Supporting Information

A Combined Experimental and Computational Study on the Catalytic Dehydration of Glycerol on Microporous Zeolites: An investigation of the Reaction Mechanism and Acrolein Selectivity

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Figure S1. The XRD patterns of the HNa-β-k zeolites.

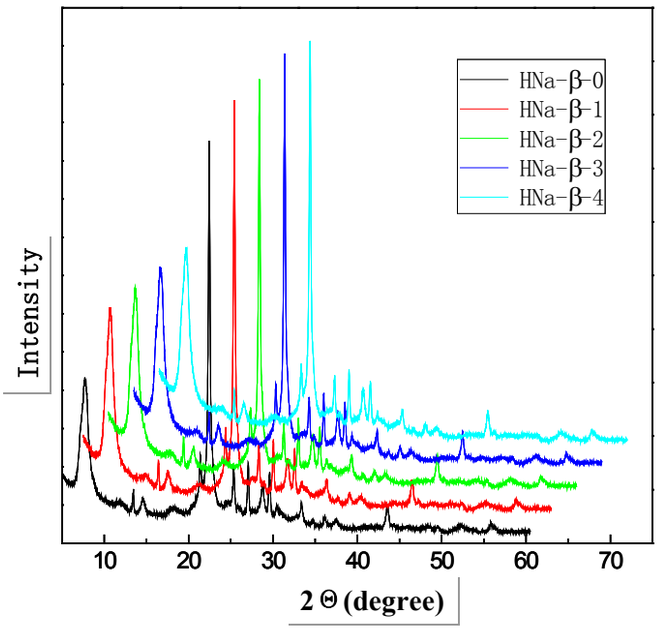


Figure S2. Schematic diagrams presenting the optimized geometries of the reactant complexes, transition states and product complexes of reaction XI with the involvement of additional one (m=1) and two (m=2) water molecules (See Scheme 2 as well). Key distances are indicated in Å. See the geometries for the m=0 case in Figure 5 in the paper. See note under Figure 2.

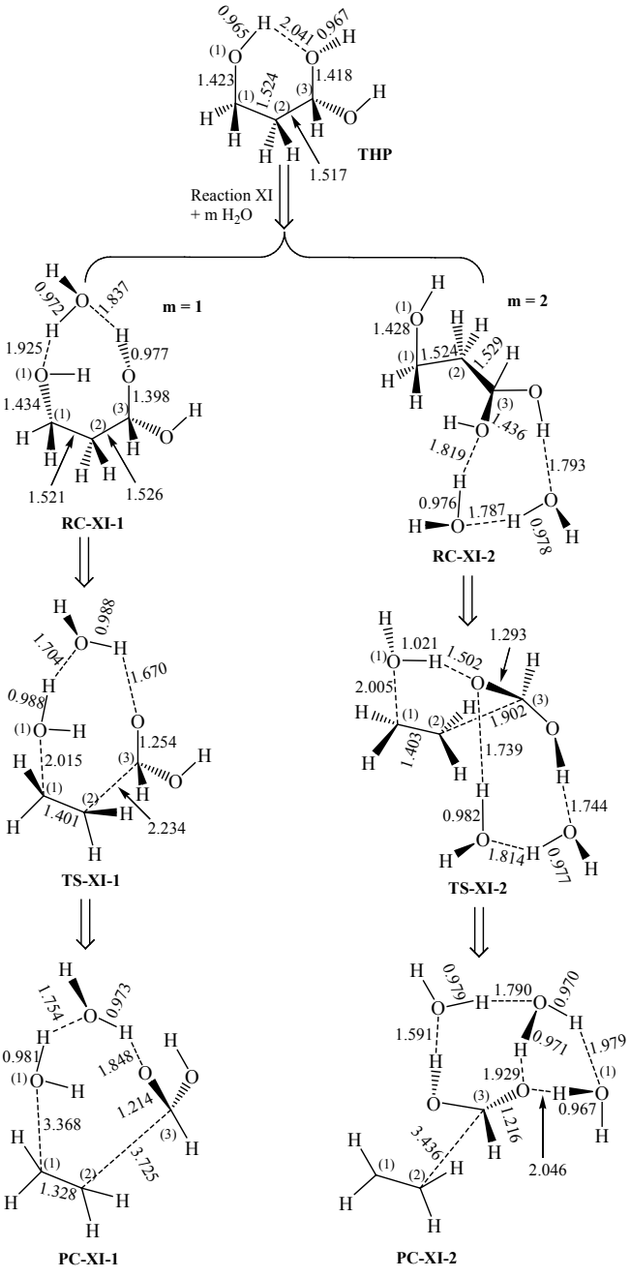
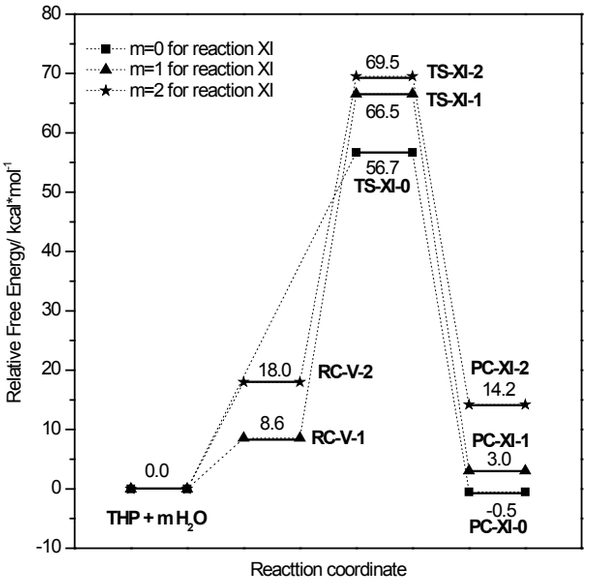


Figure S3. Relative free energy (at 473 K) profiles for the effect of different number of water molecules incorporated into reaction XI.



Temperature programmed reaction study of glycerol

1. Experiment

A typical experiment of temperature programmed reaction (TPRxn) of glycerol on zeolite was carried out as follows. First, 1 g of the as-prepared zeolite was immersed into the 40% glycerol solution for ~ 12h, and then the obtained slurry was filtered with a Buchner funnel, and put into a vacuum oven at 0.1 atm and at 40 ^{o}C for 4h to remove most of the liquid. Then 20 mg of the obtained sample was put into a small ceramic boat, and the ceramic boat was fixed into a reaction chamber. The temperature of the ceramic boat was controlled by a temperature controller. A 30 ml/L He flow was used as the carrier gas to bring possible gas products to the detector. An on-line mass spectroscope (MS, Netzsh, Germany) was used as the product detector, and a few m/z values were set according to the molecular weights of the possible products (such as light alkane, alkene, H_2, etc). In order to remove all air in the reaction chamber and obtain a stable background, He was purged into the reaction chamber at 40 ^{o}C for ~2h until the microbalance under the ceramic boat showed its mass was unchanged. No observable organic compound from the catalyst was found from the MS detector at 40 ^{o}C. The temperature range of 40 – 240 ^{o}C was examined for the TPRxn study with an increasing rate of 5 K/min. The MS signal of the gas product and the temperature of the ceramic boat were recorded simultaneously by the Aeolos32 software (Netzsh, Germany). Only HNa-β-0 and HNa-β-2 were examined in the TPRxn study.

2. Results and the hint to the reaction mechanism

In the catalytic reaction test shown in Section 3.1.2 only liquid products were gathered and analyzed. In the gas-phase dehydration of glycerol which is typically carried out at high temperatures (> 290 ^{o}C) gas phase product such as light alkenes can be observed in a quite low selectivity.[13] However, the gas phase products were not observed, despite of several attempts, by off-line or on-line

GC in this work. This can be due to the fact that the reaction is carried out at a much lower temperature ($\leq$ 200 ^{o}C) and in liquid phase. In Section 3.2 we have proposed a new reaction mechanism for liquid phase glycerol dehydration catalyzed by zeolites as shown in Scheme 2. Obviously it would be helpful if an experimental observation supports the existence of a reaction intermediate contained in Scheme 2. In order to observe possible reaction intermediates as well as minor gas phase products generated in the reaction, temperature-programmed reaction (TPRxn) study of glycerol on HNa-β-0 and HNa-β-2 were performed. The m/z ratios selected for the MS detector were set equal to the molecular weight of C_1-C_3 alkanes, C_2~C_3 alkenes, and H_2 in different experiments. No observable MS signal was found for the case of C_1~C_3 alkane, C_3 alkene and H_2. The only gas phase product detected has the m/z ratio of 28.

