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脂肪酰胺水解酶催化三联体膦酰化失活的机理：一个模型体系的理论研究

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Phosphonylation and Activity Loss Mechanism of the Catalytic Triad of Fatty Acid Amide Hydrolase: Theoretical Study of a Model System

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RC-A

SCF Done: E(RB+HF-LYP) = -1075.5824659

Sum of electronic and zero-point Energies= -1075.297026

Sum of electronic and thermal Energies= -1075.272247

Sum of electronic and thermal Enthalpies= -1075.271302

Sum of electronic and thermal Free Energies= -1075.356018

1	15	0	-2.095553	-0.430693	-0.194081
2	8	0	1.292133	-2.287304	-0.029314
3	9	0	-2.727070	1.043037	-0.433246
4	1	0	1.900796	-1.514952	-0.049651
5	8	0	2.863698	-0.061140	-0.133992
6	6	0	2.062838	-3.477137	-0.062722
7	1	0	2.639827	-3.572800	-0.992561
8	1	0	2.760088	-3.541157	0.782914
9	1	0	1.375527	-4.323521	-0.003568
10	6	0	3.475432	0.260683	-1.372066
11	1	0	4.088813	-0.589036	-1.679733
12	1	0	2.741757	0.457702	-2.165907
13	1	0	4.131770	1.135696	-1.283508
14	7	0	1.235722	1.986017	0.740620
15	1	0	0.812734	2.510478	-0.024219
16	1	0	2.312718	0.715148	0.167093
17	8	0	-3.117326	-1.475566	-0.035856
18	6	0	-0.954815	-0.554280	-1.572129
19	1	0	-0.448337	0.402212	-1.709268
20	1	0	-0.222200	-1.331798	-1.336540
21	1	0	-1.511143	-0.817484	-2.472824
22	8	0	-1.227981	-0.073801	1.110077
23	6	0	-0.950970	-1.097778	2.108717
24	1	0	-0.633889	-0.561865	3.001407
25	1	0	-1.856398	-1.667671	2.315746
26	1	0	-0.154086	-1.743566	1.738654
27	8	0	-0.735835	2.990607	-1.347181
28	1	0	-0.909333	3.214330	-2.266187
29	1	0	-1.566219	2.626565	-1.014918
30	1	0	0.468635	1.460171	1.154120
31	6	0	1.830111	2.897607	1.729604
32	1	0	2.265193	2.317825	2.546870
33	1	0	2.639499	3.463000	1.262310
34	1	0	1.118024	3.614740	2.157542

TS1-A

SCF Done: E(RB+HF-LYP) = -1075.5484585

Frequencies -- -929.0604

Sum of electronic and zero-point Energies= -1075.266723

Sum of electronic and thermal Energies= -1075.245158

Sum of electronic and thermal Enthalpies= -1075.244214

Sum of electronic and thermal Free Energies= -1075.317335

1	15	0	-1.508875	0.011608	0.288709
2	8	0	-0.719204	1.739787	-0.097269
3	9	0	-1.695369	-1.721314	0.736502
4	1	0	0.498092	1.706618	-0.052067
5	8	0	1.681391	1.621335	0.001780
6	6	0	-1.194335	2.421023	-1.256793
7	1	0	-0.807389	3.443506	-1.244430
8	1	0	-0.862943	1.919313	-2.173038
9	1	0	-2.283678	2.437820	-1.229535
10	6	0	2.257618	2.351504	1.071735
11	1	0	1.699342	3.279017	1.231354
12	1	0	2.249427	1.786736	2.014353
13	1	0	3.293384	2.618207	0.835053
14	7	0	2.302228	-0.731441	-0.532088
15	1	0	1.898662	-1.413540	0.128783
16	1	0	2.053068	0.420606	-0.191058
17	8	0	-2.923840	0.367869	0.023413
18	6	0	-0.710510	0.194642	1.927237
19	1	0	0.234792	-0.347488	1.948625
20	1	0	-0.561619	1.242483	2.167839
21	1	0	-1.384551	-0.270966	2.644836
22	8	0	-0.569560	-0.503077	-0.984093
23	6	0	-1.060127	-1.572089	-1.817975
24	1	0	-0.736770	-2.542011	-1.436428
25	1	0	-2.148522	-1.552845	-1.878328
26	1	0	-0.641989	-1.399819	-2.811906
27	8	0	0.818248	-2.691948	0.960109
28	1	0	0.905336	-3.208588	1.765569
29	1	0	-0.131761	-2.453260	0.900674
30	1	0	1.742738	-0.832432	-1.376722
31	6	0	3.734472	-0.985926	-0.786649
32	1	0	4.111545	-0.255703	-1.503364
33	1	0	4.289034	-0.874709	0.145594
34	1	0	3.900653	-1.991819	-1.177178

