

Supporting information

The First Dehydration and the Competing Reaction Pathways of Glucose Homogeneously and Heterogeneously Catalyzed by Acids

Xufeng Lin^{1,2,3*}, Yuanyuan Qu^{2,4}, Yanhong Lu^{2,4}, Yanyan Xi^{1,4},

David L. Phillips⁵, Chenguang Liu^{1,2,4}

¹State Key Laboratory of Heavy Oil Processing, ²Key Laboratory of Catalysis of China National Petroleum Corporation, ³Chemistry Department, ⁴College of Chemical Engineering, China University of Petroleum (East China), Qingdao, P. R. China, 266555

⁵Department of Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong, P. R. China

Table of Contents:

Figure 1S.....	Page S2
Table 1S.....	Page S3
Figure 2S.....	Page S4
Figure 3S.....	Page S5
Figure 4S.....	Page S6
Figure 5S.....	Page S7
Figure 6S.....	Page S8

Figure 7S.....	Page S9
Figure 8S.....	Page S10
Figure 9S.....	Page S11
Figure 10S.....	Page S12
Figure 11S.....	Page S13
Figure 12S.....	Page S14
Full citation of Ref. 50	Page S15

Cartesian coordinates, ZPE corrected energy, enthalpy (298K), free energy (298K) for all the optimized structures reported in the manuscript and in the supporting information.....Page S16-S51.

Figure 1S. The model reaction for the benchmark work for selection of appropriate computational level of theory:
dehydration of protonated isopropanol.

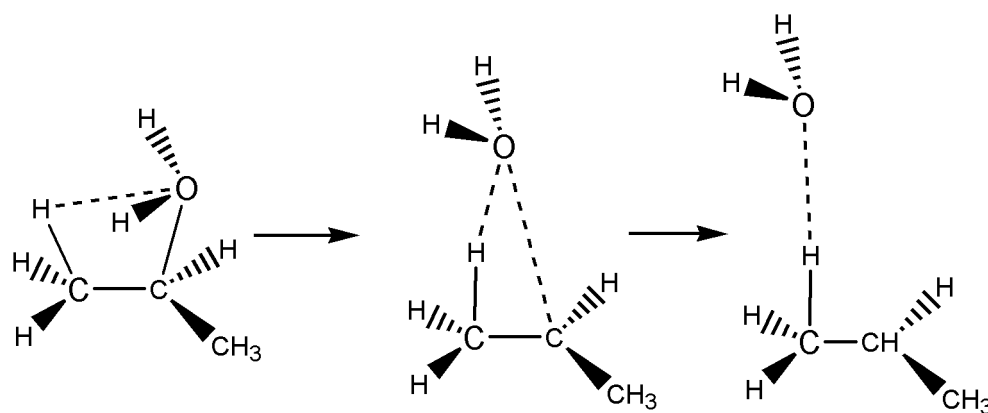


Table 1S.

Calculated reaction energy barrier for the model reaction indicated in Figure 1S with different levels of theory.

Level of theory (with gas-phase model)	Energy barrier (in kcal/mol)	Level of theory (in aqueous solution)	Energy barrier (in kcal/mol)
B3LYP/6-31G(d)	10.7		
B3LYP/6-311G(d,p)	7.7		
B3LYP/6-31+G(d,p)	6.3		
B3LYP/6-311++G(d,p)	5.4		
B3LYP/aug-cc-pvdz	6.5		
B3LYP/aug-cc-pvtz	6.0		
BLYP/6-31G(d)	8.7		
BLYP/6-311G(d,p)	6.0		
BLYP/6-31+G(d,p)	4.2		
BLYP/6-311++G(d,p)	3.4		
BLYP/aug-cc-pvdz	4.6		
BLYP/aug-cc-pvtz	3.9		
MP2/6-31G(d)	15.2		
MP2/6-311G(d,p)	13.8		
MP2/6-31+G(d,p)	11.1		
MP2/6-311++G(d,p)	11.3		
MP2/aug-cc-pvdz	11.4		
MP2/aug-cc-pvtz ^a	11.7		
B3LYP/6-31+G(d,p)	6.3	B3LYP/6-31+G(d,p)	13.4
MP2/6-31+G(d,p)	11.1	MP2/6-31+G(d,p)	19.2
BLYP/6-31+G(d,p)	4.2	BLYP/6-31+G(d,p)	10.8
M06/6-31+G(d,p)	6.9	M06/6-31+G(d,p)	14.1
M06-2X/6-31+G(d,p)	12.0	M06-2X/6-31+G(d,p)	20.3
CCSD/6-31+G(d,p)	11.9		
CCSD(T)/6-31+G(d,p)// CCSD/6-31+G(d,p) ^b	11.9		
CCSD(T)/aug-cc-pvtz// CCSD/6-31+G(d,p) ^c	12.0		

^aThe ZPE energy of MP2/aug-cc-pvdz is used.

^{b, c}The CCSD(T) single-point energy was calculated based on the geometry obtained from the CCSD method.

Figure 2S. The energy profiles for the approaching of H(A) atom in the hydrated proton to different hydroxyl groups in β -glucopyranose, presented in panels (a) for O(1) site, (b) for O(2) site, and (c) for O(5) site. The O(1)...H(A) distance was fixed while other part were allow the relax to locate the energy minimum. Computational method: PCM/BONDI//M062X/6-31+G**.

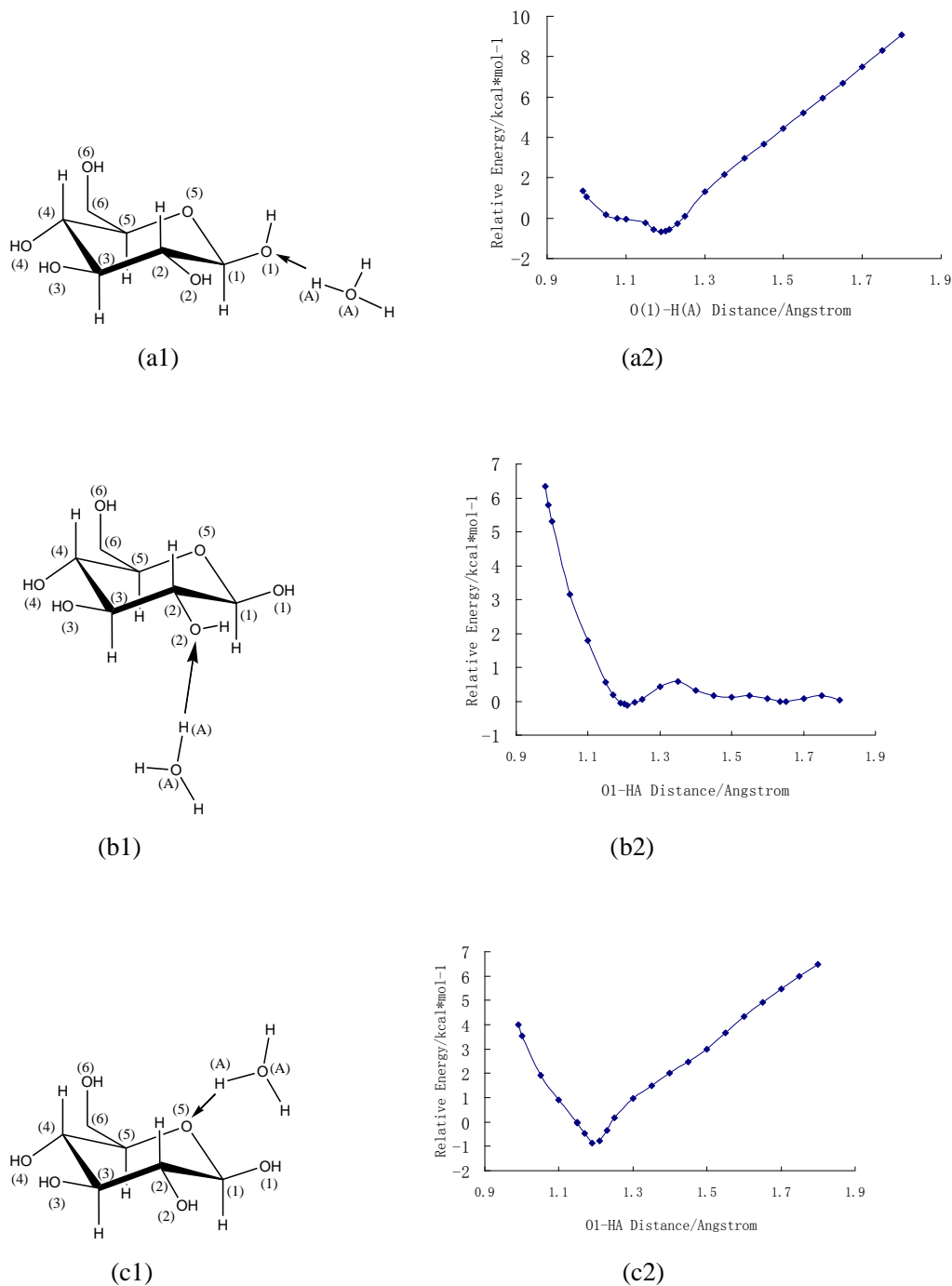


Figure 3S. Simple scheme for the optimized geometries for the species involved in the five dehydration reaction pathways of protonated β -glucopyranose, with 1 water molecule incorporated into the reaction systems. Key distances are indicated in Å. The line between atoms only represents connection here and in Figures 4S ~6S, not bonding order. See Scheme 2a for the $n = 1,2,3,4,6$ cases, and text for the notation of **RC-n-BP-kW**, **TS-n-BP-kW**, **PC-n-BP-kW** as well.

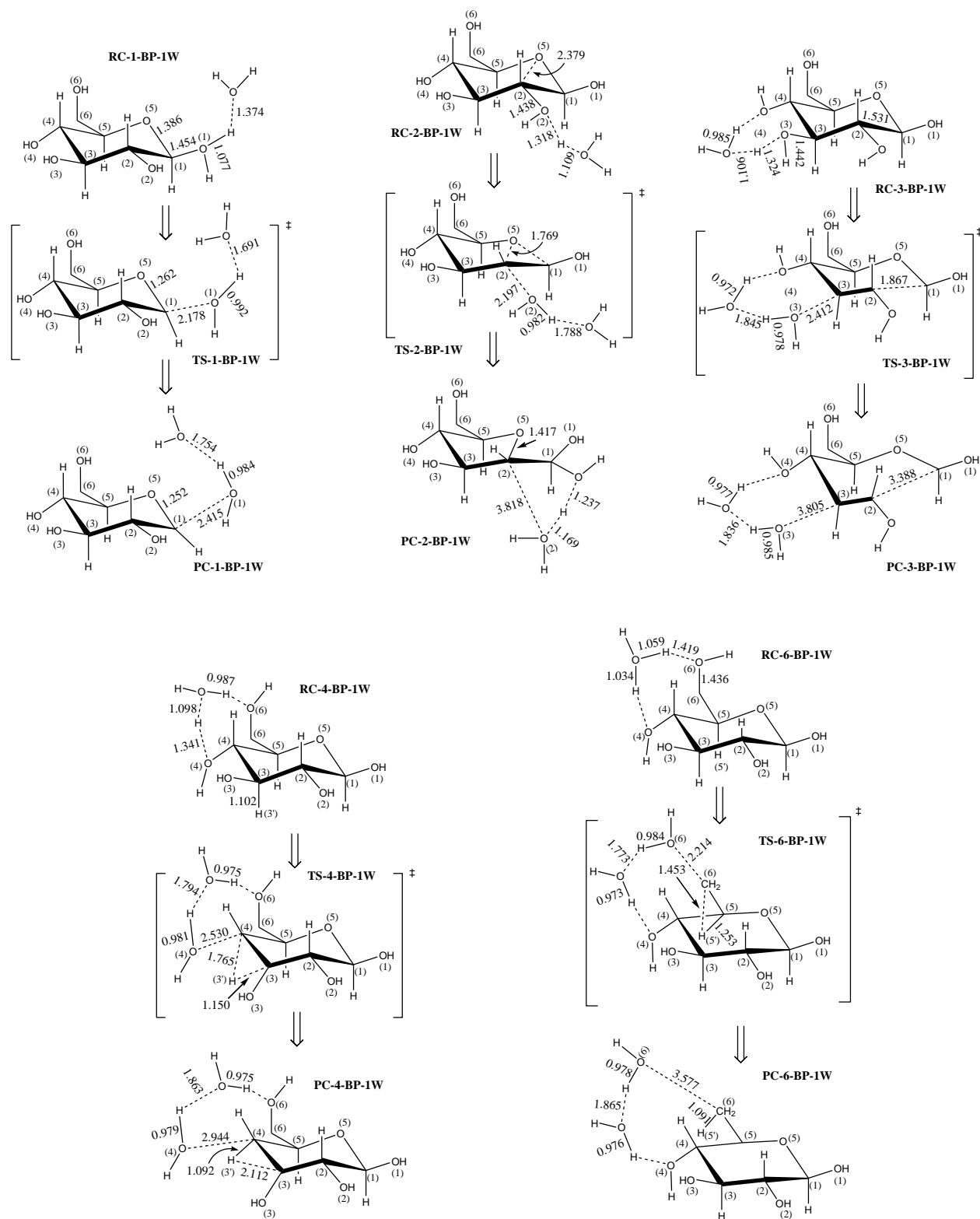


Figure 4S. Simple scheme for the optimized geometries for the species involved in the two isomerization reaction pathways of protonated β -glucopyranose, with 1 water molecule incorporated into the reaction systems. Key distances are indicated in Å. See Scheme 2a for the $n = 5-1$ and $5-2$ cases, and text for the notation of **RC-n-BP-kW**, **TS-n-BP-kW**, **PC-n-BP-kW** as well.