Obviously glycerol dehydration is not a redox reaction. However redox reactions as side reactions accompanied with glycerol dehydration are often observed. For example, the production of ethanol in this work, or the production of 1,2-propanediol elsewhere.[1] In the reaction network proposed by Corma et al,[1] the productions of alkenes, diol compounds involve the reduction process of aldehydes or ketones by H_2 or H-donor. However, they did not report the detection of H_2 or H-donor. They suspected that there could be a H_2 or H-donor generation step from glycerol similar to the process of catalytic cracking. In our work where the temperature range studied is much lower than that in Corma's work, it is not surprising that H_2 is not detected, since Brönsted acid site is unlikely a dehydrogenation catalyst in this temperature range. Although both of acetaldehyde and ethanol were found in the product mixture, it seems unlikely that ethanol is produced via the reduction of acetaldehyde by H_2. In Scheme 2 we propose a mechanism for ethanol generation which is favorable on the basis of free energy profile. This mechanism is completely different to the H_2-reduction mechanism, and it is somehow reinforced by the TPRx result.

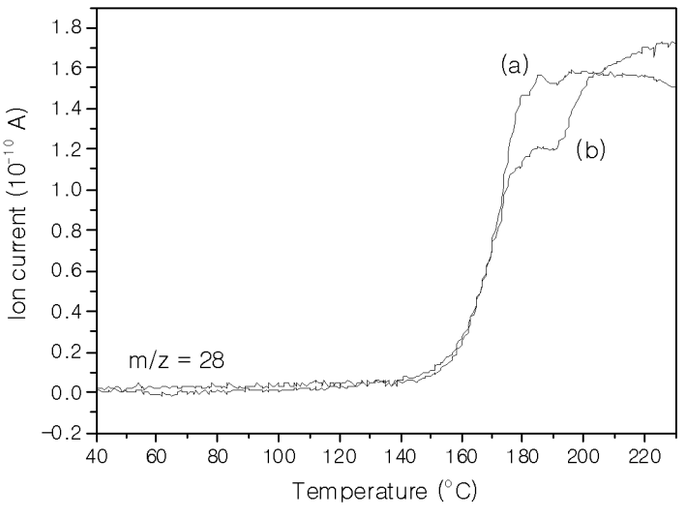


Figure S4. Temperature dependence of the m/z = 28 signal for the temperature programmed reaction of glycerol on 20 mg (a) HNa-β-0 and (b) HNa-β-2. Temperature increasing rate: 5K/min.

Figure S4 presents the temperature dependence of the m/z = 28 signal for the TPRxn of glycerol on the HNa-β-0 and HNa-β-2 catalysts. The signal appears at the temperature higher than 160 ^{o}C. This is consistent with the temperature higher than which observable glycerol conversion can be obtained in the catalytic reaction test. Excluding N_2, this signal can be assigned to either C_2H_4 or CO or their mixture. Obviously a further isotropic labeling study can help one distinguish this product. And from the present experimental and computational results, it is reasonable to imply that the signal should be assigned to C_2H_4 rather than CO, since ethanol has a significant content in the product mixture. In addition, the production of C_2H_4 is consistent with our proposed mechanism.

Reference

1. A. Corma, G. W. Huber, L. Sauvanaud, P. O'Connor, *J. Catal.*, 2008, **257**, 163-171.

Cartesian coordinates, ZPE corrected energy, free energy (473.15 K) for all the optimized structures reported in the manuscript and in the supplementary data

In Figure 2.

12T model

Atomic Number	Coordinates(Angstroms) X	Y	Z
14	2.934865	2.158052	2.452438
1	3.611192	2.859450	3.499289
8	1.699786	0.964746	2.857352
8	2.037874	3.104736	1.276203
8	3.910304	1.202125	1.351331
14	0.760580	0.074730	1.714345
8	-0.423424	-0.124885	3.093177
13	-1.828332	-0.829182	2.194040
8	-2.709450	-2.260865	2.547640
14	-3.407466	-3.064450	1.151724
1	-4.242092	-4.204043	1.368579
8	0.158272	1.298628	0.764206
8	2.045823	-0.628858	0.895554
8	-2.779961	0.304989	1.316223
8	-0.355336	-1.253593	1.124868
8	-4.057820	-1.699855	0.264336
8	-1.921639	-3.258082	0.248649
14	1.105384	2.513893	-0.079664
14	-3.309383	-0.210939	-0.266340
14	-0.770784	-2.136680	-0.397133
14	3.299582	0.248493	0.025707
8	-3.968544	0.988159	-1.246948
8	-1.883602	-0.941447	-0.963168
8	0.455465	-2.746946	-1.352192
8	4.285876	-0.692199	-0.959229
8	2.355649	1.498115	-0.754950
8	0.222322	3.516197	-1.097200
14	1.505124	-3.231067	-2.631661
8	3.095867	-2.850141	-2.133832
14	4.610516	-2.084127	-1.927522
14	-1.136890	4.280568	-1.834967
14	-3.852584	2.310307	-2.353877
8	-2.386767	3.123838	-2.008409
1	1.411448	-4.670130	-2.744436
1	1.137523	-2.552553	-3.853771
1	5.488914	-2.985018	-1.215088
1	5.183646	-1.626276	-3.173480
1	-1.594033	5.371584	-1.002408
1	-0.670094	4.730788	-3.128544
1	-4.989402	3.169874	-2.104230
1	-3.834001	1.786713	-3.701589
1	-0.325565	0.518759	3.801587

ZPE corrected energy = -1064.710003 a.u.
G(473.15K) = -1064.853555 a.u.

In Figure 3.

HPA

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-1.342508	0.213701	-0.128149
6	-0.113394	1.072871	-0.155961
6	1.108598	0.368484	0.411669
8	1.468969	-0.769746	-0.359827
8	-1.341089	-0.944603	0.224236
1	-2.281741	0.691502	-0.455313
1	0.052421	1.368805	-1.198658
1	-0.336085	1.994234	0.392606
1	1.964947	1.042544	0.396474
1	0.918339	0.083925	1.452232
1	0.742898	-1.396557	-0.267967

ZPE corrected energy = -268.242181 a.u.
G(473.15K) = -268.293161 a.u.

H_2O

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	0.000000	0.000000	0.119059
1	0.000000	0.755186	-0.476234
1	0.000000	-0.755186	-0.476234

ZPE corrected energy = -76.402887 a.u.
G(473.15K) = -76.433671 a.u.

RC-VII

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-0.690743	-0.304992	-2.475149
14	-0.742582	1.228013	-1.766567
13	0.188980	-1.603072	-1.436970

8	-0.571318	-1.293498	0.099904
8	-0.044392	-3.300155	-1.818602
8	1.899378	-1.295535	-1.397662
8	0.755346	1.436263	-1.185891
8	-1.082716	2.392471	-2.861450
8	-1.872699	1.273265	-0.598360
1	-1.493127	-0.596308	-3.049080
8	-2.699248	-1.200393	-3.688737
1	-3.433416	-0.589422	-3.830807
6	-3.135925	-2.300133	-2.871890
6	-3.607114	-1.827290	-1.498269
1	-3.925841	-2.838651	-3.395177
1	-2.265828	-2.952877	-2.777087
1	-2.852842	-1.149245	-1.077898
1	-4.566722	-1.312532	-1.556648
6	-3.703430	-2.983775	-0.543259
8	-4.712717	-3.298657	0.039767
1	-2.764103	-3.547305	-0.392956
14	-1.905291	2.647165	0.513252
14	-1.048074	4.058461	-2.238980
14	1.186939	2.866873	-0.250550
14	2.753610	-2.051642	-0.079677
14	0.031641	-2.099263	1.513089
14	0.665019	-4.359876	-0.606463
8	2.740458	2.985838	0.355432
14	4.157656	2.565449	1.254340
8	4.813433	1.177448	0.505680
14	5.565103	-0.307182	0.108370
8	4.350265	-1.533957	0.120181
8	2.285989	-3.700597	-0.440151
8	1.745168	-1.824310	1.326722
8	-0.012818	-3.735665	0.886519
8	-0.200202	2.836341	0.795529
8	0.506495	3.920939	-1.462313
8	-2.023355	3.763050	-0.820262
1	-1.349601	5.142393	-3.116849
1	0.552858	-5.770734	-0.831330
8	-2.883823	2.481273	1.862034
14	-3.600641	1.585710	3.160208
8	-2.516981	0.313991	3.515097
14	-1.394864	-0.761564	4.233962
8	-0.730995	-1.721287	2.967680
1	-0.349519	-0.036046	4.921362
1	-2.093825	-1.679050	5.108628
1	-4.861003	1.036526	2.713424
1	-3.745998	2.508429	4.263791
1	3.809447	2.323897	2.635099
1	5.077608	3.670230	1.088859
1	6.551873	-0.700157	1.091066
1	6.136736	-0.186723	-1.214843

ZPE corrected energy = -1332.961812 a.u.
G(473.15K) = -1333.130335 a.u.