INT-A

SCF Done: E(RB+HF-LYP) = -1075.5593955

Sum of electronic and zero-point Energies= -1075.270148

Sum of electronic and thermal Energies= -1075.248327

Sum of electronic and thermal Enthalpies= -1075.247383

Sum of electronic and thermal Free Energies= -1075.320697

1	15	0	1.324961	-0.501910	0.276610
2	8	0	0.262447	-1.772840	-0.293519
3	9	0	1.848584	1.246635	0.999633
4	1	0	-1.406244	-1.530711	-0.062711
5	8	0	-2.343378	-1.233572	0.068817
6	6	0	0.611270	-2.434395	-1.509659
7	1	0	-0.070828	-3.278360	-1.636081
8	1	0	0.513796	-1.758797	-2.366522
9	1	0	1.639482	-2.796811	-1.455312
10	6	0	-3.016129	-2.131085	0.944184
11	1	0	-3.023306	-3.148860	0.539391
12	1	0	-2.559864	-2.152900	1.940888
13	1	0	-4.049995	-1.794648	1.042218
14	7	0	-1.781536	1.389896	-0.403409
15	1	0	-1.425292	1.975021	0.387828
16	1	0	-2.208793	0.504683	-0.051692
17	8	0	2.700338	-1.022897	0.073157
18	6	0	0.468116	-0.566018	1.899607
19	1	0	-0.309428	0.193729	1.968768
20	1	0	0.051129	-1.558039	2.056581
21	1	0	1.223107	-0.337847	2.648278
22	8	0	0.726512	0.466480	-0.983857
23	6	0	1.624455	1.413957	-1.603315
24	1	0	1.536934	2.392954	-1.131952
25	1	0	2.652292	1.065296	-1.514239
26	1	0	1.340319	1.461480	-2.657059
27	8	0	-0.200613	2.749799	1.326359
28	1	0	-0.193923	3.131230	2.207643
29	1	0	0.653803	2.231453	1.236491
30	1	0	-0.898583	1.068274	-0.863002
31	6	0	-2.681073	2.130739	-1.317037
32	1	0	-2.967638	1.483910	-2.145119
33	1	0	-3.574726	2.443016	-0.777715
34	1	0	-2.165448	3.010650	-1.699008

