239	-0.929014	-3.504198
27	1	0	-3.203631	-0.597473	-3.328663
28	6	0	1.625461	1.384492	-2.716985
29	1	0	2.645516	1.010868	-2.572240

30	1	0	1.651788	2.278400	-3.350290
31	6	0	2.422278	2.730498	-0.184454
32	1	0	3.197304	2.906918	-0.943219
33	1	0	2.065710	3.699338	0.176271
34	6	0	-0.329779	2.147941	2.793110
35	1	0	-1.090432	2.739693	3.315103
36	1	0	0.063454	1.400135	3.486578
37	6	0	0.007926	-2.287944	2.769699
38	1	0	-0.594734	-3.104994	3.185902
39	1	0	1.048278	-2.618357	2.692356
40	6	0	-0.216838	-3.467980	0.059633
41	1	0	0.786226	-3.786361	0.365485
42	1	0	-0.936874	-4.257074	0.300570
43	7	0	-1.653925	2.869481	-1.013277
44	8	0	-0.275464	-3.226530	-1.339015
45	1	0	0.395718	-2.509407	-1.493172
46	8	0	-0.145768	-1.144320	3.585920
47	1	0	0.682037	-0.621881	3.431985
48	8	0	0.778202	0.430870	-3.325430
49	1	0	0.908044	-0.368377	-2.767356
50	8	0	2.937869	2.004875	0.911699
51	1	0	3.295079	1.148869	0.491746
52	8	0	-2.613710	-2.306042	-2.395990
53	1	0	-1.780663	-2.727110	-2.076443
54	8	0	0.653806	3.040094	2.312207
55	1	0	1.456211	2.539366	2.068442
56	8	0	1.272631	-1.110954	-1.162123
57	15	0	2.710823	-1.312707	-0.473354
58	8	0	3.528646	-0.021736	-0.517302
59	8	0	2.520246	-1.947798	0.896279
60	8	0	3.374711	-2.371946	-1.524790
61	1	0	4.328254	-2.225220	-1.578246
62	8	0	2.173910	-0.131191	2.795527
63	1	0	2.442485	0.697608	2.375986
64	1	0	2.402403	-0.831877	2.119520

Co-2'：E(opt)= -3267.7704493 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.062275	-0.038431	0.044394
2	15	0	-0.511298	1.813321	1.232490
3	15	0	2.216679	-0.215598	0.878748

4	15	0	1.091061	1.173232	-1.623901
5	15	0	0.148487	-2.053624	-1.041036
6	6	0	2.859243	1.508749	1.305771
7	1	0	2.723792	1.648458	2.383413
8	1	0	3.936941	1.559907	1.095815
9	6	0	0.934492	3.054875	1.187336
10	1	0	0.596526	3.928271	0.618899
11	1	0	1.124850	3.382272	2.216655
12	6	0	2.203458	2.510949	-0.850706
13	1	0	3.239748	2.356277	-1.176472
14	1	0	1.856477	3.464467	-1.259810
15	7	0	2.185824	2.597424	0.605981
16	6	0	3.387605	-0.802844	-0.503638
17	1	0	4.167416	-0.046925	-0.660290
18	1	0	3.863203	-1.712395	-0.125318
19	6	0	2.305987	0.056355	-2.542297
20	1	0	1.799564	-0.293097	-3.448277
21	1	0	3.176210	0.649853	-2.856194
22	6	0	1.886629	-2.260856	-1.794172
23	1	0	2.386164	-3.067587	-1.247036
24	1	0	1.759544	-2.593683	-2.831566
25	6	0	0.283786	2.169349	-2.997690
26	1	0	-0.473925	1.524781	-3.463512
27	1	0	1.033438	2.414202	-3.760172
28	6	0	-0.986238	-2.262858	-2.517593
29	1	0	-1.921945	-2.714369	-2.165860
30	1	0	-0.535510	-2.928976	-3.262109
31	6	0	-0.095462	-3.618658	-0.040835
32	1	0	-1.171085	-3.839448	-0.050424
33	1	0	0.429910	-4.467502	-0.492941
34	6	0	2.839030	-1.286662	2.295999
35	1	0	3.841816	-0.955550	2.594009
36	1	0	2.166764	-1.124901	3.152068
37	6	0	-0.854562	1.695635	3.057179
38	1	0	-0.881719	2.689238	3.528053
39	1	0	-1.827659	1.204328	3.176900
40	6	0	-1.999687	2.809228	0.670765
41	1	0	-2.866951	2.444450	1.237676
42	1	0	-1.864459	3.872790	0.896725
43	7	0	2.765873	-1.101787	-1.785345
44	8	0	-2.211085	2.687497	-0.725896
45	1	0	-2.385894	1.725471	-0.909502
46	8	0	0.211685	0.898784	3.610425
47	1	0	0.058300	0.802924	4.560426

48	8	0	-1.201993	-1.005771	-3.136894
49	1	0	-1.735334	-0.493645	-2.491710
50	8	0	0.389225	-3.474109	1.286753
51	1	0	-0.152342	-2.781891	1.753932
52	8	0	-0.232916	3.384563	-2.502957
53	1	0	-0.991291	3.187986	-1.908341
54	8	0	2.937227	-2.637000	1.909073
55	1	0	2.038199	-2.989113	1.713462
56	8	0	-0.928559	-1.577929	2.625236
57	1	0	-0.348869	-0.836578	2.871384
58	1	0	-1.739397	-1.149648	2.249573
59	8	0	-2.507375	0.059467	-0.946333
60	15	0	-3.369071	-0.588677	0.122034
61	8	0	-3.296093	-2.191379	-0.192029
62	8	0	-3.086747	-0.331238	1.586200
63	8	0	-4.924243	-0.190760	-0.165308
64	1	0	-3.713482	-2.697754	0.518767
65	1	0	-5.348889	0.059182	0.666818