TS-VII

Atomic	Coordinates(Angstroms)		
Number	X	Y	Z
8	-0.510089	0.024277	-2.631982
14	-0.214548	1.474775	-1.795772
13	-0.018729	-1.542059	-1.758561
8	-1.053773	-1.286940	-0.275887
8	-0.452454	-3.142974	-2.273074
8	1.657194	-1.486838	-1.386408
8	1.225575	1.341843	-1.080750
8	-0.245527	2.757331	-2.802110
8	-1.438418	1.612795	-0.728697
1	-1.534794	0.050839	-2.886802
8	-2.947481	0.261403	-2.988238
1	-3.174719	1.023487	-2.436030
6	-3.750280	-0.864655	-2.539986
6	-3.610584	-1.162403	-1.071103
1	-4.778513	-0.631670	-2.827110
1	-3.415165	-1.709521	-3.144319
1	-2.219925	-1.191523	-0.628803
1	-4.084589	-0.433534	-0.412139
6	-3.891834	-2.520027	-0.710654
8	-4.318194	-2.924195	0.372372
1	-3.618520	-3.269011	-1.483501
14	-1.367413	2.886541	0.494157
14	0.006320	4.337017	-2.023718
14	1.786251	2.592829	0.030705
14	2.279386	-2.473648	-0.096671
14	-0.614118	-2.223903	1.174280
14	-0.052200	-4.390689	-1.095318
8	3.265951	2.403883	0.782066
14	4.513062	1.697733	1.751239
8	4.889641	0.208521	1.008392
14	5.351653	-1.373370	0.559782
8	3.889274	-2.264952	0.340251
8	1.598339	-3.976970	-0.674011
8	1.109565	-2.147095	1.160232
8	-0.812977	-3.745264	0.349685
8	0.306833	2.721268	0.929942
8	1.417181	3.834657	-1.135197
8	-1.147314	4.100460	-0.735898
1	-0.003408	5.523317	-2.815877
1	-0.348525	-5.743066	-1.457058
8	-2.497289	2.827151	1.726955
14	-3.533216	2.040917	2.870074
8	-2.811429	0.526770	3.191429
14	-2.105596	-0.878427	3.862571
8	-1.506982	-1.793092	2.525496
1	-1.041650	-0.535717	4.778893
1	-3.119933	-1.712583	4.469648
1	-4.834380	1.843790	2.272869
1	-3.567170	2.893496	4.037250
1	4.043348	1.516429	3.104849
1	5.640948	2.598670	1.658535
1	6.085706	-2.052854	1.604617
1	6.095826	-1.314452	-0.678411

ZPE corrected energy = -1332.932251 a.u.
G(473.15K) = -1333.097864 a.u.

PC-VII

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-0.382455	-1.047684	-2.225060
14	-1.482731	-0.956609	-1.037674
13	1.088432	-0.103846	-1.980589
8	0.698997	1.471686	-1.378972
8	1.924004	-0.976824	-0.492571
8	2.415819	0.027164	-3.092864
1	-1.519901	-1.624979	-3.790774
8	-2.403329	-1.862049	-4.101742
1	-2.820512	-2.204153	-3.300939
1	1.531483	-1.837289	-0.285202
8	0.904897	-3.557694	-0.649086
6	0.635994	-3.652321	-1.816686
1	1.253080	-3.151433	-2.580784
6	-0.517438	-4.399737	-2.322101
1	-1.125673	-4.929830	-1.597130
6	-0.809400	-4.344510	-3.621247
1	-1.676081	-4.842293	-4.037463
1	-0.180910	-3.784568	-4.306644
8	-2.148348	0.541970	-0.921174
8	-2.759963	-2.004060	-1.194582
8	-0.764343	-1.313907	0.404527
14	-1.561339	-1.218110	1.969233
14	-3.154580	1.034520	0.439078
14	-3.994948	-2.007763	0.086051
14	1.835104	2.564503	-0.670201
14	3.252625	-0.087241	0.350812
14	3.800508	0.982958	-2.603568
8	-4.281406	-0.283056	0.213225
8	-2.953360	-2.161995	1.482460
8	-2.289155	0.356265	1.791562
1	-5.110849	-2.890222	-0.050220
8	4.155905	0.142380	-1.098498
8	3.069896	2.411204	-1.901423
8	2.555248	1.474866	0.498080
8	-3.485634	2.678918	0.511195
14	-3.138698	4.350179	0.235115
8	-1.453952	4.554129	0.435016
14	0.146478	5.057295	0.763631
8	1.226217	4.029091	-0.110607
8	-0.691110	-1.600112	3.346758
14	0.568611	-1.685032	4.521894
1	0.313896	-2.880407	5.295002
1	0.550214	-0.493833	5.340733
8	2.045692	-1.820119	3.675693
14	3.661840	-1.905892	3.134100
1	0.375451	6.390922	0.250929
1	0.431470	4.953454	2.177051
1	-3.884986	5.097643	1.223838
1	-3.524154	4.706070	-1.112045
1	4.570752	-1.326831	4.097838
1	4.009929	-3.264412	2.786001
1	4.862487	1.151176	-3.545845
8	3.726327	-0.953036	1.696178

ZPE corrected energy = -1332.993908 a.u.
G(473.15K) = -1333.157268 a.u.

RC-VIII

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-0.816299	0.686441	-2.491775
13	-1.552201	-0.906687	-2.041467
14	0.477483	0.802148	-1.262457
8	-0.150893	0.973142	0.271846
8	0.591762	2.480890	-1.706446
8	2.118341	0.503147	-1.155927
8	0.157630	-1.038530	-1.348595
8	-1.896816	-2.272849	-3.026767
8	-2.633348	-0.806589	-0.699506
1	-1.234952	1.543036	-2.782014
8	-2.248471	2.761790	-3.146602
1	-1.878376	3.620466	-2.899968
6	-3.434184	2.573409	-2.362068
6	-3.128733	2.576701	-0.874735
1	-4.154475	3.356411	-2.607982
1	-3.853102	1.613943	-2.666323
6	-2.547820	3.878212	-0.414473
1	-2.422809	1.783182	-0.597637
1	-4.033762	2.381771	-0.289891
8	-2.326456	4.806963	-1.161629
1	-2.317283	3.961474	0.660818
14	-2.544017	-2.129107	0.438782
14	-1.877254	-3.812045	-2.182157
14	0.487404	-2.559822	-0.440161
14	3.212192	1.305409	-0.033380
14	1.437004	3.732996	-0.795825
14	0.558919	1.896261	1.586961
8	-0.831217	-2.377475	0.663986
8	-0.258408	-3.683088	-1.530092
8	-2.779010	-3.405903	-0.734444
1	-2.240276	-4.984234	-2.914898
8	0.736821	3.439831	0.787727
8	2.225947	1.402049	1.406807
8	2.990882	2.947692	-0.574678
1	1.437171	5.077657	-1.284325
8	4.722170	0.570854	0.100800
14	5.710552	-0.847125	0.057101
8	4.675440	-2.167749	0.392023
14	3.443354	-3.151145	1.058637
8	2.031885	-2.905787	0.098837
8	-3.356254	-1.890220	1.893955
14	-3.700614	-1.030341	3.351411
8	-2.412651	0.066507	3.614851
14	-1.200062	1.051537	4.315700
8	-0.253412	1.731523	3.046574
1	-0.333628	0.273523	5.173851

1	-1.816769	2.159067	5.013626
1	-3.790901	-2.007223	4.414343
1	-4.932825	-0.294566	3.169748
1	6.730195	-0.687328	1.070220
1	6.277750	-1.031020	-1.259719
1	3.172791	-2.829225	2.440472
1	3.863676	-4.523769	0.874310

ZPE corrected energy = -1332.970828 a.u.
G(473.15K) = -1333.133917 a.u.