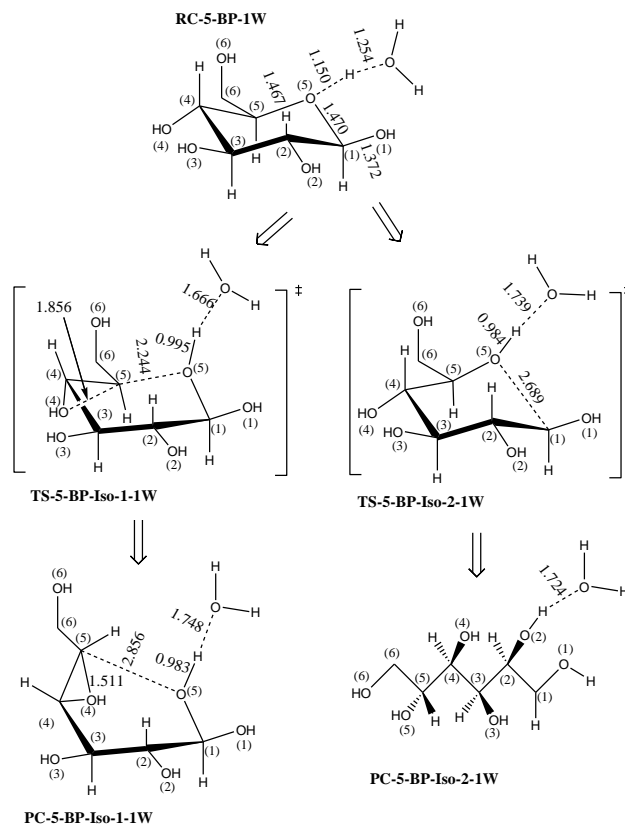


Figure 5S. Simple scheme for the optimized geometries for the species involved in the five dehydration reaction pathways of protonated β -glucopyranose, with 2 water molecules incorporated into the reaction systems. Key distances are indicated in Å. See Scheme 2a for the $n = 1, 2, 3, 4, 6$ cases, and text for the notation of **RC-n-BP-kW**, **TS-n-BP-kW**, **PC-n-BP-kW** as well.

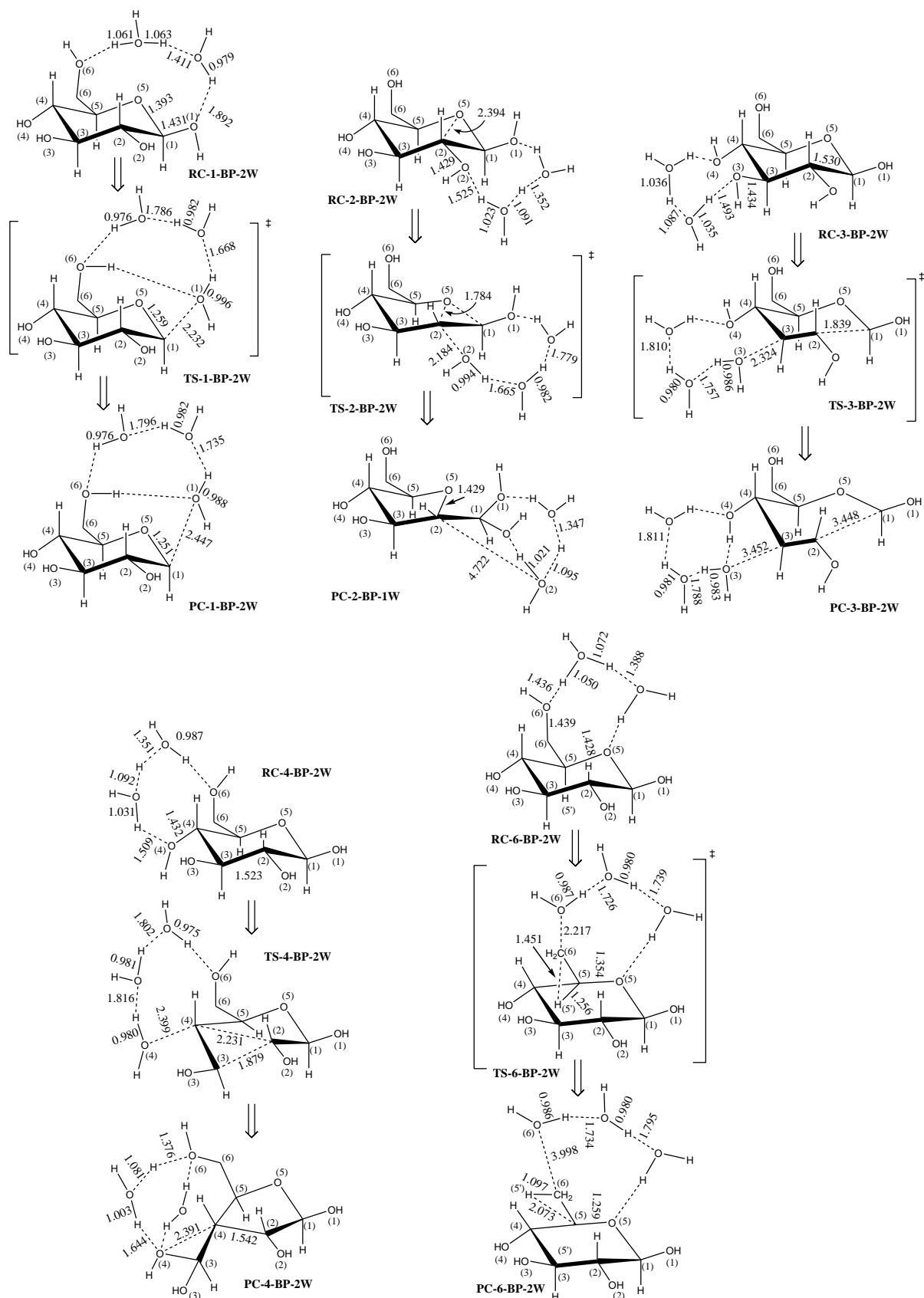


Figure 6S. Simple scheme for the optimized geometries for the species involved in the two isomerization reaction pathways of protonated β -glucopyranose, with 2 water molecules incorporated into the reaction systems. Key distances are indicated in Å. See Scheme 2a for the $n = 5-1$ and $5-2$ cases, and text for the notation of **RC-n-BP-kW**, **TS-n-BP-kW**, **PC-n-BP-kW** as well.

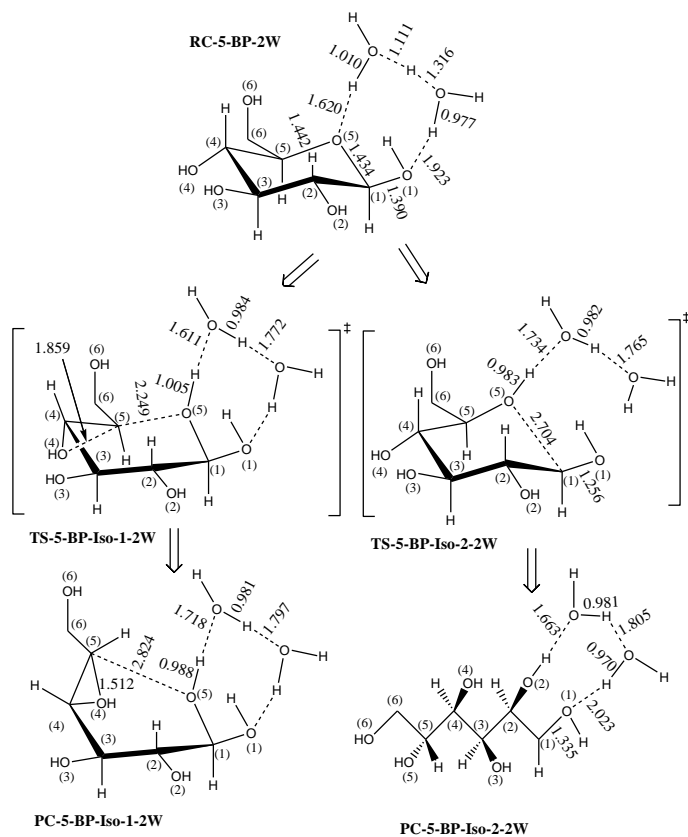
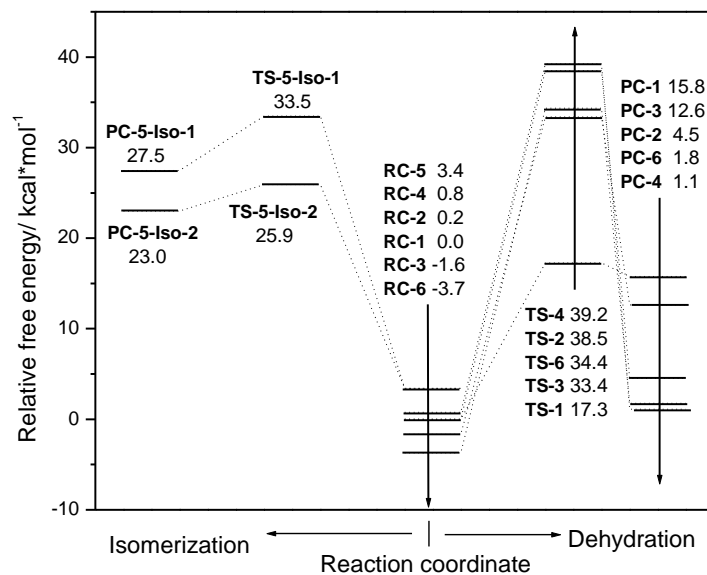
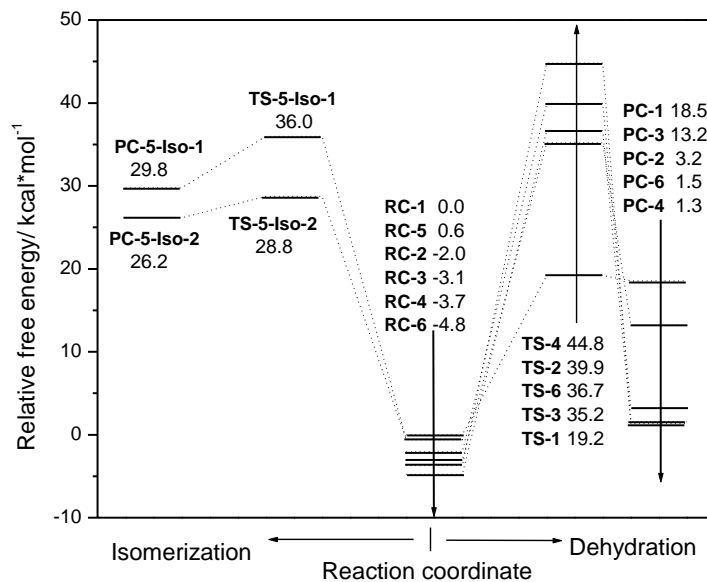


Figure 7S. Relative free energy (298K) profiles for the dehydration and isomerization reactions of protonated β -glucopyranose. (a) One water molecule and (b) two water molecules were incorporated into the reaction systems. The suffixes “-BP-1W” for (a) and “-BP-2W” for (b) in the notations of all species here are omitted for clarity. See Scheme 2a and Figures 3S~6S for the structural details.