Co-3_{dp}'： E(opt)= -3267.8063889 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	-0.234152	-0.021639	-0.016449
2	15	0	0.279602	-1.624052	1.373196
3	15	0	-2.195790	0.505337	0.862734
4	15	0	-1.337366	-1.183437	-1.451622
5	15	0	-0.001516	1.837269	-1.113862
6	6	0	-3.063259	-1.060706	1.465433
7	1	0	-2.968381	-1.096450	2.556923
8	1	0	-4.136073	-1.011053	1.224741
9	6	0	-1.270119	-2.740044	1.545645
10	1	0	-1.016151	-3.719690	1.122786
11	1	0	-1.472929	-2.879848	2.615460
12	6	0	-2.524403	-2.367853	-0.550463
13	1	0	-3.556375	-2.200283	-0.892064
14	1	0	-2.224228	-3.378614	-0.846105
15	7	0	-2.508269	-2.292900	0.911942
16	6	0	-3.354484	1.162766	-0.494943
17	1	0	-4.251804	0.530978	-0.554064
18	1	0	-3.660284	2.169678	-0.192493
19	6	0	-2.486537	-0.058078	-2.445747
20	1	0	-2.005801	0.115526	-3.416040

21	1	0	-3.447481	-0.562018	-2.635638
22	6	0	-1.689896	2.230615	-1.944681
23	1	0	-2.066370	3.169871	-1.522281
24	1	0	-1.499397	2.399056	-3.013025
25	6	0	-0.704856	-2.339296	-2.791815
26	1	0	0.046012	-1.773504	-3.362340
27	1	0	-1.525329	-2.603312	-3.474357
28	6	0	1.164308	1.814444	-2.599483
29	1	0	2.126969	2.221790	-2.265732
30	1	0	0.773032	2.456499	-3.400010
31	6	0	0.432947	3.547510	-0.415666
32	1	0	1.504968	3.723331	-0.579685
33	1	0	-0.116260	4.341254	-0.935876
34	6	0	-2.610927	1.727480	2.230590
35	1	0	-3.653565	1.592197	2.550465
36	1	0	-1.964246	1.485675	3.087738
37	6	0	0.750543	-1.429164	3.187200
38	1	0	0.568884	-2.359352	3.741385
39	1	0	1.825338	-1.207377	3.226073
40	6	0	1.613717	-2.854340	0.865914
41	1	0	2.533334	-2.543752	1.375935
42	1	0	1.347528	-3.864650	1.201869
43	7	0	-2.755000	1.240503	-1.825565
44	8	0	1.823322	-2.913393	-0.538987
45	1	0	2.226097	-2.042327	-0.808241
46	8	0	-0.026614	-0.412901	3.816753
47	1	0	0.294003	0.429303	3.441204
48	8	0	1.306428	0.508869	-3.126593
49	1	0	1.839968	0.016307	-2.461511
50	8	0	0.110984	3.682525	0.973918
51	1	0	0.666523	3.048912	1.475378
52	8	0	-0.206351	-3.543978	-2.247879
53	1	0	0.545869	-3.328307	-1.645176
54	8	0	-2.483718	3.067324	1.794735
55	1	0	-1.551828	3.245567	1.535678
56	8	0	1.419339	1.537359	2.204759
57	1	0	0.823489	1.054653	1.540610
58	1	0	2.218855	0.952337	2.181106
59	8	0	2.880729	-0.544610	-1.107811
60	15	0	3.600165	0.200191	-0.000748
61	8	0	3.312798	1.815710	-0.121532
62	8	0	3.407225	-0.190261	1.449749
63	8	0	5.187595	0.146645	-0.388416
64	1	0	2.669734	2.045985	0.572378

65	1	0	5.698346	0.466705	0.367474

Co-2$_{pt}$'： E(opt)= -3268.1618865 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.006312	-0.037009	0.003455
2	15	0	-0.434825	1.572698	1.503999
3	15	0	1.926731	-0.587365	0.988008
4	15	0	1.380174	1.323943	-1.262671
5	15	0	0.142392	-1.808385	-1.367105
6	6	0	2.692900	0.878305	1.885172
7	1	0	2.393776	0.831712	2.936292
8	1	0	3.782639	0.757981	1.843443
9	6	0	1.054887	2.678810	1.835888
10	1	0	0.856122	3.646374	1.364612
11	1	0	1.137759	2.844741	2.916449
12	6	0	2.525118	2.319201	-0.104684
13	1	0	3.565884	2.064705	-0.333328
14	1	0	2.368011	3.368228	-0.368051
15	7	0	2.315430	2.165871	1.330782
16	6	0	3.270662	-1.035260	-0.284658
17	1	0	4.091577	-0.319203	-0.173738
18	1	0	3.633109	-2.025897	0.002480
19	6	0	2.567141	0.242643	-2.255559
20	1	0	2.124998	0.104495	-3.246317
21	1	0	3.511220	0.787987	-2.380881
22	6	0	1.903432	-2.130098	-1.962316
23	1	0	2.265678	-3.051745	-1.496972
24	1	0	1.870137	-2.291293	-3.045035
25	6	0	0.830620	2.690625	-2.441629
26	1	0	0.015287	2.302813	-3.063211
27	1	0	1.674124	2.916617	-3.103330
28	6	0	-0.789183	-1.500691	-2.970038
29	1	0	-1.827818	-1.815954	-2.831738
30	1	0	-0.342214	-2.109775	-3.761811
31	6	0	-0.565442	-3.432569	-0.728977
32	1	0	-1.630413	-3.415579	-0.981686
33	1	0	-0.093582	-4.256684	-1.275093
34	6	0	2.028495	-2.044047	2.167989
35	1	0	2.932039	-1.899054	2.773047
36	1	0	1.159265	-1.994480	2.832037
37	6	0	-1.037248	1.027699	3.171639