TS-VIII

Atomic Number	X	Y	Z
8	0.477662	-0.942626	-2.282087
13	1.263825	0.559880	-1.719328
14	-0.727211	-1.498755	-1.319908
8	-0.181231	-1.562224	0.229745
8	-1.240716	-3.013236	-1.720515
8	-2.049731	-0.530977	-1.377074
8	0.005189	1.626680	-1.198856
8	2.469769	1.480102	-2.565819
8	2.178089	0.057369	-0.132876
1	1.089363	-1.980487	-3.223106
8	1.601822	-2.667643	-3.767429
1	1.632183	-3.462786	-3.210983
6	3.202284	-2.066309	-3.811027
6	3.746481	-1.844736	-2.498284
1	3.611680	-2.873447	-4.408024
1	2.961929	-1.192858	-4.409828
6	2.683474	-2.543071	-1.024235
1	3.869405	-0.800102	-2.227275
1	4.614112	-2.454303	-2.259840
8	2.256163	-3.616009	-1.273606
1	2.344264	-0.923638	-0.128470
14	2.646231	1.390737	0.987321
14	3.059910	2.929851	-1.777240
14	0.262255	3.064837	-0.274086
14	-3.392624	-0.708213	-0.248598
14	-2.525411	-3.728966	-0.721314
14	-1.186496	-2.006518	1.603873
8	1.226795	2.358120	1.005337
8	1.584848	3.697801	-1.228300
8	3.532050	2.228770	-0.232841
1	4.024460	3.724704	-2.471574
8	-1.798965	-3.459199	0.844177
8	-2.554675	-0.984984	1.254655
8	-3.647843	-2.383695	-0.677460
1	-3.019346	-5.024443	-1.067449
8	-4.524565	0.530991	-0.275280
14	-5.022003	2.173553	-0.496332
8	-3.756849	3.192726	0.031361
14	-2.659464	4.236759	0.825009
8	-1.089690	3.968052	0.156520
8	3.233633	0.766002	2.419207
14	3.304116	-0.027317	3.949586
8	1.921403	-1.028388	4.024032
14	0.536721	-1.912891	4.495355
8	-0.507767	-2.011286	3.129827
1	-0.198239	-1.242033	5.545038
1	0.937398	-3.252176	4.865150
1	3.301552	0.967052	4.998428
1	4.499421	-0.841195	3.953559
1	-6.209780	2.351386	0.309992
1	-5.265034	2.423065	-1.899201
1	-2.639795	3.988266	2.248524
1	-3.004167	5.605398	0.504536

ZPE corrected energy = -1332.897258 a.u.
G(473.15K) = -1333.064915 a.u.

PC-VIII

Atomic Number	X	Y	Z
8	-0.210418	-0.703663	-2.420081
13	1.371911	-0.177241	-1.834233
14	-1.485614	-0.460358	-1.458898
8	-1.211689	-1.265157	-0.017423
8	-2.930797	-1.016275	-2.028764
8	-1.701270	1.125738	-1.105055
8	1.307848	1.490115	-1.344548
8	2.940891	-0.474107	-2.511329
8	1.444014	-1.097936	-0.142499
1	-0.904500	-1.682459	-3.973441
8	-1.630255	-2.119640	-4.439849
1	-2.358040	-2.047481	-3.809735
6	1.425152	-3.282482	-3.437291
6	2.109379	-3.672119	-2.368191
1	0.544070	-3.813753	-3.780272
1	1.717401	-2.401013	-3.999978
6	-0.895563	-4.101001	-0.965577
1	2.970807	-3.111975	-2.021425
1	1.822086	-4.549013	-1.797041
8	-1.503281	-3.837386	-1.872413
1	0.565502	-1.439628	0.096110
14	2.782330	-0.689276	0.997391
14	4.366978	0.071760	-1.658119
14	2.468829	2.204791	-0.276574
14	-2.830081	1.719824	0.108488
14	-4.384455	-0.808555	-1.023990
14	-2.304938	-1.131619	1.365365
8	2.537061	1.012355	1.004957
8	3.902262	1.674740	-1.130442
8	4.062085	-0.784587	-0.151697
1	5.637267	-0.110643	-2.287382
8	-3.750604	-1.496316	0.452041
8	-2.505435	0.600597	1.402500
8	-4.196222	0.875161	-0.585214

1	-5.632950	-1.271030	-1.541784
8	-2.739187	3.363858	0.429903
14	-2.058715	4.951499	0.361553
8	-0.386682	4.788673	0.674179
14	1.265546	5.002669	1.060090
8	2.156640	3.784225	0.219767
8	2.725052	-1.609706	2.385727
14	2.263459	-2.569936	3.740160
8	0.558570	-2.542315	3.786544
14	-1.108988	-2.588316	4.145879
8	-1.931629	-1.959666	2.768486
1	-1.416285	-1.765613	5.294471
1	-1.563355	-3.951301	4.307524
1	2.831083	-1.970151	4.926939
1	2.745885	-3.913077	3.510795
1	-2.724257	5.714485	1.395127
1	-2.269065	5.521768	-0.950150
1	1.467850	4.856954	2.484127
1	1.761306	6.267234	0.560343

ZPE corrected energy = -1332.990436 a.u.
G(473.15K) = -1333.166043 a.u.

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Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.158288	-0.944323	-0.278324
6	-1.558351	-0.651588	0.246414
8	-2.066161	0.601251	-0.197309
6	0.895579	-0.041645	0.334722
8	2.140531	-0.424141	-0.182311
8	0.645552	1.329991	0.071551
1	0.880847	-0.116709	1.426463
1	-0.135435	-0.822389	-1.366740
1	0.104559	-1.979462	-0.046126
1	-2.251548	-1.410861	-0.116953
1	-1.556077	-0.698176	1.343061
1	-1.393831	1.258033	0.020962
1	2.820128	0.085751	0.272971
1	0.698345	1.452348	-0.885959

ZPE corrected energy = -344.656659 a.u.
G(473.15K) = -344.711595 a.u.

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Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.249224	-0.996583	-0.206902
6	-1.646567	-0.560301	0.231086
8	-1.979107	0.713215	-0.303952
6	0.776214	-0.091065	0.432553
8	2.125128	-0.273258	-0.334029
8	0.666219	1.226480	0.158061
1	0.993387	-0.347383	1.476362
1	-0.170200	-0.898683	-1.293398
1	-0.063561	-2.035542	0.073610
1	-2.387991	-1.273039	-0.132325
1	-1.704142	-0.546874	1.327657
1	-1.171733	1.245980	-0.205886
1	2.870124	-0.406275	0.274426
1	1.853657	0.818011	-0.421517

ZPE corrected energy = -344.592671 a.u.
G(473.15K) = -344.646643 a.u.

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Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.774095	0.247096	1.005712
6	-1.250419	-0.919215	0.155038
8	-0.203435	-1.429078	-0.675105
6	-0.226125	1.375870	0.183439
8	2.261743	-0.358082	0.363088
8	-0.221876	1.383382	-1.026996
1	0.183553	2.232538	0.745082
1	0.011310	-0.058093	1.703831
1	-1.592441	0.646656	1.615005
1	-1.572942	-1.740505	0.793833
1	-2.097583	-0.613529	-0.464353
1	-0.111418	-0.807984	-1.407986
1	2.484288	0.219851	-0.373108
1	1.507601	-0.871207	0.034662

ZPE corrected energy = -344.652178 a.u.
G(473.15K) = -344.712085 a.u.

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Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-1.195735	0.150276	0.262268
6	-0.524705	1.171165	-0.366639
6	1.249363	0.430692	0.319216
8	1.342485	-0.745517	-0.167837
8	-1.025771	-1.093844	-0.084682
1	-1.776733	0.328394	1.167759
1	-0.192862	1.034992	-1.388186
1	-0.661724	2.184217	-0.011971
1	1.759013	1.257612	-0.182591
1	1.123776	0.561986	1.399636
1	0.041276	-1.165101	-0.253564

ZPE corrected energy = -268.183197 a.u.

G(473.15K) = -268.232520 a.u.

PC-v-0

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-1.689094	-0.164872	0.161087
6	-1.498639	1.114903	-0.152475
6	2.098691	0.296260	0.474765
8	1.723539	-0.130246	-0.591639
8	-0.794969	-1.172578	0.025246
1	-2.627743	-0.523018	0.571806
1	-0.562026	1.469621	-0.567725
1	-2.297296	1.826115	0.006079
1	3.102937	0.724814	0.593903
1	1.447331	0.272853	1.361332
1	0.042496	-0.825540	-0.334508

ZPE corrected energy = -268.207923 a.u.
G(473.15K) = -268.265921 a.u.

In Figure 5.

RC-IV-1

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.475021	-0.864245	-0.832772
6	-0.127824	-1.202044	0.587613
8	-0.808805	-0.883124	1.537020
6	-1.711075	0.011830	-0.944570
8	-1.566170	1.224257	-0.198529
8	2.830572	-0.413781	-0.475817
1	0.805687	-1.769390	0.735132
1	0.404467	-0.394769	-1.282288
1	-0.619269	-1.810596	-1.367066
1	-1.874576	0.298193	-1.982658
1	-2.593084	-0.531068	-0.595466
1	-1.705229	0.987842	0.726774
1	2.942738	-0.224829	-1.412085
1	2.282938	0.322200	-0.150983
8	1.161319	1.614608	0.496684
1	1.050160	1.501766	1.446595
1	0.254348	1.611731	0.145562

ZPE corrected energy = -421.064106 a.u.
G(473.15K) = -421.133144 a.u.