TS2-A

SCF Done: E(RB+HF-LYP) = -1075.5588627

Frequencies -- -119.4538

Sum of electronic and zero-point Energies= -1075.270811

Sum of electronic and thermal Energies= -1075.249625

Sum of electronic and thermal Enthalpies= -1075.248681

Sum of electronic and thermal Free Energies= -1075.321065

1	15	0	1.370268	0.388236	-0.271561
2	8	0	0.553049	1.801451	0.244173
3	9	0	1.549041	-1.682735	-1.031241
4	1	0	-1.203191	1.740233	0.043194
5	8	0	-2.160277	1.538111	-0.064406
6	6	0	1.015388	2.447904	1.435778
7	1	0	0.482444	3.396391	1.519504
8	1	0	0.807963	1.832592	2.316725
9	1	0	2.088796	2.633053	1.367156
10	6	0	-2.751919	2.492956	-0.939394
11	1	0	-2.651000	3.510029	-0.545246
12	1	0	-2.312120	2.458262	-1.942863
13	1	0	-3.815262	2.260209	-1.017330
14	7	0	-1.936315	-1.168897	0.471906
15	1	0	-1.613455	-1.796079	-0.329314
16	1	0	-2.268566	-0.251384	0.116656
17	8	0	2.829793	0.612856	-0.162920
18	6	0	0.524694	0.425455	-1.887496
19	1	0	-0.383894	-0.172836	-1.879147
20	1	0	0.301590	1.462067	-2.137921
21	1	0	1.211929	-0.018930	-2.600869
22	8	0	0.706276	-0.485710	0.988017
23	6	0	1.493569	-1.538146	1.599819
24	1	0	1.246429	-2.497198	1.150016
25	1	0	2.553415	-1.339393	1.451488
26	1	0	1.252188	-1.515721	2.664768
27	8	0	-0.658271	-2.701326	-1.242156
28	1	0	-0.786244	-3.041522	-2.130573
29	1	0	0.316097	-2.327163	-1.189021
30	1	0	-1.042653	-0.938912	0.947994
31	6	0	-2.917184	-1.831563	1.360471
32	1	0	-3.162021	-1.176712	2.196105
33	1	0	-3.823909	-2.054578	0.799073
34	1	0	-2.491573	-2.761744	1.734124

PC-A

SCF Done: E(RB+HF-LYP) = -1075.588624

Sum of electronic and zero-point Energies= -1075.302227

Sum of electronic and thermal Energies= -1075.278708

Sum of electronic and thermal Enthalpies= -1075.277763

Sum of electronic and thermal Free Energies= -1075.358580

1	15	0	1.447887	-0.877302	-0.194532
2	8	0	1.963272	0.637960	0.148553
3	9	0	-1.981794	-2.594795	-1.310706
4	1	0	0.811641	2.088572	-0.295627
5	8	0	0.065067	2.656463	-0.544364
6	6	0	2.925767	0.814745	1.213452
7	1	0	3.264561	1.847664	1.156576
8	1	0	2.450973	0.629745	2.179037
9	1	0	3.766458	0.134755	1.072715
10	6	0	0.537012	3.728366	-1.350766
11	1	0	1.228535	4.380825	-0.803111
12	1	0	1.035370	3.371535	-2.260255
13	1	0	-0.329441	4.321984	-1.645364
14	7	0	-2.026812	1.037630	0.910093
15	1	0	-2.850491	0.088983	-0.232098
16	1	0	-1.534364	1.803945	0.450628
17	8	0	2.510728	-1.906393	-0.222072
18	6	0	0.503267	-0.604042	-1.699529
19	1	0	-0.034698	0.342114	-1.628245
20	1	0	1.185463	-0.583598	-2.550071
21	1	0	-0.214877	-1.418778	-1.814089
22	8	0	0.370153	-1.067206	1.008154
23	6	0	-0.103116	-2.400306	1.344245
24	1	0	-0.821115	-2.732095	0.593690
25	1	0	0.740108	-3.088760	1.406219
26	1	0	-0.583160	-2.312252	2.317732
27	8	0	-3.305623	-0.527447	-0.891541
28	1	0	-3.469780	-0.008293	-1.683934
29	1	0	-2.533198	-1.810337	-1.153263
30	1	0	-1.297040	0.419977	1.261197
31	6	0	-2.866228	1.535402	2.009996
32	1	0	-2.309508	2.094135	2.772704
33	1	0	-3.641736	2.191058	1.607782
34	1	0	-3.367166	0.696082	2.497222