38	1	0	-1.009776	1.876729	3.867636
39	1	0	-2.072760	0.691549	3.045639
40	6	0	-1.784588	2.770563	0.992506
41	1	0	-2.744857	2.347775	1.310166
42	1	0	-1.637508	3.722237	1.512192
43	7	0	2.845725	-1.063870	-1.665972
44	8	0	-1.757995	3.030211	-0.399516
45	1	0	-1.933751	2.170567	-0.837506
46	8	0	-0.188732	-0.040847	3.619364
47	1	0	-0.320031	-0.157239	4.571182
48	8	0	-0.687065	-0.143870	-3.357291
49	1	0	-1.235608	0.337153	-2.711483
50	8	0	-0.360974	-3.652081	0.647498
51	1	0	-0.990571	-3.121268	1.206329
52	8	0	0.506944	3.859761	-1.737003
53	1	0	-0.358341	3.732508	-1.296496
54	8	0	2.143968	-3.247538	1.466055
55	1	0	1.235459	-3.538067	1.209975
56	8	0	-1.857424	-2.235399	2.403398
57	1	0	-1.215946	-1.659959	2.851988
58	1	0	-2.504331	-1.600098	2.026196
59	8	0	-1.815108	0.358639	-0.871866
60	15	0	-3.151214	-0.177530	-0.297323
61	8	0	-3.307982	-1.646449	-0.968456
62	8	0	-3.356312	-0.219211	1.187251
63	8	0	-4.248434	0.757837	-1.022919
64	1	0	-4.061376	-2.137143	-0.607608
65	1	0	-5.025431	0.918324	-0.468323
66	1	0	-0.607986	-0.953748	0.928250

Co-3'： E(opt)= -3268.3612445 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.126768	-1.633954	1.537595
2	15	0	-2.255643	0.662026	0.831536
3	15	0	-1.317882	-1.241987	-1.338422
4	15	0	0.063588	1.757281	-1.282896
5	6	0	-3.158952	-0.825282	1.547340
6	1	0	-3.048631	-0.794887	2.636403
7	1	0	-4.231986	-0.753647	1.322148
8	6	0	-1.479419	-2.627696	1.736477
9	1	0	-1.287315	-3.635932	1.353056

10	1	0	-1.700248	-2.715146	2.806834
11	6	0	-2.632849	-2.248741	-0.392585
12	1	0	-3.623570	-1.988791	-0.784241
13	1	0	-2.431404	-3.295811	-0.636480
14	7	0	-2.655507	-2.106572	1.057334
15	6	0	-3.333246	1.166640	-0.649526
16	1	0	-4.203798	0.501707	-0.708876
17	1	0	-3.690124	2.179811	-0.442940
18	6	0	-2.345345	-0.148830	-2.481084
19	1	0	-1.774786	-0.027111	-3.407525
20	1	0	-3.278011	-0.674345	-2.727588
21	6	0	-1.609863	2.166447	-2.084996
22	1	0	-1.969787	3.101956	-1.645201
23	1	0	-1.436407	2.344408	-3.153568
24	6	0	-0.638996	-2.583226	-2.472355
25	1	0	0.244801	-2.174651	-2.975537
26	1	0	-1.396247	-2.792001	-3.238150
27	6	0	1.195770	1.497069	-2.757404
28	1	0	2.202453	1.807482	-2.454059
29	1	0	0.867282	2.122871	-3.595266
30	6	0	0.642610	3.408278	-0.605638
31	1	0	1.729480	3.436905	-0.742660
32	1	0	0.197336	4.221096	-1.189930
33	6	0	-2.609805	2.077924	2.006534
34	1	0	-3.667262	2.062156	2.298006
35	1	0	-2.007979	1.923719	2.912914
36	6	0	0.518040	-1.029991	3.266104
37	1	0	0.147870	-1.732318	4.020311
38	1	0	1.611937	-0.974450	3.356024
39	6	0	1.450263	-2.932664	1.231555
40	1	0	2.362474	-2.581160	1.726728
41	1	0	1.147153	-3.882580	1.686046
42	7	0	-2.662038	1.168762	-1.944378
43	8	0	1.676134	-3.160110	-0.146591
44	1	0	2.050087	-2.312999	-0.522934
45	8	0	-0.101806	0.221307	3.513127
46	1	0	0.144316	0.786811	2.754341
47	8	0	1.157350	0.146369	-3.174570
48	1	0	1.655216	-0.343365	-2.479298
49	8	0	0.296671	3.618846	0.756266
50	1	0	0.959673	3.137599	1.303482
51	8	0	-0.395021	-3.774879	-1.768478
52	1	0	0.397877	-3.641341	-1.196226
53	8	0	-2.361828	3.308549	1.364913

54	1	0	-1.393067	3.420099	1.230961
55	8	0	2.465289	2.403613	1.916841
56	1	0	3.071640	2.989859	2.387129
57	1	0	2.876810	2.227639	1.012780
58	8	0	2.443345	-0.796209	-0.962545
59	15	0	3.439250	0.045659	-0.178255
60	8	0	4.893180	-0.570561	-0.537333
61	8	0	3.410964	1.554074	-0.343022
62	8	0	3.316644	-0.290210	1.419340
63	1	0	5.603664	-0.051425	-0.136530
64	1	0	2.910276	0.475154	1.873411
65	1	0	0.650946	0.859168	1.054634
66	27	0	-0.137247	0.025812	0.096208

Co-TS'： E(opt)= -3268.3255374 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.107002	-1.773373	1.480766
2	15	0	-2.022516	0.966329	0.894706
3	15	0	-1.408580	-1.007060	-1.382192
4	15	0	0.371930	1.765414	-1.290779
5	6	0	-3.150968	-0.384408	1.565239
6	1	0	-3.005026	-0.433367	2.648434
7	1	0	-4.196979	-0.105155	1.380614
8	6	0	-1.848265	-2.479648	1.632971
9	1	0	-1.842714	-3.480717	1.188472
10	1	0	-2.082035	-2.589603	2.697994
11	6	0	-2.892515	-1.780547	-0.454992
12	1	0	-3.809995	-1.319746	-0.837517
13	1	0	-2.889746	-2.834104	-0.749125
14	7	0	-2.902668	-1.706761	0.995829
15	6	0	-3.035385	1.644343	-0.571973
16	1	0	-3.988430	1.105137	-0.621563
17	1	0	-3.248403	2.689763	-0.331614
18	6	0	-2.265613	0.271950	-2.471685
19	1	0	-1.682013	0.351088	-3.394052
20	1	0	-3.257473	-0.119392	-2.734542
21	6	0	-1.231743	2.445564	-2.017792
22	1	0	-1.441240	3.399287	-1.523836
23	1	0	-1.060536	2.650291	-3.081882
24	6	0	-0.989764	-2.416415	-2.560362
25	1	0	-0.048453	-2.161029	-3.059048