TS-IV-1

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.696857	-0.809343	-0.641755
6	0.245852	-0.678397	0.543435
8	0.349593	0.541877	1.061909
6	-2.093786	-0.342924	-0.241460
8	-2.123037	1.052996	0.023925
8	1.638276	-1.101964	-0.067677
1	0.080219	-1.470048	1.284824
1	-0.332026	-0.177736	-1.458945
1	-0.727162	-1.845950	-0.984392
1	-2.798425	-0.535234	-1.051859
1	-2.431783	-0.910462	0.636387
1	-1.323962	1.216102	0.553179
1	2.213082	-1.393532	0.655383
1	2.022302	-0.086829	-0.429392
8	2.078019	1.192953	-0.514260
1	1.262408	1.190896	0.170796
1	1.761279	1.509894	-1.368475

ZPE corrected energy = -421.031707 a.u.
G(473.15K) = -421.090551 a.u.

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Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.615512	-0.554161	-0.845080
6	0.259550	-0.937972	0.334865
8	0.360049	0.098296	1.290812
6	-2.031696	-0.185093	-0.420358
8	-2.089108	1.044691	0.292319
8	1.534452	-1.270717	-0.173970
1	-0.169914	-1.788094	0.872543
1	-0.154891	0.293021	-1.363183
1	-0.651841	-1.400642	-1.535120
1	-2.658409	-0.060846	-1.304201
1	-2.459087	-0.998493	0.180358
1	-1.442839	0.969737	1.005870
1	2.065584	-1.616575	0.553281
1	2.217387	0.616909	-0.668419
8	2.072500	1.532765	-0.389225
1	0.832219	0.830188	0.851432
1	1.724585	1.977874	-1.168613

ZPE corrected energy = -421.069715 a.u.
G(473.15K) = -421.132512 a.u.

RC-IV-2

Atomic Number	Coordinates(Angstroms) X	Y	Z

```
---------------------------------------
  6     0.418742  -1.595421  0.010875
  6     0.368320  -0.708051  1.219883
  8     -0.662289  -0.284933  1.694254
  6     -0.906971  -1.687431  -0.726953
  8     -1.275034  -0.445569  -1.320583
  8     3.104346  0.518953  0.037383
  1     1.337658  -0.464361  1.683212
  1     1.223610  -1.238936  -0.637988
  1     0.732084  -2.585542  0.365480
  1     -0.820506  -2.410766  -1.537618
  1     -1.690996  -2.029682  -0.046158
  1     -1.642130  0.142546  -0.639660
  1     3.432143  0.074230  -0.749641
  1     2.275600  0.936816  -0.257002
  8     0.683118  1.562327  -0.882101
  1     -0.019865  1.926958  -0.322520
  1     0.220482  0.840106  -1.335080
  8     -1.839379  1.768652  0.337329
  1     -2.588660  2.370462  0.284425
  1     -1.826059  1.428152  1.239460
---------------------------------------
ZPE corrected energy = -497.477680 a.u.
G(473.15K) = -497.553430 a.u.
```

TS-IV-2

```
---------------------------------------
Atomic       Coordinates(Angstroms)
Number      X         Y         Z
---------------------------------------
  6     -1.558568  -1.040452  0.149739
  6     -0.176835  -0.413071  0.235929
  8     0.003306  0.643170  -0.540709
  6     -2.619983  0.004314  0.479571
  8     -2.678186  1.013477  -0.519686
  8     0.809145  -1.516381  -0.240410
  1     0.128128  -0.262102  1.285876
  1     -1.711190  -1.399120  -0.872476
  1     -1.635672  -1.887085  0.837565
  1     -3.604543  -0.463403  0.532326
  1     -2.407720  0.446093  1.463102
  1     -1.744560  1.199209  -0.724961
  1     0.743498  -2.295475  0.331781
  1     1.899534  -1.078064  -0.171411
  8     2.983816  -0.515509  -0.039622
  1     2.728745  0.475284  0.141977
  1     3.477596  -0.543182  -0.868336
  8     2.035985  1.765221  0.300491
  1     1.906835  1.999986  1.224795
  1     1.119137  1.383285  -0.052186
---------------------------------------
ZPE corrected energy = -497.453084 a.u.
G(473.15K) =  -497.519422 a.u.
```

PC-IV-2

```
---------------------------------------
Atomic       Coordinates(Angstroms)
Number      X         Y         Z
---------------------------------------
  6     -1.640827  -1.024249  0.170153
  6     -0.211330  -0.522492  0.255659
  8     -0.032167  0.523042  -0.647894
  6     -2.656606  0.069270  0.479341
  8     -2.750073  1.030755  -0.564791
  8     0.710938  -1.554232  -0.108078
  1     0.021378  -0.185327  1.274045
  1     -1.809191  -1.409525  -0.840287
  1     -1.763752  -1.848978  0.877263
  1     -3.648951  -0.368663  0.593353
  1     -2.395241  0.556013  1.428591
  1     -1.837991  1.254366  -0.794013
  1     0.641624  -2.268908  0.537017
  1     2.440029  -0.975953  -0.186095
  8     3.305266  -0.527299  -0.160066
  1     2.671768  1.073037  0.294053
  1     3.585490  -0.478910  -1.079852
  8     2.078332  1.842937  0.409817
  1     1.938708  1.916703  1.359377
  1     0.710328  1.079342  -0.326273
---------------------------------------
ZPE corrected energy = -497.482235 a.u.
G(473.15K) = -497.554637 a.u.
```

RC-V-1

```
---------------------------------------
Atomic       Coordinates(Angstroms)
Number      X         Y         Z
---------------------------------------
  6     -0.865734  0.439026  0.827986
  6     -0.366490  1.419097  -0.188879
  8     0.805730  1.609461  -0.428579
  6     -1.446918  -0.784727  0.105807
  8     -0.519948  -1.346734  -0.805303
  1     -1.137960  1.961096  -0.763118
  1     -0.045550  0.141938  1.483920
  1     -1.656098  0.908235  1.419567
  1     -1.765030  -1.513704  0.858152
  1     -2.324490  -0.492716  -0.474793
  1     1.870002  0.053977  0.144529
  8     1.970585  -0.876674  0.398425
  1     2.737884  -1.191075  -0.090480
  1     0.345157  -1.396546  -0.363602
---------------------------------------
ZPE corrected energy = -344.652191 a.u.
G(473.15K) = -344.711468 a.u.
```

TS-V-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.065515	-0.347178	0.885320
6	0.781706	-1.253159	-0.133361
8	-0.385527	-1.432759	-0.634436
6	1.043498	1.226445	-0.108705
8	-0.103364	1.429826	-0.667630
1	1.579327	-1.769881	-0.663527
1	0.267197	-0.121743	1.584374
1	2.062032	-0.411283	1.305302
1	1.319185	1.829086	0.769655
1	1.907569	1.077374	-0.771281
1	-1.106035	-0.871120	-0.138283
8	-1.920310	0.173132	0.529387
1	-2.788847	0.275618	0.125145
1	-1.311136	0.873707	0.110525

ZPE corrected energy = -344.597383 a.u.
G(473.15K) = -344.652926 a.u.

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Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.508109	-0.507200	0.995175
6	-1.656788	-0.267571	-0.309182
8	-1.042425	0.700566	-1.018490
6	1.244018	-1.474365	0.164122
8	1.662623	-0.644445	-0.608862
1	-2.311994	-0.869223	-0.931715
1	-0.863361	0.108480	1.612050
1	-2.053651	-1.319262	1.455778
1	1.244916	-1.304490	1.250561
1	0.859714	-2.442017	-0.189615
1	-0.412232	1.182072	-0.439334
8	0.911213	1.748247	0.574739
1	1.276489	2.608734	0.344995
1	1.534120	1.095578	0.217494

ZPE corrected energy = -344.618933 a.u.
G(473.15K) = -344.682627 a.u.

RC-V-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.012196	0.241476	0.912616
6	-1.190717	1.333487	-0.093883
8	-0.289468	1.990188	-0.568499
6	-1.535600	-1.073634	0.325538
8	-0.889205	-1.382685	-0.894549
1	-2.228518	1.517374	-0.423588
1	0.041215	0.158156	1.185711
1	-1.598906	0.497629	1.801074
1	-1.403985	-1.871069	1.063737
1	-2.603104	-0.983510	0.111552
1	1.437550	1.422797	-0.154568
8	1.646992	-1.676911	0.090289
1	2.281181	-2.184769	-0.424926
1	0.048791	-1.540433	-0.673801
8	2.281286	0.996104	0.075017
1	1.972664	-0.754764	0.072262
1	2.487350	1.317044	0.958864

ZPE corrected energy = -421.067113 a.u.
G(473.15K) = -421.135139 a.u.