RC-I

SCF Done: E(RB+HF-LYP) = -903.2126328

Sum of electronic and zero-point Energies= -903.017600

Sum of electronic and thermal Energies= -903.000658

Sum of electronic and thermal Enthalpies= -902.999714

Sum of electronic and thermal Free Energies= -903.065985

1	15	0	-1.583577	-0.402739	-0.172411
2	6	0	-0.570408	-0.930470	-1.547316
3	1	0	0.396305	-1.281701	-1.171114
4	1	0	-1.086333	-1.744866	-2.057911
5	1	0	-0.421784	-0.103971	-2.243357
6	8	0	-0.770694	0.869673	0.423141
7	6	0	-1.145415	1.415913	1.717248
8	1	0	-2.038333	2.032669	1.607683
9	1	0	-1.325705	0.606619	2.424246
10	1	0	-0.303905	2.024776	2.040965
11	8	0	2.430581	-1.401656	-0.358734
12	9	0	-2.815405	0.329606	-0.892859
13	1	0	2.486495	-0.447651	-0.174523
14	8	0	2.026209	1.324417	0.141565
15	1	0	1.062016	1.222330	0.139156
16	6	0	2.805483	-2.108472	0.814269
17	1	0	3.840225	-1.892590	1.111137
18	1	0	2.147701	-1.889648	1.665973
19	1	0	2.732230	-3.175052	0.594306
20	6	0	2.384998	2.371872	-0.756236
21	1	0	1.944585	3.329102	-0.454494
22	1	0	3.470497	2.468473	-0.724406
23	1	0	2.085961	2.153853	-1.788519
24	8	0	-2.029296	-1.382529	0.829647

TS-I

SCF Done: E(RB+HF-LYP) = -903.1269801

Frequencies -- -742.8886

Sum of electronic and zero-point Energies= -902.934964

Sum of electronic and thermal Energies= -902.920669

Sum of electronic and thermal Enthalpies= -902.919725

Sum of electronic and thermal Free Energies= -902.975322

1	15	0	0.978077	-0.106974	0.185825
2	6	0	1.118910	-1.085576	1.745605
3	1	0	1.668964	-1.991142	1.487693
4	1	0	1.691671	-0.484710	2.448701
5	1	0	0.158028	-1.341713	2.186072
6	8	0	0.130324	0.888188	-0.872312
7	6	0	0.604764	2.230260	-1.045535
8	1	0	0.421862	2.812224	-0.139948
9	1	0	1.669581	2.230682	-1.286042
10	1	0	0.039810	2.650813	-1.878824
11	8	0	-0.193453	-1.392448	-0.413452
12	9	0	-0.050968	1.067551	1.477261
13	1	0	-1.226876	-0.940859	0.109644
14	8	0	-1.989196	-0.304133	0.776014
15	1	0	-1.334305	0.375532	1.186327
16	6	0	-0.273053	-1.695981	-1.823825
17	1	0	-0.855296	-2.612791	-1.923139
18	1	0	-0.732647	-0.873887	-2.371618
19	1	0	0.737068	-1.860657	-2.198083
20	6	0	-3.001288	0.389178	0.012910
21	1	0	-2.533906	1.009248	-0.752785
22	1	0	-3.645789	-0.362806	-0.440301
23	1	0	-3.587738	1.003260	0.695704
24	8	0	2.379967	-0.022088	-0.307882