26	1	0	-1.777994	-2.453346	-3.322629
27	6	0	1.419629	1.325687	-2.781952
28	1	0	2.463260	1.464738	-2.474271
29	1	0	1.186413	2.005911	-3.609356
30	6	0	1.207237	3.290130	-0.597287
31	1	0	2.282483	3.120005	-0.713160
32	1	0	0.912728	4.152946	-1.208848
33	6	0	-2.163617	2.412462	2.082226
34	1	0	-3.210316	2.545074	2.382336
35	1	0	-1.587454	2.171640	2.986794
36	6	0	0.342294	-1.341196	3.242968
37	1	0	-0.001290	-2.135426	3.914143
38	1	0	1.432673	-1.264270	3.288489
39	6	0	1.012953	-3.216324	1.053219
40	1	0	1.963416	-3.022660	1.563015
41	1	0	0.575635	-4.146811	1.433039
42	7	0	-2.405226	1.595907	-1.883474
43	8	0	1.193432	-3.339493	-0.341594
44	1	0	1.599797	-2.462814	-0.647386
45	8	0	-0.302341	-0.137902	3.653823
46	1	0	0.210736	0.594615	3.284058
47	8	0	1.157047	0.001768	-3.192627
48	1	0	1.537745	-0.538641	-2.448328
49	8	0	0.885872	3.540115	0.756619
50	1	0	1.663867	3.191521	1.287130
51	8	0	-0.966069	-3.649195	-1.891089
52	1	0	-0.143875	-3.672620	-1.340688
53	8	0	-1.745546	3.592986	1.441520
54	1	0	-0.770511	3.568563	1.291939
55	8	0	3.017208	2.493936	1.768097
56	1	0	3.780638	3.021010	2.028984
57	1	0	3.326239	1.897419	1.018409
58	8	0	1.973108	-0.946787	-0.880541
59	15	0	3.175686	-0.433370	0.016911
60	8	0	4.431577	-1.431488	-0.302615
61	8	0	3.575157	1.000258	-0.339042
62	8	0	2.764682	-0.638835	1.483326
63	1	0	5.068521	-0.970404	-0.864453
64	1	0	1.474357	0.296789	1.311316
65	1	0	0.873174	0.893289	1.226784
66	27	0	0.015067	0.003163	0.091933

Fe-1'：E(opt)= -3245.6565326 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.800926	2.103561	-1.050270
2	15	0	-2.262661	0.229363	-0.899345
3	15	0	-0.905629	1.051526	1.810214
4	15	0	-0.554005	-2.339566	0.711057
5	6	0	-2.623408	2.084541	-1.024754
6	1	0	-2.484223	2.377470	-2.070000
7	1	0	-3.681873	2.242222	-0.778217
8	6	0	-0.551616	3.405738	-0.728722
9	1	0	-0.128709	4.146563	-0.042314
10	1	0	-0.747910	3.912783	-1.680304
11	6	0	-1.818923	2.628128	1.242109
12	1	0	-2.861780	2.567106	1.575193
13	1	0	-1.337952	3.447297	1.783974
14	7	0	-1.801729	2.931111	-0.178656
15	6	0	-3.477051	-0.380323	0.443484
16	1	0	-4.115952	0.462644	0.731651
17	1	0	-4.098922	-1.128424	-0.055622
18	6	0	-2.265682	-0.032818	2.554238
19	1	0	-1.806316	-0.594860	3.372952
20	1	0	-3.028325	0.626187	2.990290
21	6	0	-2.292403	-2.267476	1.482525
22	1	0	-2.949316	-2.883304	0.860167
23	1	0	-2.226771	-2.744721	2.466547
24	6	0	0.033652	1.720288	3.303199
25	1	0	0.721967	0.934163	3.640659
26	1	0	-0.681494	1.911271	4.111123
27	6	0	0.555947	-2.875855	2.119419
28	1	0	1.428896	-3.389975	1.700980
29	1	0	0.034574	-3.558990	2.796797
30	6	0	-0.589540	-3.720046	-0.552691
31	1	0	0.401899	-4.192737	-0.564434
32	1	0	-1.326018	-4.487971	-0.298140
33	6	0	-3.026014	-0.555506	-2.437284
34	1	0	-3.956150	-0.029533	-2.681075
35	1	0	-2.326669	-0.407868	-3.272546
36	6	0	1.136227	2.215210	-2.876291
37	1	0	1.105483	3.251498	-3.237100
38	1	0	2.132617	1.797448	-3.070186
39	6	0	2.382124	2.752471	-0.274711
40	1	0	3.221221	2.441368	-0.912070
41	1	0	2.381473	3.845352	-0.225460