TS-V-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.139646	-0.344039	1.079948
6	-1.789927	0.446503	0.137779
8	-1.199445	1.266736	-0.648639
6	-0.559437	-1.644187	-0.107498
8	0.257848	-1.159096	-0.983722
1	-2.842651	0.285654	-0.088340
1	-0.183628	0.003624	1.457128
1	-1.776062	-0.861809	1.787434
1	-0.145568	-2.262409	0.703977
1	-1.508641	-2.056977	-0.473048
1	-0.205430	1.437787	-0.382310
8	2.299941	-0.531069	0.344153
1	3.122913	-0.679458	-0.130858
1	1.544837	-0.868578	-0.261059
8	1.150561	1.794018	0.004362
1	1.699518	0.979812	0.177080
1	1.157540	2.307976	0.819396

ZPE corrected energy = -421.014707 a.u.
G(473.15K) = -421.078679 a.u.

PC-V-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.340958	-0.063148	1.378481
6	1.992240	-0.076309	0.212209
8	1.552552	-0.610569	-0.942693
6	-0.138757	2.013251	-0.076188
8	-0.754839	1.425721	-0.935978
1	2.970045	0.383151	0.100691
1	0.360709	-0.513737	1.485612
1	1.799981	0.398751	2.241655

1	-0.496398	2.055240	0.962892
1	0.792706	2.549159	-0.306335
1	0.701501	-1.084293	-0.785040
8	-2.382856	-0.172087	0.629532
1	-3.324864	-0.273800	0.461263
1	-2.068059	0.475969	-0.023712
8	-0.677924	-2.028629	-0.432042
1	-1.359157	-1.467615	-0.008932
1	-0.438566	-2.681085	0.234350

ZPE corrected energy = -421.032182 a.u.
G(473.15K) = -421.103720 a.u.

In Figure 6.

THP = PC-IV-0

RC-X

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-1.374363	-1.622602	-0.498265
14	0.264833	-1.800586	-0.855670
13	-1.855549	-0.017703	0.333550
1	-1.991056	-2.375262	-0.845643
8	-2.787559	-3.495742	-1.363383
1	-2.945576	-4.149770	-0.672449
6	-4.034357	-3.168437	-2.015568
6	-4.718222	-1.997433	-1.335396
6	-5.004253	-2.229686	0.140224
8	-5.624078	-1.112807	0.712361
8	-5.864990	-3.335057	0.229924
1	-5.992506	-3.531113	1.164495
1	-4.889026	-0.492128	0.936379
1	-4.071637	-2.439924	0.687516
1	-4.104832	-1.094015	-1.433532
1	-5.670190	-1.795258	-1.833728
1	-3.784509	-2.926885	-3.047026
1	-4.669647	-4.053283	-2.003543
8	-0.621190	0.014000	1.551140
8	-1.657342	1.249591	-0.841273
8	-3.403241	0.280837	1.143994
8	0.722998	-0.426942	-1.592393
8	1.134666	-2.072116	0.489757
8	0.474832	-3.062574	-1.876154
14	2.144289	-3.343023	-2.421911
14	2.900082	-2.044727	0.411439
14	2.390190	-0.154857	-2.096882
14	-0.318034	1.481688	2.426783
14	-1.396198	2.851993	-0.208225
14	-3.429287	1.834348	1.983610
8	-2.870008	2.932750	0.735332
8	-1.968685	1.763449	2.945546
8	3.141144	-0.657701	-0.611475
8	2.470116	-1.700015	-2.904073
8	2.901057	-3.247179	-0.850689
1	2.430201	-4.431431	-3.300028
1	-4.641213	2.182143	2.663822
8	-0.928992	4.016832	-1.334989
14	-0.113634	4.597950	-2.738237
8	1.263639	3.611829	-2.977901
8	-0.284276	2.637462	1.119887
14	2.825717	2.969914	-3.233754
8	2.758384	1.286893	-2.855466
8	3.717868	-2.072246	1.870697
14	3.986436	-1.687633	3.535409
8	3.060506	-0.292487	3.871410
14	2.504339	1.287869	4.223644
8	0.920755	1.453931	3.567361
1	3.178347	3.047146	-4.634177
1	3.797309	3.628013	-2.388866
1	-0.998420	4.481202	-3.877006
1	0.271631	5.966346	-2.470276
1	3.395226	2.283325	3.668680
1	2.352135	1.428185	5.656204
1	5.402640	-1.440870	3.685309
1	3.522087	-2.784919	4.354526

ZPE corrected energy = -1409.385400 a.u.
G(473.15K) = -1409.559453 a.u.

TS-X

Atomic Number	Coordinates(Angstroms) X	Y	Z
14	-0.681088	-1.323968	-1.710440
8	0.607362	-0.577610	-2.366070
13	1.148880	0.895719	-1.522105
1	1.825401	-2.084416	-1.929526
8	2.050651	-2.704972	-1.204283
1	1.507026	-2.389719	-0.441476
6	3.664702	-2.569897	-0.949114
6	4.075990	-1.185814	-0.922744
6	4.604805	-0.670524	-2.228378
1	3.964618	-3.181261	-1.798837
1	3.745733	-3.119661	-0.017686
1	4.739825	-0.955120	-0.088759
8	4.851053	0.721893	-2.220848
1	3.995569	1.187829	-2.164404
1	3.900209	-0.906618	-3.043329
8	5.848470	-1.287411	-2.524976
1	6.127217	-0.974794	-3.393201
1	2.881584	-0.337675	-0.345402
8	2.040131	0.298272	0.002334
8	-0.265866	1.744167	-1.000655
8	2.322821	2.081765	-2.085242
8	-2.062548	-0.452483	-1.666794
8	-0.232265	-1.708010	-0.145910

8	-1.057260	-2.769066	-2.410895
14	-2.342738	-3.755167	-1.677845
14	-1.324919	-2.439158	1.032142
14	-3.477367	-0.940328	-0.734215
14	-0.314991	3.011873	0.171694
14	2.585598	3.458147	-1.015847
14	2.134097	1.428551	1.392716
8	0.602000	2.215002	1.431972
8	0.980294	3.955530	-0.530432
8	3.010191	2.604414	0.462870
1	3.487311	4.468989	-1.477211
8	-2.730482	-1.447451	0.755914
8	-3.563855	-2.515265	-1.487750
8	-1.774137	-3.758763	-0.024820
1	-2.693991	-4.988330	-2.308015
8	2.636699	0.674730	2.799773
14	2.761548	-0.511939	4.045703
8	1.426852	-1.566344	3.870453
14	0.000244	-2.476308	4.120753
8	-0.745867	-2.680758	2.581413
8	-4.737689	0.161131	-0.638860
14	-5.453385	1.734975	-0.647593
8	-4.372497	2.810012	0.122512
14	-3.409298	3.728655	1.196466
8	-1.794496	3.693210	0.588718
1	-3.840786	5.108185	1.122716
1	-3.461106	3.202718	2.541543
1	-6.695652	1.614661	0.083494
1	-5.648684	2.186875	-2.006747
1	2.735601	0.193190	5.307728
1	3.980695	-1.264441	3.849419
1	-0.922090	-1.802790	5.007393
1	0.358797	-3.795155	4.594195

ZPE corrected energy = -1409.328062 a.u.
G(473.15K) = -1409.496042 a.u.