PC-I

SCF Done: E(RB+HF-LYP) = -903.2125259

Sum of electronic and zero-point Energies= -903.017430

Sum of electronic and thermal Energies= -903.001201

Sum of electronic and thermal Enthalpies= -903.000257

Sum of electronic and thermal Free Energies= -903.062046

1	15	0	1.249873	-0.208217	-0.068100
2	6	0	0.922491	-1.187130	-1.547146
3	1	0	1.428223	-0.723759	-2.394744
4	1	0	1.333547	-2.188025	-1.403033
5	1	0	-0.149706	-1.265504	-1.729600
6	8	0	0.145652	-0.631869	1.032895
7	6	0	-0.047905	-2.003430	1.437112
8	1	0	-0.696139	-2.498265	0.712961
9	1	0	0.906446	-2.524797	1.542822
10	1	0	-0.542284	-1.969812	2.406454
11	8	0	0.636267	1.258715	-0.455289
12	9	0	-2.233296	-1.511510	-0.942071
13	1	0	-1.250764	1.214991	-0.530742
14	8	0	-2.195124	0.981402	-0.501376
15	1	0	-2.274129	-0.561612	-0.805006
16	6	0	1.295299	2.463222	0.002980
17	1	0	0.979753	3.260144	-0.668249
18	1	0	0.988389	2.689903	1.025899
19	1	0	2.376921	2.336838	-0.034424
20	6	0	-2.695333	1.288600	0.805602
21	1	0	-2.089168	0.814675	1.582330
22	1	0	-2.719522	2.370983	0.965513
23	1	0	-3.714303	0.905601	0.858302
24	8	0	2.654078	-0.171009	0.396316

RC-R

SCF Done: E(RB+HF-LYP) = -903.2114604

Sum of electronic and zero-point Energies= -903.016659

Sum of electronic and thermal Energies= -902.999538

Sum of electronic and thermal Enthalpies= -902.998594

Sum of electronic and thermal Free Energies= -903.064795

1	15	0	1.559973	-0.130470	-0.275349
2	8	0	-2.188700	1.416729	0.261870
3	9	0	0.495971	-1.360488	-0.208486
4	1	0	-2.352565	0.489557	0.016144
5	8	0	-2.390793	-1.316548	-0.399052
6	1	0	-1.456610	-1.479077	-0.575296
7	6	0	-2.148889	2.185913	-0.935834
8	1	0	-3.056487	2.047785	-1.537442
9	1	0	-2.093361	3.238465	-0.648754
10	1	0	-1.272364	1.947954	-1.550001
11	6	0	-2.812094	-2.207539	0.632626
12	1	0	-2.233281	-2.075083	1.553979
13	1	0	-3.858058	-1.982866	0.842174
14	1	0	-2.739045	-3.253204	0.312671
15	8	0	1.206812	0.818704	-1.342641
16	6	0	3.105118	-1.036279	-0.407187
17	1	0	3.223515	-1.711468	0.440082
18	1	0	3.105308	-1.604341	-1.337872
19	1	0	3.928259	-0.321319	-0.423798
20	8	0	1.565849	0.392166	1.223827
21	6	0	0.783410	1.549163	1.652786
22	1	0	0.851828	1.551216	2.738217
23	1	0	1.233096	2.454916	1.245125
24	1	0	-0.254193	1.462945	1.324996

TS-R

SCF Done: E(RB+HF-LYP) = -903.1455843

Frequencies -- -158.4545

Sum of electronic and zero-point Energies= -902.951306

Sum of electronic and thermal Energies= -902.936169

Sum of electronic and thermal Enthalpies= -902.935225

Sum of electronic and thermal Free Energies= -902.994761

1	15	0	-1.174898	0.241739	0.098911
2	8	0	0.492905	1.047979	-0.230734
3	9	0	0.374300	-1.102022	0.694459
4	1	0	1.378512	0.642788	0.096946
5	8	0	2.597695	-0.051266	0.676553
6	1	0	1.894778	-0.722982	0.891585
7	6	0	0.608262	2.411787	-0.711818
8	1	0	1.072278	3.018938	0.065989
9	1	0	1.215455	2.402315	-1.617061
10	1	0	-0.402586	2.749421	-0.921133
11	6	0	3.515234	-0.622114	-0.256619
12	1	0	3.005646	-1.009536	-1.146203
13	1	0	4.215418	0.157844	-0.558861
14	1	0	4.081150	-1.434397	0.209084
15	8	0	-1.960083	1.434598	-0.318208
16	6	0	-1.595035	-0.107881	1.833414
17	1	0	-1.496188	-1.165855	2.055840
18	1	0	-0.898433	0.441392	2.467613
19	1	0	-2.606600	0.266197	1.991080
20	8	0	-1.480109	-0.889748	-0.989575
21	6	0	-1.091875	-2.272871	-1.052781
22	1	0	-1.684318	-2.690899	-1.866541
23	1	0	-0.029159	-2.360757	-1.260278
24	1	0	-1.313961	-2.788393	-0.119318