(a) 1 water molecule incorporated



(b) 2 water molecules incorporated

Figure 8S: Optimized geometries for the species involved in the dehydration of BP at C(2) site catalyzed by the acid site on the 12T model. Key distances are indicated in (Å).

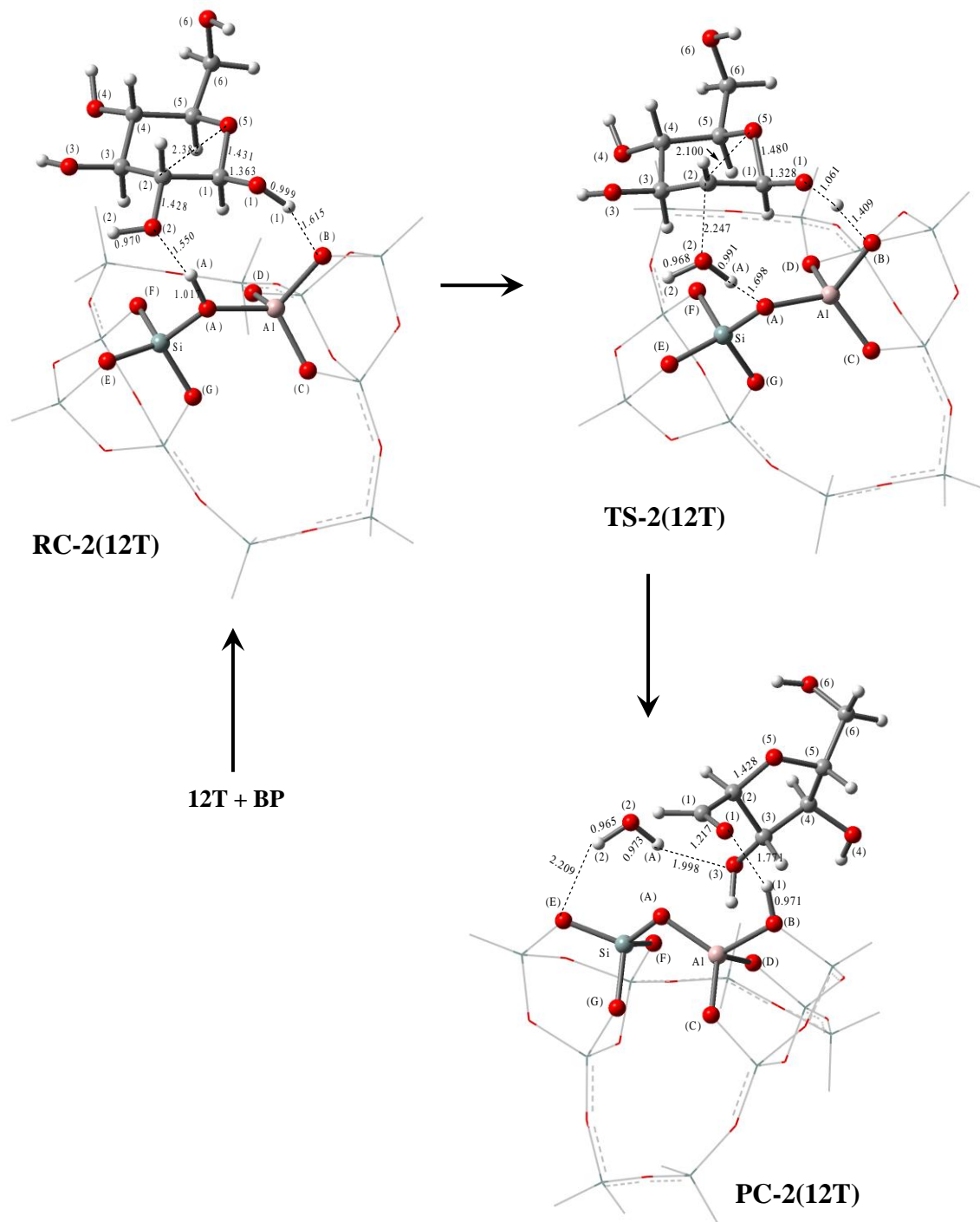


Figure 9S: Optimized geometries for the species involved in the dehydration of BP at C(3) site catalyzed by the acid site on the 12T model. Key distances are indicated in (Å)

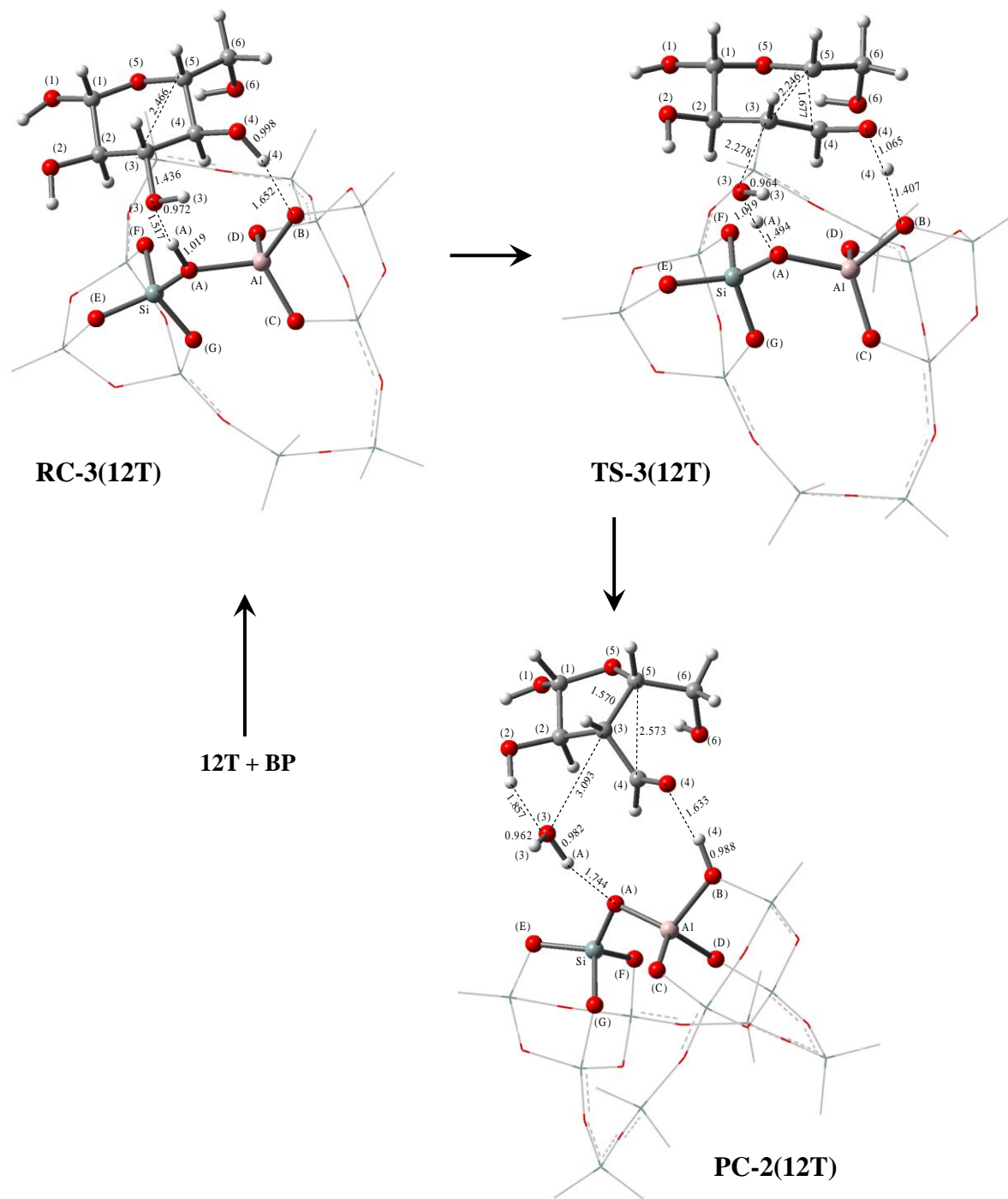


Figure 10S: Optimized geometries for the species involved in the dehydration of BP at C(4) site catalyzed by the acid site on the 12T model. Key distances are indicated in (Å).

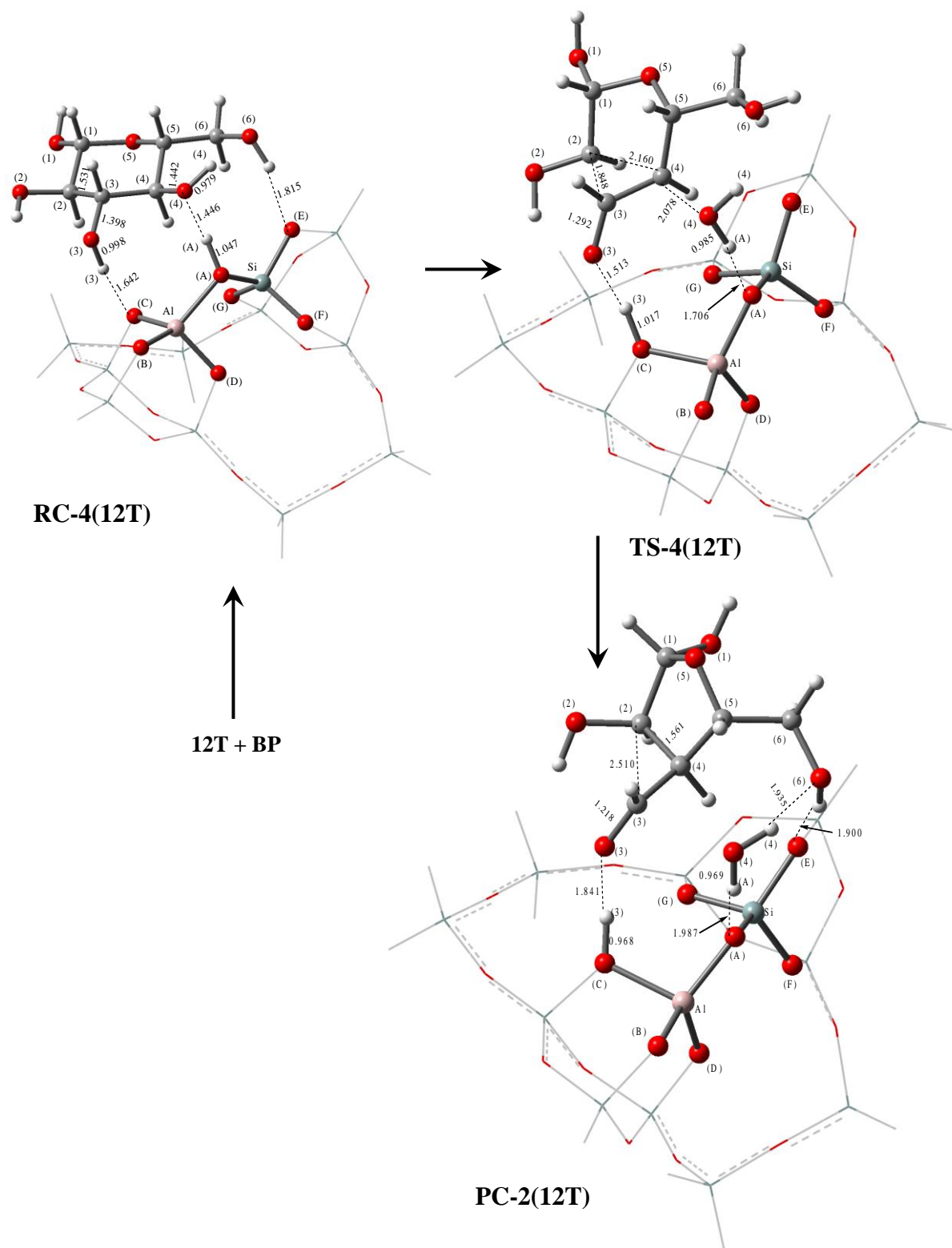


Figure 11S: Optimized geometries for the species involved in the dehydration of BP at C(6) site catalyzed by the acid site on the 12T model. Key distances are indicated in (Å).