42	7	0	-2.899685	-0.961367	1.634726
43	8	0	2.531956	2.269003	1.050275
44	1	0	2.567258	1.289154	1.015235
45	8	0	0.108624	1.424403	-3.507992
46	1	0	0.162193	1.549792	-4.466364
47	8	0	0.919369	-1.725406	2.869636
48	1	0	1.530916	-1.213368	2.309883
49	8	0	-0.936523	-3.210987	-1.837073
50	1	0	-0.278439	-2.528021	-2.095536
51	8	0	0.663945	2.935048	2.988436
52	1	0	1.427486	2.757472	2.401421
53	8	0	-3.340266	-1.900014	-2.194716
54	1	0	-2.515358	-2.433036	-2.152373
55	8	0	0.659719	-1.022248	-2.262185
56	1	0	0.388989	-0.305697	-2.872165
57	1	0	1.660764	-1.024965	-2.260331
58	8	0	2.138301	-0.437213	0.567219
59	15	0	3.274376	-1.063126	-0.274983
60	8	0	3.211391	-2.626499	0.136146
61	8	0	3.230308	-0.853127	-1.764408
62	8	0	4.645013	-0.489836	0.348801
63	1	0	3.836087	-3.174049	-0.362001
64	1	0	5.303364	-0.291609	-0.332926
65	26	0	0.170277	-0.132167	-0.139482

Fe-1$_{dp}$'： E(opt)= -3245.2483948 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.591004	1.799084	0.479419
2	15	0	1.438062	0.358509	1.781905
3	15	0	1.481789	1.420619	-1.147569
4	15	0	1.350561	-2.069933	-0.706820
5	6	0	1.341424	2.197642	2.218293
6	1	0	0.629057	2.289578	3.044214
7	1	0	2.325644	2.522195	2.584248
8	6	0	-0.509281	3.285033	0.975765
9	1	0	-0.655251	4.074809	0.231084
10	1	0	-0.909511	3.649747	1.928193
11	6	0	1.687842	2.995088	-0.092166
12	1	0	2.751989	3.115546	0.148083
13	1	0	1.389457	3.818843	-0.747667
14	7	0	0.919510	3.072867	1.134778

15	6	0	3.254608	0.093020	1.246113
16	1	0	3.802672	1.022909	1.444649
17	1	0	3.640005	-0.681766	1.914982
18	6	0	3.230691	0.690852	-1.143572
19	1	0	3.393217	0.246695	-2.130792
20	1	0	3.940155	1.523600	-1.037956
21	6	0	3.189626	-1.684198	-0.474645
22	1	0	3.567330	-2.336253	0.319707
23	1	0	3.722598	-1.943835	-1.397018
24	6	0	1.299247	2.159144	-2.868572
25	1	0	1.073371	1.325676	-3.547392
26	1	0	2.255425	2.602470	-3.173034
27	6	0	1.087733	-2.453007	-2.524288
28	1	0	0.293130	-3.210299	-2.586306
29	1	0	1.993208	-2.862431	-2.985942
30	6	0	1.002398	-3.655240	0.236387
31	1	0	0.442053	-4.330564	-0.423813
32	1	0	1.930091	-4.156425	0.529162
33	6	0	1.392658	-0.610745	3.389467
34	1	0	2.051927	-0.147513	4.132902
35	1	0	0.363576	-0.569498	3.772925
36	6	0	-2.839483	1.792787	1.867695
37	1	0	-3.155279	2.822489	2.083428
38	1	0	-3.716352	1.232579	1.520592
39	6	0	-2.597815	2.326016	-1.015837
40	1	0	-3.584246	1.856901	-0.902318
41	1	0	-2.729256	3.413199	-1.044642
42	7	0	3.511413	-0.308482	-0.126150
43	8	0	-1.993368	1.929009	-2.237216
44	1	0	-1.914481	0.934730	-2.215653
45	8	0	-2.263577	1.225101	3.023297
46	1	0	-2.537512	0.272715	2.989821
47	8	0	0.744439	-1.265564	-3.211319
48	1	0	-0.149409	-1.011742	-2.879616
49	8	0	0.269074	-3.384148	1.425944
50	1	0	-0.545497	-2.900207	1.140760
51	8	0	0.328261	3.172857	-2.864547
52	1	0	-0.556269	2.752107	-2.734918
53	8	0	1.857781	-1.918410	3.153823
54	1	0	1.197771	-2.426185	2.626600
55	8	0	-1.575302	-0.651166	-1.841787
56	15	0	-2.466847	-1.531056	-0.904100
57	8	0	-1.532159	-1.701806	0.388995
58	8	0	-3.843407	-1.052533	-0.559171

59	8	0	-2.492590	-3.013456	-1.595198
60	1	0	-3.383526	-3.383238	-1.532002
61	8	0	-3.186292	-1.226807	2.446797
62	1	0	-2.492924	-1.496099	1.801458
63	1	0	-3.941655	-1.117259	1.847268
64	26	0	-0.170660	-0.216749	-0.009566

Fe-2'：E(opt)= -3245.8261528 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.535958	1.854748	1.206088
2	15	0	2.258227	-0.164329	0.884964
3	15	0	1.068845	1.205686	-1.646877
4	15	0	0.175054	-2.130016	-0.991852
5	6	0	2.876047	1.580238	1.267019
6	1	0	2.763617	1.738492	2.344879
7	1	0	3.947691	1.650493	1.031600
8	6	0	0.917066	3.091872	1.159437
9	1	0	0.577014	3.973396	0.604282
10	1	0	1.116109	3.406597	2.190913
11	6	0	2.171910	2.555622	-0.891598
12	1	0	3.207056	2.417445	-1.228799
13	1	0	1.804755	3.503116	-1.298395
14	7	0	2.165819	2.643437	0.565023
15	6	0	3.395595	-0.750878	-0.528792
16	1	0	4.161471	0.014010	-0.710019
17	1	0	3.888268	-1.649234	-0.145505
18	6	0	2.276438	0.069624	-2.557366
19	1	0	1.750089	-0.296172	-3.445282
20	1	0	3.141030	0.657029	-2.898890
21	6	0	1.909148	-2.261170	-1.783624
22	1	0	2.450965	-3.053453	-1.255447
23	1	0	1.769935	-2.589884	-2.820500
24	6	0	0.245538	2.161156	-3.040024
25	1	0	-0.499936	1.493013	-3.493648
26	1	0	0.990042	2.406872	-3.807196
27	6	0	-0.964283	-2.410041	-2.453049
28	1	0	-1.891147	-2.864833	-2.082662
29	1	0	-0.511260	-3.085921	-3.187161
30	6	0	0.019917	-3.683244	0.044855
31	1	0	-1.039826	-3.973561	0.034762
32	1	0	0.601258	-4.511681	-0.375170