PC-R

SCF Done: E(RB+HF-LYP) = -903.212655

Sum of electronic and zero-point Energies= -903.017537

Sum of electronic and thermal Energies= -903.001297

Sum of electronic and thermal Enthalpies= -903.000353

Sum of electronic and thermal Free Energies= -903.063116

1	15	0	1.485987	-0.138724	-0.228256
2	8	0	0.340904	1.054744	-0.185378
3	9	0	-2.283240	-1.968586	-0.394502
4	1	0	-1.435687	0.813748	-0.538544
5	8	0	-2.365983	0.539490	-0.642947
6	1	0	-2.391375	-1.024347	-0.531736
7	6	0	0.746512	2.387978	0.213007
8	1	0	-0.028023	3.067388	-0.140190
9	1	0	0.827422	2.447626	1.300378
10	1	0	1.704907	2.635574	-0.241901
11	6	0	-3.180592	1.240560	0.300109
12	1	0	-2.864475	1.054323	1.332256
13	1	0	-3.163023	2.316961	0.104586
14	1	0	-4.201625	0.881209	0.175431
15	8	0	2.846756	0.376561	-0.468902
16	6	0	0.799022	-1.258188	-1.461112
17	1	0	-0.209256	-1.590566	-1.209124
18	1	0	0.788681	-0.752419	-2.427386
19	1	0	1.457101	-2.126302	-1.524835
20	8	0	1.362545	-0.871609	1.198843
21	6	0	0.112951	-1.187066	1.845264
22	1	0	-0.259512	-0.304726	2.371097
23	1	0	-0.640108	-1.542789	1.140041
24	1	0	0.333181	-1.970732	2.567746

RC-B

SCF Done: E(RB+HF-LYP) = -903.2214687

Sum of electronic and zero-point Energies= -903.026138

Sum of electronic and thermal Energies= -903.009463

Sum of electronic and thermal Enthalpies= -903.008519

Sum of electronic and thermal Free Energies= -903.073344

1	15	0	-1.444722	-0.164029	-0.302206
2	6	0	-1.487317	1.286157	-1.342966
3	1	0	-1.792768	0.994688	-2.348587
4	1	0	-2.186087	2.019940	-0.940743
5	1	0	-0.471696	1.690665	-1.357115
6	8	0	-1.261560	0.411598	1.172912
7	6	0	-0.645354	-0.370212	2.227177
8	1	0	-0.537852	0.308642	3.069999
9	1	0	-1.291427	-1.204610	2.505303
10	1	0	0.330136	-0.734565	1.904414
11	8	0	1.680498	1.598359	-0.613652
12	9	0	-2.963497	-0.668199	-0.297964
13	1	0	1.974109	0.682039	-0.452646
14	8	0	2.086732	-1.082137	0.012448
15	6	0	2.170412	2.409250	0.439940
16	1	0	3.267783	2.409193	0.487520
17	1	0	1.843081	3.434110	0.251699
18	1	0	1.783623	2.103974	1.421879
19	6	0	3.048187	-2.037744	-0.419731
20	1	0	3.109998	-2.092047	-1.513175
21	1	0	4.019592	-1.726800	-0.032328
22	1	0	2.824325	-3.037102	-0.029113
23	8	0	-0.536452	-1.273523	-0.679745
24	1	0	1.200173	-1.332985	-0.314560