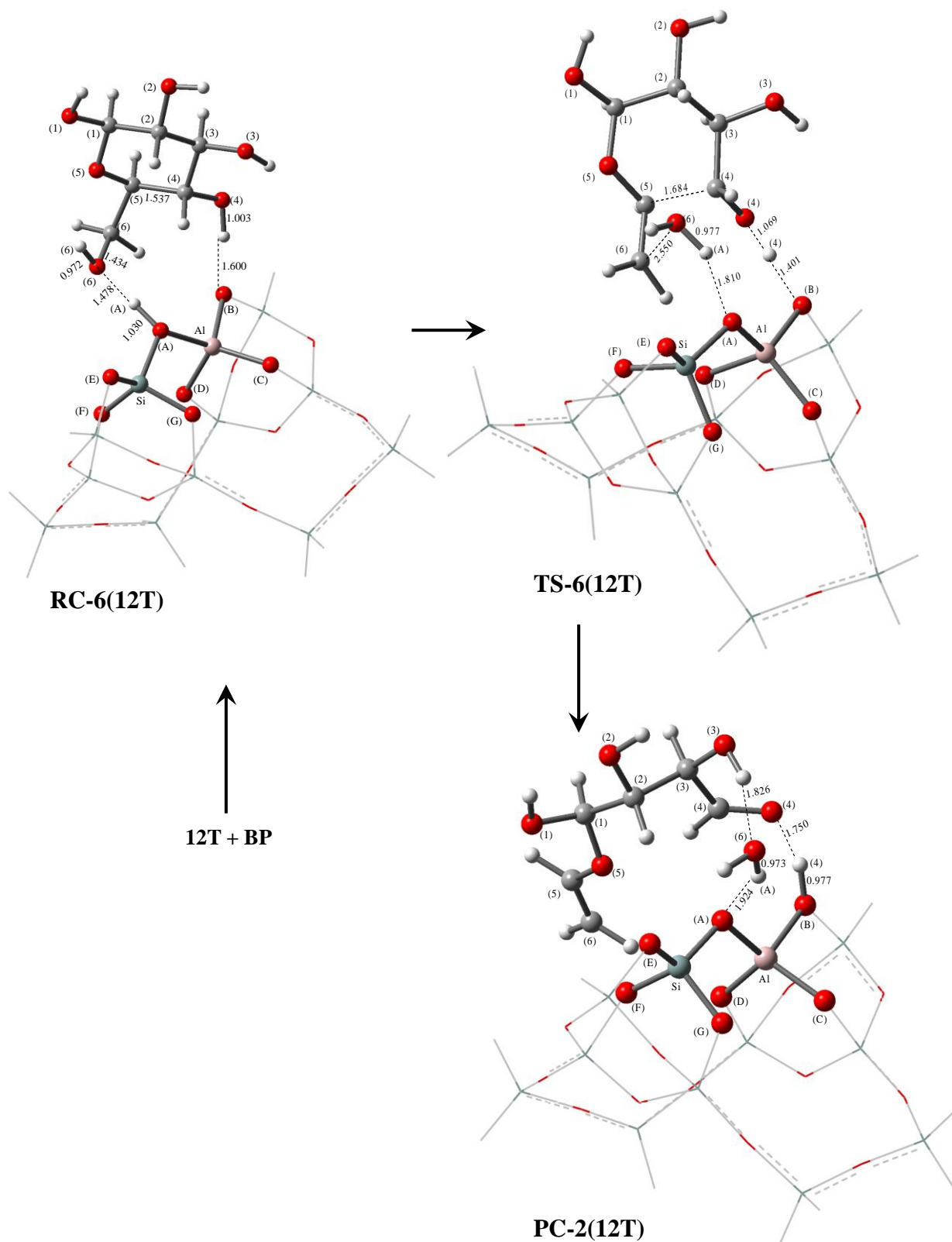
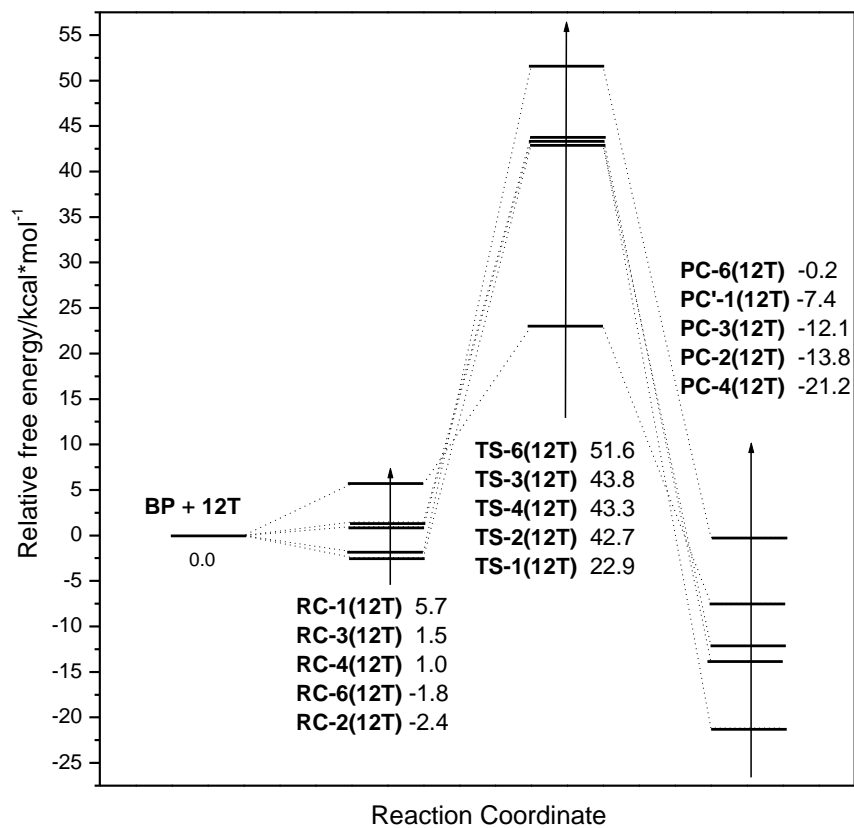


Figure 12S. Relative free energy (298 K) profiles for the first dehydration of BP catalyzed by the acid site on the 12T model. See Figure 13 in the text, and Figures S8-S11 as well for the structural information.



Full citation of Reference 50:

[50] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision C.01, Gaussian, Inc., Wallingford, CT, 2010.

Cartesian coordinates, ZPE corrected energy, enthalpy (298 K), free energy (298 K) for all the optimized structures reported in the manuscript. See the computational method and the notations of the species in the manuscript as well.

Note: In order to clarified the computational method for a certain species, in this paper, if a species notation does not contain a bracket, then this species is calculated with the PCM model in aqueous solution. If there is “(12T)” immediately followed a species notation, it is species is calculated with the gas-phase model for heterogeneous reaction on surface.

In Figure 1.

RC-1-BP (RC-n-BP, n = 1)

```
-----  
C      -1.179344  -1.096883  -0.312516  
C      -1.632094  0.255261  0.200146  
C      -0.573102  1.273736  -0.227401  
C      0.799368  0.805058  0.260145  
C      1.091124  -0.617429  -0.231971  
O      0.033356  -1.482326  0.215111  
H      -1.685168  0.209334  1.296946  
O      -0.878479  2.573160  0.231800  
H      -0.560883  1.338543  -1.322263  
H      0.806118  0.799215  1.361712  
O      1.831460  1.638535  -0.234157  
H      1.137041  -0.630019  -1.330761  
C      2.382822  -1.194290  0.337403  
H      -1.211060  -1.167380  -1.405528  
O      -2.905186  0.480115  -0.361543  
H      -3.366457  1.161028  0.147120  
H      -0.903544  2.576001  1.200503  
H      1.690837  2.536387  0.098989  
H      2.422113  -2.260298  0.102252  
O      3.522409  -0.593646  -0.249945  
H      2.383820  -1.073770  1.428683  
H      3.446999  0.366116  -0.133975  
O      -2.144324  -2.082485  0.210656  
H      -2.104214  -2.948566  -0.249406  
H      -3.062131  -1.726149  0.155520  
-----
```

E + ZPE = -687.173151 a.u.
H(298K) = -687.159527 a.u.
G(298K) = -687.211146 a.u.

TS-1-BP (TS-n-BP, n = 1)

```
-----  
C      1.519941  -0.627254  -0.111818  
C      0.416063  -1.432626  0.567482  
O      -0.581751  -0.899130  1.152513  
-----
```

```
C      -1.059828  0.464927  0.856097  
C      -0.175835  1.163325  -0.175493  
C      1.288940  0.858437  0.100897  
C      -2.515933  0.325839  0.446850  
O      -2.677541  -0.232642  -0.841112  
O      -0.353230  2.559761  -0.052454  
O      2.134098  1.549378  -0.787880  
O      2.735799  -0.997628  0.489995  
O      -0.523926  -2.264733  -1.010397  
H      1.946742  2.495081  -0.694813  
H      1.526192  1.115385  1.144372  
H      1.521237  -0.831395  -1.186638  
H      -0.062686  -2.273541  -1.865125  
H      0.678450  -2.415140  0.952379  
H      3.106844  -1.767546  0.036569  
H      -0.987324  0.984017  1.814999  
H      -1.031439  2.857142  -0.672869  
H      -0.430050  0.828131  -1.188969  
H      -2.948360  1.329381  0.419443  
H      -3.042126  -0.257545  1.210829  
H      -2.259238  -1.107319  -0.873880  
H      -0.725922  -3.192584  -0.805713  
-----
```

E + ZPE = -687.167405 a.u.
H(298K) = -687.153466 a.u.
G(298K) = -687.205626 a.u.

PC-1-BP (PC-n-BP, n = 1)

```
-----  
C      -1.704166  -0.510186  0.026782  
C      -0.558399  -1.524383  -0.079041  
O      0.513945  -1.211629  -0.823604  
C      1.007241  0.157141  -0.856700  
C      0.288707  1.038230  0.167176  
C      -1.210812  0.933361  -0.067832  
C      2.511762  0.094834  -0.668072  
O      2.865977  -0.370498  0.624537  
O      0.639018  2.393477  -0.046994  
O      -1.938205  1.708015  0.863753  
O      -2.598312  -0.745300  -1.039844  
O      -0.029734  -1.675509  1.388723  
H      -1.636127  2.624272  0.779911  
-----
```


H	-1.407784	1.283551	-1.091708
H	-2.202208	-0.647690	0.992949
H	-0.675686	-2.089166	1.997898
H	-0.901055	-2.524802	-0.338831
H	-3.152647	-1.511928	-0.834612
H	0.791451	0.543974	-1.859363
H	1.365450	2.638152	0.540662
H	0.538856	0.736453	1.190408
H	2.914249	1.104851	-0.785853
H	2.944894	-0.539316	-1.447515
H	3.005554	-1.324780	0.588544
H	0.787551	-2.215998	1.401064

E + ZPE = -687.171202 a.u.
H(298K) = -687.158161 a.u.
G(298K) = -687.208438 a.u.

RC-2-BP (RC-n-BP, n = 2)

C	-1.156458	-1.260508	-0.286498
C	-1.583501	0.101414	0.236381
C	-0.627536	1.191316	-0.210292
C	0.771007	0.818742	0.279620
C	1.121879	-0.590624	-0.217216
O	0.130977	-1.507111	0.246465
H	-1.713177	0.073214	1.321818
O	-1.081787	2.455840	0.220766
H	-0.616061	1.237075	-1.305930
H	0.784124	0.817242	1.380017
O	1.741413	1.714043	-0.227035
H	1.152390	-0.591460	-1.317857
C	2.461152	-1.084317	0.321263
H	-1.114315	-1.264024	-1.384864
O	-2.044873	-2.198214	0.203360
O	-2.896937	0.441189	-0.352194
H	-1.996849	-3.006080	-0.327582
H	-3.634558	-0.095054	0.010122
H	-1.011753	2.519955	1.186029
H	1.651880	2.567540	0.219722
H	2.557561	-2.147564	0.089671
O	3.553456	-0.422633	-0.292719
H	2.482711	-0.960568	1.412363
H	3.416064	0.531772	-0.191505
H	-3.095258	1.396917	-0.220696

E + ZPE = -687.179695 a.u.
H(298K) = -687.166322 a.u.
G(298K) = -687.217323 a.u.