33	6	0	2.935251	-1.222292	2.289192
34	1	0	3.944599	-0.882550	2.553433
35	1	0	2.288165	-1.060922	3.164432
36	6	0	-0.895166	1.781858	3.034163
37	1	0	-0.914640	2.780498	3.494914
38	1	0	-1.872606	1.299031	3.155790
39	6	0	-2.022775	2.845046	0.620140
40	1	0	-2.889080	2.514832	1.210191
41	1	0	-1.879327	3.916973	0.795439
42	7	0	2.751582	-1.073937	-1.789354
43	8	0	-2.251561	2.663648	-0.768758
44	1	0	-2.393013	1.691786	-0.916282
45	8	0	0.160301	0.980269	3.604897
46	1	0	0.003211	0.903316	4.555955
47	8	0	-1.202268	-1.168762	-3.101683
48	1	0	-1.730361	-0.640780	-2.466033
49	8	0	0.482469	-3.470789	1.372814
50	1	0	-0.077401	-2.772935	1.806239
51	8	0	-0.294150	3.371843	-2.563866
52	1	0	-1.046766	3.168117	-1.963379
53	8	0	3.028003	-2.572148	1.903926
54	1	0	2.124565	-2.934998	1.748242
55	8	0	-0.887981	-1.548730	2.651384
56	1	0	-0.350162	-0.778876	2.907744
57	1	0	-1.722219	-1.158647	2.287758
58	8	0	-2.451279	-0.000412	-0.900120
59	15	0	-3.360712	-0.631491	0.143528
60	8	0	-3.322450	-2.231574	-0.180673
61	8	0	-3.103912	-0.383963	1.612974
62	8	0	-4.895038	-0.188599	-0.184128
63	1	0	-3.763338	-2.732644	0.519638
64	1	0	-5.329038	0.087728	0.634809
65	26	0	-0.015714	-0.069005	0.044218

Fe-3_{dp}'： E(opt)= -3245.86679 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.347858	-1.846255	1.139659
2	15	0	-2.149783	0.376091	0.903968
3	15	0	-1.296982	-1.035320	-1.552605
4	15	0	-0.026051	1.964973	-1.003972
5	6	0	-2.992483	-1.265985	1.341520

6	1	0	-2.876886	-1.416205	2.421196
7	1	0	-4.070768	-1.203489	1.125992
8	6	0	-1.203118	-2.960470	1.218380
9	1	0	-0.974087	-3.902809	0.704960
10	1	0	-1.386194	-3.188106	2.276065
11	6	0	-2.463702	-2.342977	-0.807627
12	1	0	-3.497952	-2.148904	-1.126261
13	1	0	-2.152257	-3.308948	-1.219161
14	7	0	-2.441255	-2.432296	0.652757
15	6	0	-3.341856	1.140264	-0.379342
16	1	0	-4.225668	0.495933	-0.490786
17	1	0	-3.666910	2.102534	0.028795
18	6	0	-2.471452	0.146511	-2.449382
19	1	0	-1.996389	0.424217	-3.398316
20	1	0	-3.417700	-0.363060	-2.689576
21	6	0	-1.736733	2.395998	-1.751424
22	1	0	-2.117770	3.275859	-1.218874
23	1	0	-1.583164	2.681957	-2.800992
24	6	0	-0.631275	-2.014690	-3.016181
25	1	0	0.106627	-1.368882	-3.515037
26	1	0	-1.445616	-2.212881	-3.727560
27	6	0	1.122856	2.155106	-2.490964
28	1	0	2.061464	2.601622	-2.136052
29	1	0	0.683870	2.823899	-3.242882
30	6	0	0.389686	3.564198	-0.084522
31	1	0	1.477857	3.701749	-0.153708
32	1	0	-0.084886	4.430710	-0.561870
33	6	0	-2.701822	1.422821	2.379530
34	1	0	-3.749141	1.202188	2.629949
35	1	0	-2.086134	1.129706	3.245215
36	6	0	0.873699	-1.900050	2.949439
37	1	0	0.856375	-2.935595	3.316146
38	1	0	1.907081	-1.531902	2.996009
39	6	0	1.691874	-2.993041	0.470545
40	1	0	2.596071	-2.818925	1.072542
41	1	0	1.404014	-4.044067	0.598675
42	7	0	-2.771503	1.369830	-1.705614
43	8	0	1.969756	-2.797797	-0.909554
44	1	0	2.304277	-1.869061	-1.019908
45	8	0	0.002193	-1.147140	3.784823
46	1	0	0.209072	-0.209549	3.609137
47	8	0	1.348603	0.902891	-3.117025
48	1	0	1.858568	0.372187	-2.466444
49	8	0	-0.035103	3.567596	1.278813

50	1	0	0.437559	2.847035	1.758371
51	8	0	-0.103182	-3.266121	-2.623178
52	1	0	0.672015	-3.103216	-2.035631
53	8	0	-2.632240	2.811658	2.103094
54	1	0	-1.723169	3.049060	1.819800
55	8	0	0.893024	1.324977	2.596660
56	1	0	0.227628	0.927966	1.975533
57	1	0	1.738398	0.934332	2.244892
58	8	0	2.882766	-0.283511	-1.092924
59	15	0	3.539020	0.376051	0.094125
60	8	0	3.543707	1.995151	-0.209636
61	8	0	3.086184	0.176280	1.526264
62	8	0	5.127348	-0.042946	0.047347
63	1	0	3.493393	2.458301	0.637675
64	1	0	5.436611	-0.110628	0.960781
65	26	0	-0.154473	0.006413	0.026015