PC-X

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	0.421728	-0.415806	-2.442004
14	-0.873920	-1.184730	-1.856853
13	1.095229	0.874268	-1.453590
8	2.291677	-2.382123	-0.936373
1	2.430167	-1.942812	-1.789764
1	1.377749	-2.697360	-0.933685
6	5.372235	-1.363003	0.078543
6	5.180967	-0.502092	-0.911554
6	4.865529	-0.920851	-2.317842
8	5.836884	-0.337539	-3.152991
8	3.572256	-0.514115	-2.709544
1	5.315488	-2.433625	-0.091074
1	5.579984	-1.028149	1.088235
1	4.874111	-2.010627	-2.409902
1	5.649176	-0.619155	-4.055590
1	5.230387	0.572588	-0.746934
1	3.463438	0.437233	-2.498832
8	1.776756	0.022254	0.113291
1	1.960853	-0.926604	-0.043054
8	2.479302	1.870678	-1.884885
8	-0.147020	1.923940	-0.867288
8	-0.464137	-1.832677	-0.382210
8	-2.153313	-0.178023	-1.630101
8	-1.440060	-2.450814	-2.751294
14	-2.823371	-3.372360	-2.119958
14	-3.602953	-0.624620	-0.736564
14	-1.612302	-2.596833	0.712470
14	0.001346	3.096235	0.391993
14	2.132724	1.053961	1.549895
14	2.963268	3.114187	-0.740936
8	3.197782	2.087454	0.670659
8	1.456688	3.842433	-0.227226
8	0.753609	2.075562	1.601055
8	2.487635	0.091290	2.865948
8	-1.040788	-3.111923	2.197622
14	-0.254930	-3.204169	3.727488
8	1.066603	-2.119765	3.692462
14	2.474798	-1.203758	4.006136
8	-1.382383	3.934918	0.851639
14	-2.996232	4.082572	1.450871
14	-5.248793	2.240078	-0.308543
8	-4.706250	0.604916	-0.443607
8	-4.009890	3.154296	0.432938
8	-3.896111	-2.051103	-1.706108
8	-2.235975	-3.690093	-0.503638
8	-2.905374	-1.427005	0.644618
1	-3.329230	-4.452320	-2.907342
1	-5.498628	2.792322	-1.621235
1	-6.440346	2.198093	0.510794
1	-3.347279	5.480121	1.318681
1	-3.065617	3.619496	2.818410
1	0.221560	-4.560867	3.880815
1	-1.199588	-2.824457	4.754632
1	3.652354	-2.015887	3.796047
1	2.430328	-0.605242	5.321446
1	4.032890	3.985513	-1.117571

ZPE corrected energy = -1409.414109 a.u.
G(473.15K) = -1409.590217 a.u.

RC-IX

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-0.854835	0.889129	-2.334014
14	0.459261	0.978312	-1.124248
13	-1.440020	-0.804074	-2.041497
1	-1.302740	1.736026	-2.614454
8	-1.683210	3.294625	-2.872230
1	-0.905847	3.448057	-2.296248
6	-2.848850	3.922585	-2.319050

6	-3.866631	2.875735	-1.903432
6	-3.463269	2.125812	-0.645823
8	-3.638554	3.012693	0.440569
1	-3.185546	2.635090	1.202678
1	-2.407842	1.833326	-0.687192
8	-4.259967	0.984320	-0.493596
1	-3.665344	0.210583	-0.385974
1	-3.268517	4.577569	-3.083722
1	-2.563263	4.532781	-1.459174
1	-4.838629	3.343534	-1.721972
1	-3.985737	2.154278	-2.715836
8	0.301438	-0.858403	-1.429657
8	-2.447407	-0.966373	-0.628354
8	-1.734981	-2.075486	-3.152346
8	0.404755	2.736801	-1.329694
8	-0.133488	0.905347	0.425215
8	2.116772	0.847652	-1.112128
14	1.170753	3.919042	-0.259241
14	3.177056	1.578862	0.090787
14	0.538057	1.688890	1.847055
14	0.823481	-2.439950	-0.738807
14	-2.177921	-2.413033	0.326278
14	-1.517732	-3.697192	-2.516613
8	2.791482	3.252848	-0.199160
8	0.548527	3.339425	1.274870
1	1.038890	5.313627	-0.548447
8	2.230926	1.377615	1.545549
8	0.116114	-3.484099	-1.928090
8	-0.442127	-2.518943	0.436930
8	-2.368174	-3.544036	-0.992480
1	-1.812746	-4.802807	-3.372097
8	2.420009	-2.694354	-0.315060
14	3.895523	-2.943634	0.541868
8	4.997723	-1.750612	0.004046
14	5.883954	-0.297262	-0.162342
8	4.752290	0.987045	0.077290
14	-3.289012	-1.874444	3.413104
8	-2.126705	-0.670738	3.771773
14	-0.971392	0.342613	4.524452
8	-0.198818	1.268304	3.293698
1	-1.640072	1.291412	5.388604
1	0.020260	-0.440295	5.228335
1	6.433726	-0.230730	-1.497378
1	6.906681	-0.170277	0.852003
1	3.666722	-2.867298	1.965891
1	4.432949	-4.223179	0.130734
1	-4.611141	-1.287908	3.407369
1	-3.183340	-2.995803	4.320574
8	-2.944778	-2.450348	1.822306

ZPE corrected energy = -1409.392320 a.u.
G(473.15K) = -1409.557888 a.u.

TS-IX

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	-0.867507	0.859782	-2.151577
14	-0.045446	1.771458	-1.092042
13	-0.818298	-0.885612	-1.829599
1	-2.305210	2.045175	-3.136124
8	-2.849841	2.833755	-2.976284
1	-2.614514	3.087939	-2.063760
6	-4.880555	2.475666	-2.708016
6	-5.147064	1.592985	-1.644350
6	-3.654025	1.148208	-0.810571
8	-3.185717	2.424796	-0.383225
1	-2.570471	2.232416	0.339737
1	-3.078662	0.808839	-1.676818
8	-3.849979	0.301824	0.122171
1	-2.603158	-0.674739	-0.034683
1	-4.891842	2.133273	-3.733329
1	-4.957979	3.545074	-2.565923
1	-5.665780	2.046605	-0.805234
1	-5.507371	0.614502	-1.942319
8	0.813989	-1.279061	-1.390731
8	-1.830153	-1.274509	-0.265722
8	-1.402981	-2.109405	-2.922613
8	-0.330251	3.399662	-1.183504
8	-0.495451	1.330460	0.443626
8	1.582936	1.600018	-1.233566
14	0.477863	4.449157	0.004181
14	2.724373	2.213758	-0.040516
14	0.268229	1.920611	1.917021
14	1.380127	-2.801738	-0.805533
14	-1.476158	-2.849279	0.543916
14	-1.131741	-3.783541	-2.479296
8	2.118845	3.851130	-0.147829
8	0.068118	3.605081	1.480518
1	0.241215	5.856767	-0.076750
8	1.940708	1.773311	1.451636
8	0.545054	-3.799771	-1.975617
8	0.236446	-2.974060	0.509472
8	-1.852576	-3.762328	-0.872802
1	-1.577803	-4.788279	-3.394215
8	3.021826	-2.952270	-0.469350
14	4.526486	-2.519921	0.259016
8	4.947741	-0.975922	-0.341382
14	5.549064	0.586456	-0.676505
8	4.316642	1.719505	-0.238439
14	-2.779308	-2.268565	3.561050
8	-1.745828	-0.962354	3.940560
14	-0.635171	0.148874	4.612746
8	-0.273488	1.294793	3.373788
1	-1.264801	0.905843	5.672994
1	0.565508	-0.526878	5.049721
1	5.818165	0.701640	-2.091989
1	6.703422	0.911286	0.132170
1	4.404194	-2.505909	1.698761
1	5.490916	-3.496222	-0.201839
1	-4.137660	-1.793882	3.422981
1	-2.650519	-3.343657	4.519305
8	-2.244330	-2.865662	2.030020

ZPE corrected energy = -1409.326107 a.u.

G(473.15K) = -1409.497438 a.u.

PC-XI

Atomic Number	Coordinates(Angstroms) X	Y	Z
8	0.502163	-0.730795	-2.305807
14	-0.614769	-1.415294	-1.351760
13	1.132316	0.834481	-1.780631
1	0.973978	-2.062657	-3.679431
8	0.915665	-2.985739	-3.965254
1	0.212584	-3.335993	-3.400312
6	3.379698	-0.814027	-3.928239
6	4.076039	-0.816728	-2.796910
6	2.450205	-3.025382	-0.857597
8	2.543199	-4.324996	-0.640610
1	3.000009	-4.476330	0.202648
1	1.923650	-2.819458	-1.794351
8	2.908927	-2.185926	-0.120967
1	2.296586	-0.518292	-0.077936
1	2.829842	0.066609	-4.245051
1	3.329343	-1.688718	-4.567797
1	4.629154	-1.691618	-2.472499
1	4.114074	0.060789	-2.158551
8	-0.230573	1.763903	-1.230000
8	2.089213	0.427845	-0.174627
8	2.222733	1.933409	-2.573702
8	-0.965900	-2.981671	-1.787420
8	-0.035065	-1.499076	0.190712
8	-2.052791	-0.624442	-1.325582
14	-2.126561	-3.888971	-0.790401
14	-3.331861	-1.018132	-0.178819
14	-0.939265	-2.120351	1.565232
14	-0.149472	3.194571	-0.265395
14	2.419688	1.793945	0.959918
14	2.634382	3.431729	-1.766622
8	-3.405128	-2.695893	-0.666128
8	-1.406857	-3.612042	0.778793
1	-2.468706	-5.219405	-1.184577
8	-2.428231	-1.252843	1.292847
8	1.082674	4.012296	-1.200825
8	0.895674	2.584982	1.002050
8	3.196198	2.757418	-0.240018
1	3.497805	4.344671	-2.448505
8	-1.600416	3.910384	0.197137
14	-3.157287	3.980209	0.939950
8	-4.148574	2.802987	0.193127
14	-5.317606	1.642781	-0.261478
8	-4.608725	0.070741	-0.123682
14	3.364102	0.288984	3.802708
8	2.026505	-0.762523	3.955680
14	0.673725	-1.665616	4.480377
8	-0.206101	-2.108242	3.067533
1	1.126577	-2.890841	5.101415
1	-0.186650	-0.891023	5.346603
1	-5.695689	1.884037	-1.635901
1	-6.454866	1.653343	0.632355
1	-3.038694	3.740195	2.360165
1	-3.691899	5.291706	0.640959
1	4.567291	-0.488070	3.605253
1	3.461926	1.200082	4.920768
8	3.086268	1.224671	2.380177

ZPE corrected energy = -1409.413358 a.u.
G(473.15K) = -1409.594954 a.u.