TS-2-BP (TS-n-BP, n = 2)

C	-1.167212	-1.347750	-0.426341
C	-1.315403	-0.119783	0.344912
C	-0.623761	1.135633	-0.135933
C	0.881657	0.929420	0.147692
C	1.181442	-0.526913	-0.195770
O	0.078895	-1.258976	0.393925
H	-1.711983	-0.180174	1.354212
O	-1.149197	2.298429	0.445979

H	-0.765618	1.234671	-1.216750
H	1.050575	1.080722	1.223877
O	1.703558	1.773698	-0.613265
H	1.192500	-0.678495	-1.281224
C	2.465567	-1.063452	0.426213
H	-0.941021	-1.272639	-1.488345
O	-1.882516	-2.451306	-0.156924
O	-3.237566	0.594661	-0.316674
H	-2.242104	-2.437883	0.744238
H	-3.957685	0.137829	0.142083
H	-0.951712	2.318387	1.394819
H	1.708340	2.657425	-0.219619
H	2.545372	-2.133241	0.224767
O	3.591631	-0.443099	-0.165544
H	2.439668	-0.905945	1.511544
H	3.522618	0.516310	-0.050854
H	-3.261113	1.512844	-0.003362

E + ZPE = -687.135749 a.u.
H(298K) = -687.121075 a.u.
G(298K) = -687.175056 a.u.

PC-2-BP (PC-n-BP, n = 2)

C	-2.226977	-0.611070	-0.369773
C	-0.818072	-0.370820	0.143522
C	-0.336877	1.035492	-0.194913
C	1.162015	0.890633	0.022672
C	1.400806	-0.551987	-0.475784
O	0.111097	-1.207364	-0.504872
H	-0.803698	-0.521018	1.236855
O	-1.049132	2.021951	0.553282
H	-0.531622	1.258542	-1.248829
H	1.380029	0.971820	1.097944
O	1.958650	1.784809	-0.717792
H	1.784886	-0.512744	-1.500630
C	2.338302	-1.366923	0.405855
H	-2.316907	-0.464164	-1.446240
O	-2.813016	-1.786310	-0.035819
O	-2.988167	0.516737	0.286318
H	-2.625919	-2.024553	0.886773
H	-3.785124	0.774641	-0.214074
H	-0.733600	2.054121	1.472753
H	1.961371	2.644791	-0.276232
H	2.424381	-2.376531	-0.002232
O	3.643251	-0.810837	0.412431
H	1.924779	-1.431441	1.420296
H	3.654587	-0.018749	0.966349
H	-2.349827	1.341445	0.469405

E + ZPE = -687.176522 a.u.
H(298K) = -687.163463 a.u.
G(298K) = -687.214232 a.u.

RC-3-BP (RC-n-BP, n = 3)

C	-0.993996	-1.345619	-0.375772
C	-1.566854	-0.080795	0.284613

C	-0.767052	1.094199	-0.218689
C	0.711729	0.947821	0.044196
C	1.162852	-0.369740	-0.609683
O	0.387357	-1.439846	-0.074216
H	-1.451285	-0.168716	1.373676
O	-1.226274	2.294636	0.524431
H	-0.967736	1.291559	-1.276304
H	0.889932	0.894433	1.124072
O	1.334673	2.081385	-0.523916
H	1.009005	-0.301125	-1.697215
C	2.624843	-0.667414	-0.358764
H	-1.145590	-1.302254	-1.462564
O	-1.628073	-2.492673	0.070262
O	-2.908050	0.158661	-0.075010
H	-1.538969	-2.561276	1.033822
H	-3.487254	-0.421870	0.438093
H	-2.190653	2.444260	0.412184
H	2.135718	2.295076	-0.026820
H	3.229188	0.085384	-0.878504
O	2.863685	-0.636868	1.040762
H	2.853823	-1.653151	-0.778302
H	3.780793	-0.891319	1.202849
H	-0.732647	3.095923	0.241110

E + ZPE = -687.182442 a.u.
H(298K) = -687.168634 a.u.
G(298K) = -687.220605 a.u.

TS-3-BP (TS-n-BP, n = 3)

C	1.181236	-1.385900	0.386387
C	1.721202	0.223272	-0.323052
C	0.683599	0.906374	0.303286
C	-0.716831	0.688936	-0.101680
C	-1.068270	-0.793972	0.308391
O	-0.042998	-1.657159	-0.133977
H	1.627422	-0.017981	-1.382678
O	0.606509	3.136232	-0.480674
H	0.866442	1.355581	1.278158
H	-0.827278	0.768853	-1.190548
O	-1.534332	1.603092	0.581947
H	-1.163657	-0.828728	1.400096
C	-2.345160	-1.260372	-0.375540
H	1.232693	-1.272579	1.469360
O	2.134424	-2.233096	-0.035888
O	2.982981	0.471038	0.139796
H	2.018928	-2.449283	-0.977645
H	3.618339	-0.080213	-0.339615
H	1.246563	3.685212	-0.007635
H	-2.456291	1.354542	0.396748
H	-2.591033	-2.268370	-0.026431
O	-3.363090	-0.333144	-0.029177
H	-2.179074	-1.279821	-1.458296
H	-4.137965	-0.487552	-0.584986
H	-0.257693	3.354611	-0.099494

E + ZPE = -687.142575 a.u.
H(298K) = -687.127803 a.u.
G(298K) = -687.181842 a.u.

PC-3-BP (PC-n-BP, n = 3)

C	-1.948472	1.381439	-0.485854
C	1.255078	1.713524	0.532679
C	1.029957	0.717787	-0.330209
C	0.390508	-0.557898	0.107719
C	-0.965956	-0.771227	-0.592280
O	-1.879926	0.219325	0.008516
H	0.998618	1.635684	1.587608
O	3.978483	-0.882485	-0.105301
H	1.296559	0.822888	-1.380779
H	0.212268	-0.539164	1.188527
O	1.233329	-1.654978	-0.233692
H	-0.906184	-0.567926	-1.664892
C	-1.577013	-2.132608	-0.355782
H	-1.446565	1.658530	-1.411366
O	-2.649255	2.280856	0.078388
O	1.813073	2.882188	0.139544
H	-3.075277	1.977805	0.908055
H	1.911117	3.476827	0.894868
H	4.524665	-1.666811	-0.235773
H	0.962745	-2.425039	0.290407
H	-1.064463	-2.842028	-1.014419
O	-1.390066	-2.469386	1.008978
H	-2.637353	-2.107638	-0.627175
H	-1.783506	-3.335922	1.175043
H	3.057656	-1.197485	-0.139217

E + ZPE = -687.173187 a.u.
H(298K) = -687.156631 a.u.
G(298K) = -687.216745 a.u.

RC-4-BP (RC-n-BP, n = 4)

C	-1.324908	-1.176211	-0.305266
C	-1.680056	0.225337	0.202845
C	-0.601626	1.231324	-0.190834
C	0.745333	0.721963	0.278226
C	0.978899	-0.697054	-0.255301
O	-0.044378	-1.550310	0.204957
H	-1.751804	0.187540	1.300523
O	-0.822523	2.493026	0.404512
H	-0.583931	1.322136	-1.287214
H	0.794255	0.722739	1.373843
O	1.821520	1.524609	-0.247878
H	0.992087	-0.665812	-1.356359
C	2.295380	-1.273796	0.245007
H	-1.299826	-1.192157	-1.402632
O	-2.244184	-2.131725	0.091550
O	-2.888783	0.679571	-0.368708
H	-2.368808	-2.083946	1.052257
H	-3.629924	0.205970	0.032745
H	-1.634212	2.867468	0.034102
H	1.910607	2.351368	0.252344
H	2.509684	-2.243013	-0.200453
O	3.330455	-0.339970	-0.218679
H	2.324188	-1.316609	1.334419
H	4.150617	-0.395779	0.304685
H	2.892092	0.649124	-0.212357

E + ZPE = -687.193146 a.u.
H(298K) = -687.180181 a.u.

G(298K) = -687.230178 a.u.

TS-4-BP (TS-n-BP, n = 4)

```
-----  
C      1.334755 -1.072398  0.487385  
C      1.771662  0.200150 -0.250008  
C      0.611107  1.198937 -0.320156  
C     -0.696926  0.656188 -0.435495  
C     -0.964212 -0.726291  0.053017  
O      0.151338 -1.561946 -0.140326  
H      2.038060 -0.058414 -1.283065  
O      0.862364  2.344463 -1.041381  
H      0.323504  1.453522  0.765834  
H     -1.504267  1.257031 -0.847779  
O     -2.150550  1.547429  1.453234  
H     -1.218444 -0.633575  1.123646  
C     -2.181306 -1.322193 -0.655815  
H      1.138224 -0.857371  1.545977  
O      2.297845 -2.058138  0.446242  
O      2.824465  0.859224  0.403816  
H      2.571812 -2.220146 -0.470073  
H      3.669267  0.525475  0.073142  
H      1.717121  2.701666 -0.752201  
H     -2.372504  2.485131  1.527504  
H     -2.292515 -2.354355 -0.311451  
O     -3.275505 -0.512714 -0.264918  
H     -2.037579 -1.311488 -1.740326  
H     -4.013294 -0.652443 -0.872706  
H     -2.949517  1.112066  1.114591  
-----
```

E + ZPE = -687.131098 a.u.
H(298K) = -687.115950 a.u.
G(298K) = -687.170811 a.u.

PC-4-BP (PC-n-BP, n = 4)

```
-----  
C      1.397305 -0.936711  0.604197  
C      1.945826  0.213227 -0.302266  
C      0.819519  1.153709 -0.574057  
C     -0.479411  0.632982 -1.009035  
C     -0.837297 -0.550808 -0.067666  
O      0.241236 -1.465751 -0.002146  
H      2.243670 -0.231669 -1.261391  
O      0.983778  2.379142 -0.325376  
H     -1.241109  1.412601 -1.000180  
H     -0.355151  0.229484 -2.022677  
O     -3.232084  1.236198  1.599641  
H     -1.059833 -0.160117  0.933753  
C     -2.032624 -1.323019 -0.599141  
H      1.172498 -0.532380  1.598300  
O      2.331346 -1.931959  0.769853  
O      2.970970  0.917072  0.333872  
H      2.577120 -2.308792 -0.089465  
H      3.798514  0.830418 -0.158488  
H      1.905487  2.527880  0.011089  
H     -4.104371  1.317838  2.003263  
H     -2.270168 -2.129499  0.101817  
O     -3.109081 -0.402154 -0.708410  
H     -1.782880 -1.750567 -1.577026  
-----
```

H -3.898999 -0.871608 -1.007444
H -3.354006 0.669730 0.816791

E + ZPE = -687.194108 a.u.
H(298K) = -687.178757 a.u.
G(298K) = -687.236134 a.u.

RC-6-BP (RC-n-BP, n = 6)

```
-----  
C     -0.899935 -1.319433 -0.449728  
C     -1.552588 -0.149851  0.290588  
C     -0.910203  1.159151 -0.146297  
C      0.595667  1.102030  0.061795  
C      1.159101 -0.120969 -0.662713  
O      0.508649 -1.301282 -0.212819  
H     -1.398200 -0.285063  1.371876  
O     -1.389225  2.256893  0.607684  
H     -1.115126  1.315739 -1.216416  
H      0.796914  1.015616  1.139947  
O      1.237543  2.239365 -0.475204  
H      1.036925  0.009308 -1.747600  
C      2.627001 -0.355366 -0.393684  
H     -1.085080 -1.238917 -1.528514  
O     -1.385961 -2.551791 -0.049032  
O     -2.928953 -0.064576 -0.018031  
H     -1.331057 -2.628044  0.916395  
H     -3.405770 -0.765160  0.447209  
H     -2.316057  2.409264  0.377904  
H      0.840483  3.025362 -0.073013  
H      3.223596  0.550988 -0.463906  
O      2.704854 -0.774963  1.029802  
H      3.029875 -1.169417 -0.993287  
H      3.593450 -1.083250  1.298263  
H      2.040535 -1.478966  1.212186  
-----
```

E + ZPE = -687.186078 a.u.
H(298K) = -687.172376 a.u.
G(298K) = -687.223939 a.u.