Fe-2_{pt}': E(opt)= -3246.2187113 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.432904	1.734162	1.363593
2	15	0	1.910610	-0.572359	1.043975
3	15	0	1.503995	1.222181	-1.305583
4	15	0	0.138145	-1.901912	-1.296723
5	6	0	2.675455	0.932741	1.881281
6	1	0	2.332890	0.944365	2.920011
7	1	0	3.763434	0.787685	1.888664
8	6	0	1.096409	2.792414	1.684008
9	1	0	0.959836	3.741999	1.157303
10	1	0	1.154871	3.011807	2.756446
11	6	0	2.625434	2.268450	-0.177878
12	1	0	3.667858	1.977254	-0.349787
13	1	0	2.500518	3.302058	-0.510564
14	7	0	2.351871	2.199822	1.251031
15	6	0	3.264708	-1.147014	-0.166579
16	1	0	4.117161	-0.465600	-0.069577
17	1	0	3.569746	-2.136958	0.182992
18	6	0	2.671533	0.054936	-2.215896
19	1	0	2.253478	-0.110816	-3.213162
20	1	0	3.640939	0.555521	-2.337041
21	6	0	1.906969	-2.278123	-1.842109
22	1	0	2.236381	-3.195404	-1.344141

23	1	0	1.896605	-2.470601	-2.920189
24	6	0	0.958860	2.520390	-2.561274
25	1	0	0.169002	2.083851	-3.183543
26	1	0	1.817947	2.731368	-3.208051
27	6	0	-0.780898	-1.686723	-2.918702
28	1	0	-1.821110	-1.996289	-2.772317
29	1	0	-0.333523	-2.322738	-3.688352
30	6	0	-0.591047	-3.476289	-0.561308
31	1	0	-1.651825	-3.475434	-0.832966
32	1	0	-0.115665	-4.343168	-1.032514
33	6	0	1.979261	-1.939515	2.332617
34	1	0	2.885255	-1.768331	2.926919
35	1	0	1.109913	-1.817314	2.988544
36	6	0	-1.087856	1.312165	3.050737
37	1	0	-1.071179	2.205460	3.689322
38	1	0	-2.122622	0.974779	2.920575
39	6	0	-1.744893	2.931751	0.758225
40	1	0	-2.714155	2.590203	1.141998
41	1	0	-1.552316	3.931916	1.157236
42	7	0	2.875521	-1.230190	-1.556944
43	8	0	-1.754483	3.032256	-0.658167
44	1	0	-1.970953	2.141414	-0.998667
45	8	0	-0.262899	0.269095	3.595907
46	1	0	-0.415338	0.228677	4.550685
47	8	0	-0.681475	-0.341993	-3.361139
48	1	0	-1.251026	0.164937	-2.757260
49	8	0	-0.413395	-3.594795	0.833401
50	1	0	-1.037171	-3.012573	1.342633
51	8	0	0.593995	3.708880	-1.914916
52	1	0	-0.301734	3.599164	-1.531011
53	8	0	2.071269	-3.196576	1.730653
54	1	0	1.164647	-3.473214	1.453264
55	8	0	-1.892567	-2.040600	2.501193
56	1	0	-1.270389	-1.435378	2.937437
57	1	0	-2.552964	-1.433367	2.101968
58	8	0	-1.846031	0.279813	-0.862385
59	15	0	-3.203092	-0.189444	-0.283102
60	8	0	-3.361563	-1.694736	-0.864101
61	8	0	-3.429591	-0.125521	1.196323
62	8	0	-4.267021	0.714323	-1.092178
63	1	0	-4.123456	-2.159737	-0.487273
64	1	0	-5.047788	0.932726	-0.563118
65	1	0	-0.408589	-0.829919	1.150219
66	26	0	-0.027510	-0.016440	-0.022044

Fe-3'：E(opt)= -3246.4323905 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.036894	-1.852466	1.393524
2	15	0	-2.085177	0.617616	0.860961
3	15	0	-1.278051	-1.037144	-1.455880
4	15	0	0.142678	1.933836	-1.073447
5	6	0	-3.085902	-0.859259	1.463127
6	1	0	-2.930376	-0.960433	2.541596
7	1	0	-4.152432	-0.658392	1.295302
8	6	0	-1.591643	-2.809017	1.413747
9	1	0	-1.439414	-3.748860	0.872665
10	1	0	-1.844541	-3.057253	2.451353
11	6	0	-2.680552	-2.061234	-0.649933
12	1	0	-3.643197	-1.680769	-1.010587
13	1	0	-2.554859	-3.079706	-1.026810
14	7	0	-2.718270	-2.111611	0.807153
15	6	0	-3.190764	1.302538	-0.534617
16	1	0	-4.060534	0.645061	-0.644057
17	1	0	-3.541054	2.281803	-0.198036
18	6	0	-2.237258	0.200506	-2.508618
19	1	0	-1.625617	0.413669	-3.390473
20	1	0	-3.169058	-0.271784	-2.848791
21	6	0	-1.498508	2.461698	-1.852106
22	1	0	-1.860019	3.342492	-1.312181
23	1	0	-1.310960	2.758949	-2.890882
24	6	0	-0.674202	-2.301362	-2.718004
25	1	0	0.246473	-1.916763	-3.172007
26	1	0	-1.430076	-2.369225	-3.509757
27	6	0	1.257500	1.731801	-2.574371
28	1	0	2.280577	1.961977	-2.254926
29	1	0	0.961979	2.443473	-3.353067
30	6	0	0.816813	3.543840	-0.376011
31	1	0	1.907340	3.488671	-0.466063
32	1	0	0.461483	4.371903	-1.000428
33	6	0	-2.330230	1.960527	2.149413
34	1	0	-3.358921	1.893449	2.524626
35	1	0	-1.657668	1.765208	2.994296
36	6	0	0.405791	-1.545107	3.199320
37	1	0	0.082425	-2.387709	3.819325
38	1	0	1.494873	-1.435831	3.303166