TS-XI-0

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	-0.441754	1.380992	-0.204140
6	-1.576721	0.604797	0.074832
8	-1.132575	-1.358071	0.158239
6	1.091078	0.277344	-0.268173
8	0.895399	-0.672306	-1.089661
8	1.253450	-0.136368	1.052483
1	1.788006	1.079666	-0.538396
1	-0.131760	2.057852	0.585859
1	-0.386645	1.787670	-1.208463
1	-1.975282	0.561531	1.080427
1	-2.276822	0.355817	-0.710806
1	-0.758358	-1.439993	1.044400
1	1.473585	0.626690	1.600040
1	-0.298532	-1.274078	-0.436667

ZPE corrected energy = -344.566035 a.u.
G(473.15K) = -344.621254 a.u.

PC-XI-0

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	2.547650	-0.728442	-0.362355
6	2.259264	0.505043	0.043589
8	-0.744731	2.092142	-0.105146
6	-1.173480	-0.758917	-0.259606
8	-2.371927	-0.792415	-0.303411
8	-0.517304	-0.794804	0.899569
1	-0.527936	-0.705246	-1.145151
1	3.205162	-1.374846	0.209040
1	2.138395	-1.130745	-1.283791
1	2.670859	0.908284	0.963129
1	1.596541	1.150156	-0.524445
1	-0.548073	1.714934	0.758639
1	0.439609	-0.739518	0.733786
1	-1.703469	2.031496	-0.169072

ZPE corrected energy = -344.642477 a.u.

G(473.15K) = -344.712351 a.u.

In Figure S2.

RC-XI-1

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	1.169783	0.924462	-0.526706
6	-0.262077	1.436078	-0.555804
6	1.294417	-0.532537	-0.090638
8	0.498221	-1.411967	-0.830914
8	0.946327	-0.576790	1.286660
8	-0.909529	1.370915	0.722322
8	-2.172791	-1.006052	-0.050202
1	2.323615	-0.875392	-0.223643
1	1.776697	1.536892	0.145695
1	1.587384	1.015645	-1.531950
1	-0.274177	2.477308	-0.881587
1	-0.844602	0.854250	-1.278152
1	-0.389855	0.773206	1.279492
1	0.984578	-1.494526	1.580140
1	-2.065260	-0.117692	0.328242
1	-0.440512	-1.259978	-0.605199
1	-2.768423	-0.886573	-0.797076

ZPE corrected energy = -421.070982 a.u.
G(473.15K) = -421.132389 a.u.

TS-XI-1

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	1.088088	0.945621	-0.936372
6	0.033361	1.767379	-0.517307
6	1.180876	-0.813397	-0.182480
8	0.254363	-1.568221	-0.562907
8	1.252171	-0.522276	1.207378
8	-0.941575	1.059937	1.097699
8	-2.266864	-0.809578	-0.272416
1	2.192843	-0.966933	-0.574498
1	2.079781	1.297839	-0.671501
1	0.986248	0.550031	-1.941342
1	0.229118	2.650131	0.075872
1	-0.899225	1.774030	-1.068107
1	-0.207614	0.525875	1.452413
1	0.875951	-1.299815	1.643741
1	-1.557950	0.406617	0.687152
1	-1.364398	-1.180856	-0.427450
1	-2.533464	-0.433432	-1.117359

ZPE corrected energy = -420.975881 a.u.
G(473.15K) = -421.040001 a.u.

PC-XI-1

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	1.569849	-1.154062	-0.762642
6	2.731712	-0.652558	-0.360003
6	-2.089591	-0.549751	-0.416793
8	-1.663704	0.422024	-1.007488
8	-1.640543	-1.015042	0.718486
8	0.313094	0.325423	1.770753
8	0.530999	2.019641	-0.327613
1	-2.922646	-1.147506	-0.802469
1	1.404489	-2.223916	-0.836078
1	0.741928	-0.507830	-1.036257
1	3.565651	-1.290559	-0.087541
1	2.885201	0.419595	-0.289890
1	1.081969	-0.254366	1.711381
1	-0.878835	-0.459260	1.090311
1	0.504403	1.043723	1.130010
1	-0.277748	1.593484	-0.660924
1	0.304997	2.948500	-0.215011

ZPE corrected energy = -421.067695 a.u.
G(473.15K) = -421.141197 a.u.

RC-XI-2

Atomic Number	Coordinates(Angstroms) X	Y	Z
6	0.649406	-0.351894	-0.971110
6	1.701053	0.734955	-0.782903
8	2.766766	0.305307	0.064793
6	0.326564	-1.073611	0.337918
8	-0.840089	-1.816854	0.260818
8	0.196121	-0.138340	1.419414
8	-1.315815	1.936111	0.371217
8	-2.743366	-0.097669	-0.782723
1	1.129854	-1.766863	0.596430
1	0.993185	-1.103077	-1.688046
1	-0.261324	0.099908	-1.376588
1	2.085170	1.068288	-1.750838
1	1.257236	1.596164	-0.281784
1	-1.739804	2.503238	1.022896
1	1.089013	0.163605	1.635575
1	3.180515	-0.462822	-0.343855
1	-1.542550	-1.255540	-0.126112
1	-3.588607	-0.225889	-0.340156
1	-2.379742	0.727221	-0.403615
1	-0.794023	1.290624	0.884506

```
---------------------------------------
ZPE corrected energy = -497.480591 a.u.
G(473.15K) = -497.551036 a.u.
```

TS-XI-2

```
---------------------------------------
Atomic       Coordinates(Angstroms)
Number      X         Y         Z
---------------------------------------
  6     -0.731576  -0.478420  1.279104
  6     -1.873332  0.322995  1.126040
  8     -2.430216  0.440049  -0.796953
  6     -0.109143  -1.168526  -0.379880
  8     1.058896  -1.767908  -0.028903
  8     -0.068620  -0.199743  -1.234993
  8     0.808675  2.013351  0.050571
  8     2.895372  0.224794  0.256734
  1     -0.885727  -1.929044  -0.502737
  1     -0.876084  -1.418872  1.799433
  1     0.176029  0.061237  1.531014
  1     -2.852434  -0.053155  1.394780
  1     -1.775071  1.400158  1.107393
  1     0.915937  2.777347  -0.524526
  1     -1.506938  0.231051  -1.179411
  1     -2.965017  -0.347993  -0.951526
  1     1.760134  -1.076314  0.014827
  1     3.420837  0.322656  -0.544144
  1     2.296535  0.996940  0.255668
  1     0.463252  1.295368  -0.524007
---------------------------------------
ZPE corrected energy = -497.398269 a.u.
G(473.15K) = -497.468947 a.u.
```

PC-XI-2

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---------------------------------------
Atomic       Coordinates(Angstroms)
Number      X         Y         Z
---------------------------------------
  6     -1.685091  2.135292  0.085498
  6     -0.374634  1.980096  -0.054202
  8     2.693476  0.817687  -0.399469
  6     -0.561954  -1.105420  -1.554892
  8     -1.626861  -1.098431  -0.801937
  8     0.586203  -1.045435  -1.157442
  8     1.521811  -0.853643  1.508566
  8     -1.187614  -0.685213  1.726497
  1     -0.809361  -1.175312  -2.619226
  1     -2.207771  2.980684  -0.349536
  1     -2.275666  1.416180  0.642597
  1     0.226417  2.693250  -0.609894
  1     0.147425  1.132447  0.377192
  1     2.043869  -0.081416  1.239761
  1     2.040701  0.380890  -0.963609
  1     2.566885  1.757460  -0.562419
  1     -1.403142  -0.972549  0.176830
  1     -1.527968  -1.397681  2.278415
  1     -0.220431  -0.667227  1.876634
  1     1.252994  -1.206252  0.645101
---------------------------------------
ZPE corrected energy = -497.478868 a.u.
G(473.15K) = -497.557051 a.u.
```