TS-6-BP (TS-n-BP, n = 6)

```
-----  
C     -1.048079 -1.333926 -0.376411  
C     -1.654714 -0.123838  0.333729  
C     -0.973451  1.151027 -0.145703  
C      0.525896  1.064065  0.100471  
C      1.066260 -0.244299 -0.451979  
O      0.382811 -1.371288 -0.132171  
H     -1.504172 -0.229607  1.418261  
O     -1.430697  2.285544  0.557585  
H     -1.150747  1.268934 -1.225418  
H      0.707920  1.029005  1.185290  
O      1.234593  2.115208 -0.501941  
H      1.200371 -0.115590 -1.675371  
C      2.400365 -0.380753 -0.834581  
H     -1.207576 -1.271101 -1.458562  
O     -1.561387 -2.538697  0.044210  
O     -3.024458 -0.007507  0.017323  
H     -1.537510 -2.595410  1.012598  
H     -3.529648 -0.652277  0.530801  
-----
```

H	-2.352924	2.447928	0.314995
H	0.940365	2.947969	-0.105669
H	2.970232	0.518174	-1.038326
O	3.490458	-0.627533	1.047534
H	2.751264	-1.349339	-1.173900
H	4.298775	-0.094960	1.047799
H	3.785425	-1.543187	1.154035

E + ZPE = -687.141884 a.u.
H(298K) = -687.127081 a.u.
G(298K) = -687.181457 a.u.

PC-6-BP (PC-n-BP, n = 6)

C	-1.237005	-0.505739	-0.873179
C	-1.156039	0.747303	-0.001596
C	0.190308	1.434839	-0.170051
C	1.276249	0.478145	0.300733
C	1.175018	-0.848817	-0.393072
O	0.085456	-1.268625	-0.860521
H	-1.294645	0.475128	1.051542
O	0.289567	2.578851	0.642930
H	0.354833	1.688467	-1.226785
H	1.090691	0.232908	1.363353
O	2.574214	0.971122	0.118350
H	3.041706	-1.211789	-1.223766
C	2.356141	-1.711561	-0.527850
H	-1.345882	-0.250997	-1.927987
O	-2.182001	-1.404522	-0.515722
O	-2.155853	1.643173	-0.429676
H	-2.047000	-1.630468	0.431222
H	-2.988590	1.437209	0.015757
H	-0.298275	3.261660	0.289677
H	2.705606	1.704635	0.736275
H	2.872822	-1.762812	0.434966
O	-0.870013	-1.828618	1.835425
H	2.079910	-2.695396	-0.900442
H	-1.183324	-1.606711	2.722502
H	-0.546839	-2.737892	1.897493

E + ZPE = -687.199020 a.u.
H(298K) = -687.182774 a.u.
G(298K) = -687.240526 a.u.

In Figure 3.

RC-5-BP

(RC-n-BP, n = 5)

O	0.322700	-1.388251	-0.097872
C	-1.175033	-1.272007	-0.393593
C	-1.588475	0.013572	0.303180
C	-0.764371	1.194528	-0.195491
C	0.723952	0.975215	0.050010
C	1.201353	-0.308479	-0.631942
O	-1.747999	-2.404723	0.059477
O	-2.954818	0.178834	0.009124

O	-1.236202	2.321309	0.511593
O	1.410981	2.068596	-0.519662
C	2.631028	-0.686054	-0.327874
O	2.809994	-0.691269	1.074602
H	-1.426714	-0.107980	1.385432
H	-0.934221	1.320832	-1.275279
H	0.906239	0.907872	1.128154
H	1.040749	-0.266027	-1.713052
H	-1.255661	-1.229572	-1.481201
H	-1.895379	-2.366410	1.019062
H	-3.227139	1.042313	0.354764
H	-0.849110	3.115914	0.118118
H	2.178793	2.290095	0.023566
H	3.266153	0.060253	-0.819411
H	2.854010	-1.665181	-0.767057
H	3.704643	-0.997573	1.270994
H	0.629667	-2.281155	-0.367941

E + ZPE = -687.179572 a.u.
H(298K) = -687.165882 a.u.
G(298K) = -687.217389 a.u.

TS-5-BP-Iso-1

(TS-n-BP-Iso-m, n = 5, m = 1)

O	-0.140973	-1.646888	-0.117159
C	-1.461725	-1.171832	-0.355186
C	-1.575823	0.188022	0.324280
C	-0.569582	1.216203	-0.206818
C	0.855640	0.833350	0.121107
C	1.487941	-0.195167	-0.694415
O	-2.398346	-2.019421	0.230790
O	-2.882450	0.655416	0.072939
O	-0.889465	2.436273	0.433238
O	1.800287	1.673858	-0.589394
C	2.662805	-0.976228	-0.264510
O	2.880651	-0.815088	1.112229
H	-1.411663	0.046925	1.403735
H	-0.685836	1.309022	-1.295136
H	1.063171	0.788844	1.189420
H	1.189728	-0.265794	-1.736636
H	-1.634166	-1.082043	-1.434143
H	-2.640428	-2.718958	-0.390803
H	-2.924520	1.573181	0.380949
H	-0.573656	3.176771	-0.101789
H	2.567464	1.867738	-0.022148
H	3.515114	-0.647201	-0.874493
H	2.456248	-2.018292	-0.548228
H	3.742792	-1.188585	1.337990
H	-0.017434	-2.480896	-0.596622

E + ZPE = -687.139905 a.u.
H(298K) = -687.125721 a.u.
G(298K) = -687.178722 a.u.

PC-5-BP-Iso-1

(PC-n-BP-Iso-m, n = 5, m = 1)

O	0.582898	-1.789507	-0.223020
C	1.682583	-1.096363	0.279145
C	1.638299	0.307408	-0.316049
C	0.473359	1.153671	0.211825
C	-0.856911	0.561860	-0.172873
C	-1.643156	-0.251926	0.740872
O	2.849190	-1.768426	-0.137780
O	2.852600	0.928603	0.046080
O	0.618801	2.426234	-0.387875
O	-1.985630	1.211141	0.599969
C	-2.740616	-1.143392	0.229650
O	-3.298578	-0.488988	-0.896484
H	1.554319	0.216526	-1.409212
H	0.548218	1.225630	1.304291
H	-1.095372	0.523111	-1.232878
H	-1.252680	-0.441926	1.735644
H	1.653618	-1.043936	1.377033
H	3.618051	-1.287907	0.203661
H	2.829932	1.841954	-0.275085
H	0.193318	3.096555	0.163772
H	-2.782194	1.273408	0.015853
H	-3.483647	-1.290675	1.016686
H	-2.289190	-2.106299	-0.033827
H	-4.224153	-0.746081	-0.996807
H	0.454184	-2.600371	0.288339

E + ZPE = -687.150267 a.u.
H(298K) = -687.135733 a.u.
G(298K) = -687.190026 a.u.

TS-5-BP-Iso-2

(TS-n-BP-Iso-m, n = 5, m = 2)

C	-2.057520	1.318274	-0.149452
C	-2.062944	-0.143925	-0.344525
C	-0.811121	-0.727253	0.415828
C	0.516147	-0.376833	-0.305652
C	1.453133	0.344601	0.664200
O	0.738611	1.515345	1.039165
H	-1.971854	-0.386046	-1.412442
O	-1.032148	-2.105381	0.539626
H	-0.815344	-0.312730	1.427683
H	0.315552	0.321086	-1.132728
O	1.054582	-1.573933	-0.827447
H	1.642815	-0.299381	1.534221
C	2.776008	0.742078	0.020594
H	-2.529602	1.767464	0.727166
O	-3.239935	-0.637674	0.227117
H	-3.072532	-1.570264	0.444863
H	-0.534757	-2.556596	-0.163163
H	2.018962	-1.465172	-0.916030
H	3.351118	1.354347	0.724669
O	3.479432	-0.458294	-0.296948
H	2.577139	1.329747	-0.884346
H	4.256456	-0.245184	-0.829941
O	-1.469414	2.044588	-0.988006
H	-1.452475	2.996390	-0.752886
H	1.083279	1.847473	1.878919

E + ZPE = -687.156536 a.u.
H(298K) = -687.142191 a.u.
G(298K) = -687.196212 a.u.

PC-5-BP-Iso-2

(PC-n-BP-Iso-m, n = 5, m = 2)

C	-2.494154	-1.068235	0.272257
O	-3.807408	-0.791808	-0.196248
C	-1.657924	0.139893	-0.119259
O	-2.183102	1.312651	0.475166
C	-0.231924	0.052202	0.396944
C	0.665969	1.252970	0.063995
C	2.074061	0.645714	0.048440
C	1.928057	-0.689531	-0.671977
O	2.750104	-1.637765	-0.195446
O	0.451890	-1.077037	-0.238165
O	0.333532	1.927552	-1.123418
O	2.447306	0.444894	1.387991
H	-2.095234	-1.979127	-0.189760
H	-2.485731	-1.179306	1.363247
H	-1.644862	0.232934	-1.214079
H	-0.199171	-0.155556	1.468705
H	0.594533	1.986821	0.867395
H	2.775381	1.284284	-0.498354
H	1.867035	-0.635660	-1.758004
H	-4.431344	-1.386540	0.238163
H	3.293792	-0.024362	1.418243
H	0.464046	1.381084	-1.910634
H	0.457835	-1.899186	0.249269
H	-3.144565	1.284911	0.354426
H	2.905194	-2.336282	-0.850060

E + ZPE = -687.173660 a.u.
H(298K) = -687.159880 a.u.
G(298K) = -687.211977 a.u.

In Figure 4:

P1

O	0.224020	-1.729418	-0.129241
C	-1.005882	-1.692917	0.085654
C	-1.812170	-0.445396	0.286288
C	-1.078278	0.782074	-0.252828
C	0.371791	0.712137	0.223352
C	1.065163	-0.529552	-0.325608
O	-3.064179	-0.607493	-0.317948
O	-1.695733	1.982275	0.137546
O	1.130807	1.800551	-0.254985
C	2.403031	-0.848809	0.336379
O	3.388167	0.063289	-0.100497
H	-1.892744	-0.361566	1.384782
H	-1.106834	0.765390	-1.347899
H	0.393075	0.682895	1.324030

H	1.180090	-0.463497	-1.411338
H	-1.490790	-2.669035	0.136722
H	-3.727275	-0.837046	0.347585
H	-1.735748	2.041033	1.104679
H	0.748974	2.617643	0.098709
H	2.722725	-1.845688	0.026477
H	2.286375	-0.831654	1.426593
H	3.095561	0.962677	0.111228

E + ZPE = -610.772105 a.u.
H(298K) = -610.759919 a.u.
G(298K) = -610.808612 a.u.

TS-P1-A

O	0.278977	-1.721975	0.236176
C	-1.031936	-1.697124	0.136279
C	-1.764451	-0.523461	-0.111241
C	-1.056565	0.811928	-0.269230
C	0.353782	0.711845	0.312361
C	1.021510	-0.556032	-0.218750
O	-3.058031	-0.612751	-0.400950
O	-1.843781	1.847756	0.254991
O	1.149629	1.800777	-0.098161
C	2.449269	-0.744816	0.282628
O	3.349667	0.083363	-0.425443
H	-1.594385	-0.934343	1.128718
H	-0.981660	0.990654	-1.348041
H	0.302736	0.661521	1.410209
H	1.007221	-0.567433	-1.315321
H	-1.534250	-2.656615	0.240463
H	-3.472991	0.262733	-0.291365
H	-1.835949	1.818556	1.225089
H	0.964394	2.566601	0.463283
H	2.745061	-1.779641	0.095966
H	2.490263	-0.555329	1.362812
H	3.068206	1.001889	-0.296997

E + ZPE = -610.754455 a.u.
H(298K) = -610.743031 a.u.
G(298K) = -610.789975 a.u.

P1-A

O	-0.265615	-1.676183	-0.269084
C	0.998485	-1.809832	0.346446
C	1.758788	-0.540832	0.131180
C	1.086959	0.773010	0.342483
C	-0.327546	0.718278	-0.271560
C	-1.026385	-0.564407	0.194066
O	2.950442	-0.570693	-0.261058
O	1.892835	1.778034	-0.203829
O	-1.080448	1.829412	0.151518
C	-2.425746	-0.705955	-0.400337
O	-3.349451	0.164979	0.226546
H	1.521442	-2.649635	-0.110256
H	0.968684	0.872968	1.433200
H	-0.235182	0.697069	-1.364918
H	-1.095808	-0.580134	1.292541

H	0.913993	-1.967331	1.432671
H	3.285512	0.355093	-0.392722
H	2.103244	2.442671	0.466973
H	-0.866998	2.594796	-0.400640
H	-2.772432	-1.726299	-0.222456
H	-2.384148	-0.533481	-1.483992
H	-3.007749	1.068314	0.143173

E + ZPE = -610.786003 a.u.
H(298K) = -610.774196 a.u.
G(298K) = -610.821963 a.u.