39	6	0	1.337802	-3.126111	0.938989
40	1	0	2.258434	-2.848139	1.466639
41	1	0	1.027255	-4.119152	1.280860
42	7	0	-2.552698	1.455581	-1.831454
43	8	0	1.559211	-3.196186	-0.460835
44	1	0	1.862159	-2.289535	-0.722445
45	8	0	-0.290639	-0.393081	3.647730
46	1	0	-0.036064	0.308118	3.016642
47	8	0	1.152490	0.426898	-3.115881
48	1	0	1.539144	-0.151517	-2.425278
49	8	0	0.431811	3.812944	0.965595
50	1	0	1.111589	3.401803	1.548886
51	8	0	-0.530994	-3.579578	-2.147853
52	1	0	0.258841	-3.565052	-1.560377
53	8	0	-2.160423	3.235199	1.580052
54	1	0	-1.202605	3.422086	1.441875
55	8	0	2.349135	2.235305	2.131836
56	1	0	1.625755	1.610834	1.877140
57	1	0	2.915738	2.219951	1.325819
58	8	0	2.029960	-0.610401	-0.720893
59	15	0	3.316396	-0.019141	-0.109252
60	8	0	4.482970	-0.885691	-0.813632
61	8	0	3.531959	1.466073	-0.203667
62	8	0	3.415978	-0.501770	1.447994
63	1	0	5.360991	-0.535869	-0.608867
64	1	0	3.238971	0.251373	2.039852
65	1	0	0.573663	0.745327	1.419267
66	26	0	-0.054975	0.024266	0.150694

Fe-TS’：E(opt)= -3246.4100906 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.888134	-1.700786	1.339918
2	15	0	-1.298456	1.554526	1.049791
3	15	0	-1.755479	-0.098769	-1.352616
4	15	0	1.089809	1.569164	-1.159320
5	6	0	-2.894117	0.835469	1.742635
6	1	0	-2.722433	0.585801	2.794171
7	1	0	-3.675125	1.606581	1.703478
8	6	0	-2.763576	-1.607515	1.497218
9	1	0	-3.198748	-2.426340	0.914946
10	1	0	-3.038759	-1.763072	2.547117

11	6	0	-3.416486	-0.228909	-0.412832
12	1	0	-4.023129	0.649663	-0.660626
13	1	0	-3.915167	-1.113260	-0.818374
14	7	0	-3.354892	-0.357084	1.036098
15	6	0	-1.943892	2.840061	-0.203857
16	1	0	-3.039384	2.803072	-0.202750
17	1	0	-1.633806	3.817459	0.175725
18	6	0	-1.969285	1.528329	-2.281226
19	1	0	-1.436715	1.432585	-3.232317
20	1	0	-3.036381	1.661618	-2.505466
21	6	0	-0.046772	2.959723	-1.736395
22	1	0	0.205307	3.860403	-1.167737
23	1	0	0.156720	3.164543	-2.794446
24	6	0	-2.047221	-1.406030	-2.678521
25	1	0	-1.105481	-1.559376	-3.217131
26	1	0	-2.773834	-0.994067	-3.389409
27	6	0	1.780378	0.860243	-2.754722
28	1	0	2.783445	0.482394	-2.521927
29	1	0	1.856818	1.647482	-3.513093
30	6	0	2.581306	2.480012	-0.478988
31	1	0	3.454854	1.879522	-0.754249
32	1	0	2.653936	3.456006	-0.976346
33	6	0	-0.632281	2.694277	2.381021
34	1	0	-1.478768	3.208736	2.852755
35	1	0	-0.150273	2.078276	3.151108
36	6	0	-0.309065	-1.795334	3.116315
37	1	0	-1.014354	-2.386510	3.709870
38	1	0	0.669606	-2.285482	3.117540
39	6	0	-0.526926	-3.427682	0.704512
40	1	0	0.433293	-3.732379	1.138095
41	1	0	-1.301682	-4.127162	1.036336
42	7	0	-1.472456	2.703409	-1.572614
43	8	0	-0.477580	-3.462177	-0.712495
44	1	0	0.230652	-2.806024	-0.961044
45	8	0	-0.252393	-0.499465	3.707503
46	1	0	0.547463	-0.075059	3.365650
47	8	0	0.938131	-0.160227	-3.256867
48	1	0	1.004135	-0.860893	-2.566482
49	8	0	2.542163	2.669259	0.922177
50	1	0	3.138665	1.965493	1.312290
51	8	0	-2.588665	-2.584010	-2.135664
52	1	0	-1.867252	-3.042746	-1.643560
53	8	0	0.213592	3.665650	1.822086
54	1	0	1.086730	3.262264	1.594063

55	8	0	4.215962	0.776265	1.547391
56	1	0	5.142695	1.040525	1.510291
57	1	0	4.086794	0.128921	0.798589
58	8	0	1.181980	-1.432741	-0.905230
59	15	0	2.558994	-1.692794	-0.148994
60	8	0	2.937516	-3.223581	-0.564048
61	8	0	3.670017	-0.750881	-0.583104
62	8	0	2.231972	-1.667185	1.362403
63	1	0	3.809937	-3.238748	-0.978975
64	1	0	1.462166	-0.465942	1.311627
65	1	0	1.083657	0.362172	1.273199
66	26	0	0.000805	-0.005923	0.092955

H_2：E(opt)= -1.1785394 hartree

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	1	0.000000000	0.000000000	-0.000000256
2	1	0.000000000	0.000000000	0.000000256

H_2O：E(opt)= -76.418168 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.118840
2	1	0	0.000000	0.760114	-0.475358
3	1	0	0.000000	-0.760114	-0.475358

H_2PO_4：E(opt)= -643.6373796 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.000079	-0.113027	0.126486
2	8	0	0.000410	0.847508	1.291529
3	8	0	0.000166	-1.600542	0.241927
4	8	0	1.292258	0.343136	-0.838350
5	1	0	1.648265	1.114864	-0.378627
6	8	0	-1.292760	0.342990	-0.837575
7	1	0	-1.647676	1.115819	-0.378906