TS1-B

SCF Done: E(RB+HF-LYP) = -903.1814146

Frequencies -- -1075.7755

Sum of electronic and zero-point Energies= -902.991074

Sum of electronic and thermal Energies= -902.976680

Sum of electronic and thermal Enthalpies= -902.975736

Sum of electronic and thermal Free Energies= -903.032691

1	15	0	0.632375	-0.389186	0.255420
2	6	0	0.824149	-0.184919	2.056303
3	1	0	0.981173	-1.176336	2.480056
4	1	0	1.720161	0.408956	2.246475
5	1	0	-0.044083	0.295535	2.495389
6	8	0	1.372285	0.691861	-0.701053
7	6	0	2.564475	0.418709	-1.462046
8	1	0	2.749633	1.324199	-2.038772
9	1	0	3.409798	0.209216	-0.807019
10	1	0	2.411693	-0.425117	-2.135203
11	8	0	-0.786021	0.979667	0.339875
12	9	0	1.930588	-1.437867	0.226889
13	1	0	-1.773459	0.543378	-0.348676
14	8	0	-2.394992	-0.225764	-0.913618
15	6	0	-0.530574	2.376411	0.360332
16	1	0	-1.474998	2.902548	0.531366
17	1	0	0.151230	2.628443	1.179858
18	1	0	-0.086411	2.719816	-0.577547
19	6	0	-3.558603	-0.626319	-0.182827
20	1	0	-3.321851	-0.830439	0.866446
21	1	0	-4.303816	0.169682	-0.236651
22	1	0	-3.970921	-1.527173	-0.640142
23	8	0	-0.390832	-1.375601	-0.324446
24	1	0	-1.509260	-0.928715	-0.725506

INT1-B

SCF Done: E(RB+HF-LYP) = -903.1990654

Sum of electronic and zero-point Energies= -903.002221

Sum of electronic and thermal Energies= -902.987293

Sum of electronic and thermal Enthalpies= -902.986349

Sum of electronic and thermal Free Energies= -903.044447

1	15	0	0.625233	-0.278728	0.244714
2	6	0	0.855058	-0.077037	2.048343
3	1	0	0.639415	-1.048345	2.495021
4	1	0	1.901051	0.149443	2.256613
5	1	0	0.204524	0.681492	2.475051
6	8	0	1.514147	0.602405	-0.790811
7	6	0	2.777308	0.212701	-1.359883
8	1	0	3.058684	1.033167	-2.019384
9	1	0	3.533228	0.076351	-0.586472
10	1	0	2.676881	-0.709731	-1.930143
11	8	0	-0.617536	0.939289	0.143243
12	9	0	1.814443	-1.476721	0.299495
13	1	0	-2.215109	0.496423	-0.667679
14	8	0	-2.758935	-0.259043	-0.956318
15	6	0	-0.315411	2.322875	0.284632
16	1	0	-1.261620	2.853945	0.411584
17	1	0	0.305803	2.517383	1.167616
18	1	0	0.203799	2.704525	-0.596806
19	6	0	-3.828072	-0.436163	-0.029581
20	1	0	-3.468092	-0.535727	1.001259
21	1	0	-4.538081	0.397119	-0.078448
22	1	0	-4.351744	-1.351362	-0.307106
23	8	0	-0.393887	-1.390831	-0.281077
24	1	0	-1.280826	-1.062096	-0.568643

INT2-B

SCF Done: E(RB+HF-LYP) = -903.1951397

Sum of electronic and zero-point Energies= -902.998693

Sum of electronic and thermal Energies= -902.983210

Sum of electronic and thermal Enthalpies= -902.982265

Sum of electronic and thermal Free Energies= -903.042025

1	15	0	0.544013	-0.178529	0.106307
2	6	0	-0.128973	-1.119629	1.505562
3	1	0	-0.320652	-0.442542	2.334133
4	1	0	-1.078358	-1.541895	1.164701
5	1	0	0.550305	-1.921669	1.781150
6	8	0	1.978516	0.565579	0.212540
7	6	0	3.270492	0.014095	-0.097726
8	1	0	3.980079	0.812017	0.117938
9	1	0	3.483855	-0.856447	0.521356
10	1	0	3.334782	-0.268449	-1.148225
11	8	0	-0.274572	1.190335	0.559790
12	9	0	1.333646	-1.639611	-0.449205
13	6	0	-0.146631	2.433259	-0.132155
14	1	0	-0.846898	3.126299	0.334985
15	1	0	0.869186	2.823554	-0.035939
16	1	0	-0.397923	2.324720	-1.190636
17	8	0	-0.218910	-0.194845	-1.355480
18	1	0	0.120057	-0.934160	-1.876530
19	1	0	-2.213344	-0.535060	-0.926755
20	8	0	-2.935765	-0.933886	-0.425447
21	6	0	-3.704963	0.117621	0.144954
22	1	0	-4.489703	-0.344650	0.746456
23	1	0	-3.100650	0.764318	0.792236
24	1	0	-4.187442	0.738848	-0.621662