TS-P1-B

C	0.398047	-1.400302	-0.599369
C	-0.849905	-1.092678	0.206083
C	-1.237229	0.353640	-0.091904
C	-0.041783	1.274934	0.150103
C	1.246907	0.730402	-0.491043
H	0.585029	-2.424728	-0.923236
O	-1.859611	-1.944992	-0.273144
H	-1.854152	-2.771840	0.229595
O	-2.366196	0.776446	0.632411
H	-2.188959	0.717333	1.583266
H	-1.517021	0.420117	-1.149792
H	0.116491	1.359774	1.234807
O	-0.272951	2.551849	-0.407295
H	-1.050048	2.935157	0.024953
H	1.657719	1.447904	-1.198333
C	2.290253	0.238599	0.518358
O	1.726316	-0.939939	1.083816
H	2.403705	-1.623283	1.199316
O	1.022045	-0.501555	-1.251712
H	3.229899	0.018287	0.011434
H	2.436097	0.998918	1.289375
H	-0.653338	-1.239686	1.272645

E + ZPE = -610.767564 a.u.
H(298K) = -610.756385 a.u.
G(298K) = -610.802754 a.u.

P1-B

C	0.946448	-1.104882	-0.393234
C	-0.448855	-1.254340	0.227459
C	-1.252143	0.008835	-0.088724
C	-0.436850	1.268768	0.215219
C	0.984379	1.116524	-0.363952
H	1.338230	-2.019196	-0.835924
O	-1.023278	-2.399071	-0.364136
H	-1.922165	-2.501797	-0.018950
O	-2.509020	0.012845	0.555323
H	-2.385807	0.026409	1.516368
H	-1.470917	0.003604	-1.161356
H	-0.376312	1.408235	1.303770
O	-1.024410	2.406381	-0.385287
H	-1.906724	2.530148	-0.006285
H	1.257515	1.998330	-0.941829
C	2.057077	0.764255	0.665392

O	1.873666	-0.711494	0.751443
H	2.723705	-1.197894	0.732285
O	1.062216	-0.029023	-1.236056
H	3.061178	0.943650	0.290204
H	1.898926	1.159907	1.664993
H	-0.351367	-1.383462	1.313480

E + ZPE = -610.778765 a.u.

H(298K) = -610.767814 a.u.

G(298K) = -610.813728 a.u.

In Figure 6.

RC-2-OC (RC-n-OC, n = 2)

C	-3.085227	0.570795	-0.201205
H	-3.066825	1.507728	0.363103
O	-4.228420	-0.209445	0.136783
H	-3.073746	0.790588	-1.276632
C	-1.877755	-0.279951	0.153900
O	-1.936270	-1.521154	-0.531415
C	-0.573478	0.398020	-0.257855
H	-1.865934	-0.449260	1.241669
C	0.634211	-0.483903	0.114780
H	-0.590221	0.567559	-1.341545
O	-0.495202	1.624105	0.454447
C	1.889496	-0.177166	-0.696710
O	0.913894	-0.393488	1.492822
H	0.394609	-1.528095	-0.115638
C	3.081561	-0.962283	-0.185075
H	1.739237	-0.348894	-1.765412
O	2.286745	1.230648	-0.512104
O	4.058635	-0.363627	0.208804
H	2.999054	-2.056125	-0.181362
H	-5.017238	0.208009	-0.230756
H	3.220553	1.231272	-0.153876
H	0.759034	0.527581	1.761914
H	-0.109957	2.313557	-0.101001
H	-2.838324	-1.859801	-0.431179
H	2.241861	1.766492	-1.330996

E + ZPE = -687.164341 a.u.

H(298K) = -687.149549 a.u.

G(298K) = -687.204819 a.u.

TS-2-OC (TS-n-OC, n = 2)

C	2.928564	0.735011	-0.137280
H	2.783938	1.397759	-0.996235
O	4.119178	-0.030465	-0.269410
H	2.945910	1.326539	0.786285
C	1.796729	-0.282154	-0.068495
O	1.985265	-1.155814	1.024994
C	0.468372	0.427783	0.144743
H	1.755728	-0.842338	-1.012706
C	-0.681787	-0.800974	0.273711

H	0.446897	0.964510	1.099138
O	0.189035	1.198988	-0.946427
C	-1.827152	-0.280561	0.906948
O	-0.752505	-1.482248	-0.918364
H	-0.133904	-1.376277	1.049993
C	-3.224531	-0.384650	0.362705
H	-1.705005	0.123488	1.907583
O	-2.071759	1.976726	0.311693
O	-3.410809	-0.793039	-0.763353
H	-4.039329	-0.077628	1.029151
H	4.881984	0.542456	-0.121458
H	-2.834172	2.299023	-0.193554
H	-1.615436	-1.340844	-1.340535
H	-0.538080	1.808256	-0.717893
H	2.884445	-1.511636	0.967305
H	-2.061384	2.486783	1.135877

E + ZPE = -687.110435 a.u.

H(298K) = -687.094919 a.u.

G(298K) = -687.151078 a.u.

PC-2-OC (PC-n-OC, n = 2)

C	2.748197	-1.112303	0.267645
H	2.525199	-1.913307	0.980813
O	3.664708	-0.171789	0.807575
H	3.138117	-1.545230	-0.660749
C	1.474001	-0.324175	-0.026140
O	1.724494	0.732487	-0.928917
C	0.440394	-1.223643	-0.660982
H	1.067875	0.055619	0.923913
C	-0.756369	2.127725	-0.713768
H	0.238065	-1.048886	-1.732786
O	-0.130321	-2.100393	-0.041981
C	-1.575356	1.059095	-0.421976
O	-0.289819	2.917607	0.215437
H	-0.474944	2.343634	-1.740979
C	-1.941562	0.790011	0.899223
H	-1.916048	0.431048	-1.236634
O	-2.884092	-1.909758	-0.551655
O	-2.612795	-0.230556	1.275301
H	-1.655927	1.467078	1.703752
H	4.560324	-0.526690	0.742195
H	-2.794939	-0.922788	0.510325
H	0.271367	3.617951	-0.155368
H	-2.025149	-2.370626	-0.572818
H	2.519241	1.193095	-0.619942
H	-3.566415	-2.581944	-0.411809

E + ZPE = -687.179384 a.u.

H(298K) = -687.162291 a.u.

G(298K) = -687.223458 a.u.

RC-3-OC (RC-n-OC, n = 3)

C	-2.616765	-0.732888	-0.830821
H	-2.850113	-0.495438	-1.873161
O	-3.790630	-0.952078	-0.060175

H	-1.967903	-1.613199	-0.794710
C	-1.952310	0.473406	-0.192992
O	-1.895184	0.235567	1.264889
C	-0.533825	0.785128	-0.658040
H	-2.576190	1.361374	-0.311179
C	0.467350	-0.289983	-0.200011
H	-0.541438	0.802663	-1.756177
O	-0.231729	2.055744	-0.115431
C	1.900438	-0.026032	-0.657255
O	0.439454	-0.384143	1.239284
H	0.151938	-1.265106	-0.580777
C	2.790279	-1.214686	-0.347529
H	1.892308	0.090538	-1.751707
O	2.377686	1.133709	-0.018642
O	3.820539	-1.070637	0.272338
H	2.463149	-2.194949	-0.727812
H	-4.099124	-1.857618	-0.193475
H	3.283422	0.964650	0.292871
H	0.989936	0.332617	1.607590
H	0.704609	2.261522	-0.261608
H	-2.626153	-0.372301	1.513357
H	-0.916517	-0.129715	1.498569

E + ZPE = -687.182199 a.u.
H(298K) = -687.168237 a.u.
G(298K) = -687.221078 a.u.

TS-3-OC (TS-n-OC, n = 3)

C	-3.067562	0.622876	-0.060750
H	-3.052051	1.473045	0.627896
O	-4.177363	-0.228228	0.187182
H	-3.078592	0.986903	-1.095755
C	-1.840459	-0.250752	0.152348
O	-1.858780	-1.366968	-0.705563
C	-0.556461	0.522520	-0.110295
H	-1.790986	-0.566889	1.204783
C	0.567836	-0.165962	-0.610421
H	-0.532135	0.750065	-1.295442
O	-0.474105	1.644866	0.648072
C	1.929670	0.423073	-0.769389
O	1.173036	-1.501488	1.168362
H	0.347501	-1.084480	-1.150534
C	2.999469	-0.645166	-0.520673
H	2.026560	0.684295	-1.838019
O	2.138856	1.549885	0.032556
O	3.918457	-0.392729	0.218136
H	2.898389	-1.592013	-1.067827
H	-4.983597	0.199377	-0.128117
H	2.881458	1.359640	0.634389
H	1.182020	-0.986926	1.988897
H	0.451925	1.956196	0.673755
H	-2.762977	-1.717012	-0.703375
H	0.456722	-2.144440	1.274473

E + ZPE = -687.131412 a.u.
H(298K) = -687.115558 a.u.
G(298K) = -687.172670 a.u.

PC-3-OC (PC-n-OC, n = 3)

C	-2.763497	-0.836667	-0.028053
H	-2.686212	-1.597089	-0.811505
O	-4.007952	-0.162544	-0.073592
H	-2.600953	-1.294321	0.953491
C	-1.717404	0.265324	-0.270747
O	-1.824578	1.282603	0.691313
C	-0.347920	-0.334888	-0.194517
H	-1.849644	0.654152	-1.289204
C	0.440717	-0.368192	1.067673
H	-0.002188	-1.193219	1.645940
O	0.026709	-0.990780	-1.203103
C	1.936766	-0.624463	0.868641
O	0.602651	1.888236	-0.628260
H	0.265934	0.545228	1.637853
C	2.719467	0.614248	0.467700
H	2.358017	-0.951783	1.827550
O	2.115469	-1.646184	-0.114457
O	3.494699	0.575830	-0.462645
H	2.595326	1.502437	1.102999
H	-4.659006	-0.659942	0.437366
H	2.948771	-1.467471	-0.590866
H	0.703920	2.101574	-1.565826
H	0.956488	-1.418328	-0.982886
H	-2.770529	1.467689	0.803250
H	-0.124697	2.441616	-0.306392

E + ZPE = -687.188275 a.u.
H(298K) = -687.172489 a.u.
G(298K) = -687.229140 a.u.

RC-4-OC (RC-n-OC, n = 4)

= RC-2-OC (RC-n-OC, n = 2)

TS-4-OC (TS-n-OC, n = 4)

C	3.040248	0.567809	0.049407
H	2.929004	1.558854	-0.392961
O	4.137963	-0.064680	-0.577133
H	3.200583	0.674061	1.128579
C	1.773049	-0.210197	-0.207707
O	1.786301	-1.468297	0.533742
C	0.631373	-0.021861	0.678382
H	1.558003	-0.367988	-1.263245
C	-0.716971	-0.656437	0.397020
H	0.830569	0.298673	1.696218
O	0.395536	2.099477	0.230283
C	-1.886420	0.339891	0.390254
O	-0.695356	-1.410680	-0.785239
H	-0.875554	-1.353960	1.228702
C	-3.193232	-0.425194	0.505748
H	-1.814830	0.993974	1.270750
O	-1.851440	1.073518	-0.808172
O	-4.068504	-0.275804	-0.316796
H	-3.305170	-1.096661	1.370962

H	4.362910	-0.864715	-0.082819
H	-2.739601	1.057040	-1.205626
H	-0.868614	-0.815447	-1.534001
H	-0.381169	2.241075	-0.338181
H	1.328870	-2.148457	0.003124
H	0.250725	2.631219	1.026400

E + ZPE = -687.128617 a.u.

H(298K) = -687.113510 a.u.

G(298K) = -687.169114 a.u.

PC-4-OC (PC-n-OC, n = 4)

C	2.860641	0.528639	-0.009207
H	2.650702	1.554171	-0.320639
O	3.910326	0.032177	-0.810403
H	3.119786	0.533493	1.054622
C	1.596728	-0.250852	-0.225925
O	1.598985	-1.552732	0.554609
C	0.619132	-0.455570	0.839984
H	1.300676	-0.431812	-1.255953
C	-0.805352	-0.907791	0.572503
H	0.824072	-0.027782	1.816818
O	0.553902	2.565226	0.447620
C	-1.727171	0.296184	0.377447
O	-0.832146	-1.774093	-0.537716
H	-1.133256	-1.480150	1.445811
C	-3.173984	-0.157678	0.329301
H	-1.627136	0.966270	1.245393
O	-1.366532	0.946108	-0.817923
O	-3.881652	0.141514	-0.606425
H	-3.540018	-0.748793	1.182601
H	4.249655	-0.785087	-0.420524
H	-2.176770	1.118033	-1.329227
H	-0.941031	-1.251194	-1.350186
H	-0.147938	2.299299	-0.169130
H	1.139237	-2.252228	0.028472
H	0.199008	3.322589	0.929215

E + ZPE = -687.142288 a.u.