TS2-B

SCF Done: E(RB+HF-LYP) = -903.1795929

Frequencies -- -399.8144

Sum of electronic and zero-point Energies= -902.986630

Sum of electronic and thermal Energies= -902.971060

Sum of electronic and thermal Enthalpies= -902.970116

Sum of electronic and thermal Free Energies= -903.031739

1	15	0	0.486598	0.035021	0.228237
2	6	0	-0.000457	-0.914660	1.672502
3	1	0	0.029814	-0.256600	2.540963
4	1	0	-1.027152	-1.242754	1.492027
5	1	0	0.651696	-1.774698	1.778454
6	8	0	1.993562	0.544785	0.195244
7	6	0	3.174623	-0.089827	-0.355976
8	1	0	4.012724	0.471242	0.053512
9	1	0	3.201809	-1.138626	-0.081209
10	1	0	3.155663	0.001119	-1.442322
11	8	0	-0.247737	1.424124	0.578808
12	9	0	1.260178	-1.967247	-0.456000
13	6	0	-0.158686	2.564959	-0.294399
14	1	0	-0.779331	3.339458	0.152025
15	1	0	0.875037	2.909352	-0.358225
16	1	0	-0.532814	2.315721	-1.289298
17	8	0	-0.141508	-0.344563	-1.179000
18	1	0	0.373815	-1.269350	-1.250691
19	1	0	-2.130923	-0.851052	-0.808699
20	8	0	-2.837256	-1.069635	-0.187185
21	6	0	-3.767176	0.004282	-0.172951
22	1	0	-4.563552	-0.266363	0.522261
23	1	0	-3.313757	0.942702	0.172350
24	1	0	-4.219915	0.173559	-1.158695

PC-B

SCF Done: E(RB+HF-LYP) = -903.2143213

Sum of electronic and zero-point Energies= -903.019916

Sum of electronic and thermal Energies= -903.003192

Sum of electronic and thermal Enthalpies= -903.002248

Sum of electronic and thermal Free Energies= -903.067748

1	15	0	-0.441694	-0.364319	0.401343
2	6	0	0.163181	-0.229858	2.079786
3	1	0	-0.180930	-1.073394	2.677609
4	1	0	1.253251	-0.197485	2.039062
5	1	0	-0.209221	0.701647	2.508069
6	8	0	-2.042486	-0.361512	0.519335
7	6	0	-2.922832	0.410524	-0.336930
8	1	0	-3.878723	0.448662	0.181179
9	1	0	-2.530074	1.414476	-0.489458
10	1	0	-3.044935	-0.096431	-1.296032
11	8	0	-0.029404	-1.863931	0.008626
12	9	0	-0.965330	3.003883	-0.644591
13	6	0	-0.262394	-2.380029	-1.316951
14	1	0	0.280650	-3.320537	-1.378295
15	1	0	-1.329299	-2.562915	-1.465082
16	1	0	0.110252	-1.683593	-2.070132
17	8	0	0.076143	0.660644	-0.572167
18	1	0	-0.494185	2.183221	-0.700412
19	1	0	2.007152	0.925885	-0.145331
20	8	0	2.805092	0.735003	0.369141
21	6	0	3.792680	0.216965	-0.507384
22	1	0	4.679232	-0.000447	0.091098
23	1	0	3.475158	-0.714423	-0.996346
24	1	0	4.076494	0.937926	-1.285353