H(298K) = -687.126601 a.u.

G(298K) = -687.183587 a.u.

RC-5-OC (RC-n-OC, n = 5)

= RC-3-OC (RC-n-OC, n = 3)

TS-5-OC (TS-n-OC, n = 5)

C	-3.045412	-0.472131	0.413419
H	-3.012770	-1.479731	0.846762
O	-3.951773	-0.375598	-0.661353
H	-3.277820	0.233453	1.220881

C	-1.687453	-0.140158	-0.084497
O	-1.828314	2.049415	0.161517
C	-0.502076	-0.359782	0.736295
H	-1.534453	0.091298	-1.133286
C	0.752838	0.465132	0.455160
H	-0.675643	-0.502976	1.802172
O	-0.629906	-1.652024	0.077488
C	2.002814	-0.424441	0.514519
O	0.698430	1.156152	-0.773108
H	0.799042	1.223738	1.242035
C	3.248127	0.435248	0.471462
H	2.010501	-0.981126	1.462124
O	1.970982	-1.309477	-0.584335
O	4.064042	0.298645	-0.413759
H	3.369667	1.179025	1.273530
H	-4.845140	-0.537454	-0.330835
H	2.775416	-1.171948	-1.114965
H	0.905158	0.548057	-1.501167
H	0.035719	-1.739658	-0.636784
H	-1.108475	2.351976	-0.415520
H	-2.641916	2.425225	-0.204687

E + ZPE = -687.130363 a.u.

H(298K) = -687.114917 a.u.

G(298K) = -687.171410 a.u.

PC-5-OC (PC-n-OC, n = 5)

C	-2.860170	-1.100230	-0.194840
H	-3.218357	-1.634214	-1.078841
O	-3.561393	0.126613	-0.019660
H	-2.964502	-1.742220	0.686766
C	-1.418291	-0.711991	-0.377627
O	-1.816128	2.367539	-0.005454
C	-0.559588	-0.486028	0.792230
H	-1.162221	-0.197168	-1.299934
C	0.643076	0.452340	0.693998
H	-0.959166	-0.672789	1.784713
O	-0.455992	-1.716030	0.001626
C	1.950848	-0.344071	0.665217
O	0.632735	1.240315	-0.470827
H	0.655744	1.069554	1.600230
C	3.113724	0.559322	0.313317
H	2.126544	-0.861086	1.611089
O	1.881937	-1.366346	-0.368784
O	3.707693	0.405874	-0.729323
H	3.359337	1.347865	1.038204
H	-4.472652	0.029831	-0.324124
H	2.314473	-1.055493	-1.194903
H	-0.191891	1.774658	-0.452875
H	0.845604	-1.650209	-0.460532
H	-2.107049	3.176890	-0.444312
H	-2.554280	1.734617	-0.079865

E + ZPE = -687.150110 a.u.

H(298K) = -687.134997 a.u.

G(298K) = -687.190967 a.u.

RC-6-OC (RC-n-OC, n = 6)

```
-----  
C      -2.946891  0.690086  -0.092103  
C      -1.787083  -0.256900  0.164939  
C      -0.484391  0.373857  -0.323813  
O      -0.395290  1.627261  0.334996  
O      -2.095337  -1.435647  -0.567892  
C      0.725091  -0.509070  0.008079  
O      0.931471  -0.574550  1.406889  
C      1.989824  -0.015014  -0.712045  
O      2.235776  1.350900  -0.454499  
C      3.160086  -0.861818  -0.272289  
O      4.131349  -0.366004  0.259257  
O      -4.149683  -0.131674  0.171982  
H      -2.993432  1.523303  0.602256  
H      -2.995099  1.012369  -1.133125  
H      -1.718911  -0.476339  1.236096  
H      -0.546848  0.499332  -1.414185  
H      0.528817  -1.530182  -0.336834  
H      1.852600  -0.165451  -1.792122  
H      3.080533  -1.946733  -0.444820  
H      -3.994166  -1.025612  -0.222817  
H      3.042029  1.418557  0.084933  
H      0.876872  0.325208  1.764653  
H      0.444891  2.039839  0.074022  
H      -1.808900  -2.217393  -0.076476  
H      -4.974493  0.253965  -0.184066  
-----
```

E + ZPE = -687.175705 a.u.
H(298K) = -687.161119 a.u.
G(298K) = -687.215843 a.u.

TS-6-OC (TS-n-OC, n = 6)

```
-----  
C      -2.453698  0.488824  -0.531506  
H      -2.670166  1.519378  -0.278289  
O      -4.664073  0.037328  -0.192639  
H      -2.599612  0.137585  -1.547418  
C      -1.804270  -0.331365  0.393519  
O      -1.745730  -1.655442  0.098561  
C      -0.480589  0.621557  -0.198257  
H      -1.795707  -0.057631  1.446618  
C      0.668981  -0.400294  -0.207498  
H      -0.554544  1.036864  -1.214631  
O      -0.366071  1.612119  0.773562  
C      1.958095  0.275952  -0.708310  
O      0.839915  -0.981202  1.063445  
H      0.413375  -1.203525  -0.903549  
C      3.083153  -0.735724  -0.643961  
H      1.814282  0.554659  -1.761217  
O      2.270273  1.420451  0.049516  
O      4.077047  -0.515957  0.013498  
H      2.947437  -1.670479  -1.209712  
H      -4.893516  -0.804753  -0.609751  
H      3.086055  1.245202  0.549918  
H      1.042603  -0.286849  1.710240  
H      0.478806  2.076127  0.632188  
H      -1.174745  -2.097570  0.747636  
H      -5.215184  0.698923  -0.633494  
-----
```

E + ZPE = -687.128051 a.u.

H(298K) = -687.111964 a.u.
G(298K) = -687.169871 a.u.

PC-6-OC (PC-n-OC, n = 6)

```
-----  
C      1.326143  -1.574784  -0.735061  
H      1.792088  -2.518450  -0.416022  
O      4.154880  1.739473  0.662256  
H      1.402671  -1.493041  -1.820865  
C      2.116954  -0.511853  -0.082092  
O      2.937267  0.163696  -0.735598  
C      -0.127621  -1.581981  -0.257153  
H      2.047770  -0.361475  0.997895  
C      -0.787398  -0.250203  -0.634018  
H      -0.658380  -2.400811  -0.757031  
O      -0.084721  -1.777998  1.146787  
C      -2.275108  -0.193049  -0.269294  
O      -0.076143  0.819333  -0.030796  
H      -0.695169  -0.119316  -1.717233  
C      -2.860130  1.121504  -0.734148  
H      -2.794652  -0.996995  -0.810308  
O      -2.445455  -0.346876  1.122039  
O      -3.395527  1.878138  0.047908  
H      -2.772261  1.354399  -1.806822  
H      5.085248  1.503626  0.797410  
H      -2.916606  0.433101  1.462025  
H      -0.252138  0.804620  0.923992  
H      -0.962433  -1.596182  1.518872  
H      3.502202  0.877692  -0.129191  
H      4.142220  2.648898  0.327114  
-----
```

E + ZPE = -687.197828 a.u.
H(298K) = -687.182351 a.u.
G(298K) = -687.239571 a.u.

In Figure 8.

RC-1-OC (RC-n-OC, n = 1)

= PC-5-BP-Iso-2 (PC-n-BP-Iso-m, n = 5, m = 2)

TS-1-OC (TS-n-OC, n = 1)

```
-----  
C      2.924087  -0.558940  -0.699476  
O      4.193287  -0.210066  -0.156473  
C      1.888619  0.056803  0.225618  
O      2.065948  1.461868  0.294594  
C      0.472286  -0.198707  -0.283803  
C      -0.560279  0.521765  0.603979  
C      -1.917713  0.492049  -0.084902  
C      -2.926601  -0.416893  0.260266  
O      -3.987109  -0.481514  -0.510389  
O      0.243595  -1.594555  -0.205281  
O      -0.639128  -0.063115  1.874799  
-----
```

O	-2.002399	1.252023	-1.172764
H	2.796075	-1.645127	-0.739284
H	2.807315	-0.138665	-1.706479
H	1.994961	-0.388639	1.226118
H	0.384589	0.168560	-1.312930
H	-0.278837	1.572317	0.712417
H	-2.751840	0.823487	0.866855
H	-2.814045	-1.064740	1.126078
H	4.882235	-0.426241	-0.797152
H	-2.792878	1.049352	-1.704046
H	-0.458074	-1.013919	1.784400
H	-0.344245	-1.876643	-0.918692
H	3.011142	1.624337	0.431530
H	-4.712340	-0.977674	-0.094797

E + ZPE = -687.148001 a.u.
H(298K) = -687.133849 a.u.
G(298K) = -687.187322 a.u.

PC-1-OC (PC-n-OC, n = 1)

C	3.022686	-0.148656	-0.788894
O	4.242305	0.021420	-0.074579
C	1.916807	-0.012027	0.244015
O	1.986092	1.255434	0.873472
C	0.538754	-0.116696	-0.403561
C	-0.559773	0.114489	0.668817
C	-1.882726	0.395237	0.039304
C	-3.093606	-0.430895	0.288044
O	-4.174624	0.146603	-0.393260
O	0.406705	-1.426886	-0.914360
O	-0.657769	-0.965590	1.552460
O	-1.983415	1.391286	-0.725307
H	2.976524	-1.133019	-1.264868
H	2.908470	0.632992	-1.550342
H	2.022610	-0.814054	0.989545
H	0.444341	0.641536	-1.188813
H	-0.300214	1.019971	1.233736
H	-3.264893	-0.446088	1.372035
H	-2.865818	-1.459789	-0.020291
H	4.964945	0.143767	-0.702765
H	-2.921125	1.459002	-1.049148
H	-0.487862	-1.781767	1.051657
H	-0.139481	-1.424223	-1.712868
H	2.908881	1.399395	1.130832
H	-4.453563	-0.424557	-1.122457

E + ZPE = -687.177228 a.u.
H(298K) = -687.162425 a.u.
G(298K) = -687.217718 a.u.

In Figure 12.

12T (12T)

Si	2.879446	2.180101	2.468566
H	3.542558	2.853776	3.542057
O	1.673370	0.948131	2.849424

O	1.926763	3.141615	1.355577
O	3.867654	1.316360	1.313248
Si	0.741096	0.079231	1.673144
O	-0.468419	-0.097913	3.074278
Al	-1.843588	-0.829160	2.153001
O	-2.720262	-2.264316	2.494870
Si	-3.370879	-3.110170	1.107279
H	-4.205845	-4.249543	1.326626
O	0.088121	1.309630	0.765190
O	2.035020	-0.540120	0.777425
O	-2.757928	0.248562	1.181964
O	-0.311181	-1.289838	1.140238
O	-3.983296	-1.793247	0.133466
O	-1.859269	-3.339805	0.254341
Si	0.996759	2.593748	-0.013539
Si	-3.226931	-0.311159	-0.395445
Si	-0.697043	-2.221777	-0.363249
Si	3.262713	0.417017	-0.042202
O	-3.870659	0.838632	-1.448034
O	-1.780588	-1.064205	-1.030560
O	0.557172	-2.890735	-1.252352
O	4.237702	-0.471495	-1.090839
O	2.249970	1.644134	-0.759221
O	0.037547	3.638393	-0.920280
Si	1.868010	-3.777788	-1.922070
O	3.195022	-2.741398	-2.208320
Si	4.538994	-1.685250	-2.269085
Si	-1.347589	4.392474	-1.602866
Si	-3.814660	2.201451	-2.494982
O	-2.518940	3.223917	-2.039804
H	2.259946	-4.824767	-1.005854
H	1.436042	-4.319394	-3.191235
H	5.746404	-2.397821	-1.918343
H	4.637146	-1.091793	-3.582607
H	-1.913823	5.306334	-0.636203
H	-0.923525	5.086956	-2.798486
H	-5.060553	2.923108	-2.359742
H	-3.613763	1.753128	-3.854637
H	-0.339145	0.598400	3.726817

E + ZPE = -1064.462645 a.u.
H(298K) = -1064.425794 a.u.
G(298K) = -1064.530022 a.u.

β -glucopyranose (12T)

C	-1.210799	-1.210694	-0.307599
C	-1.656266	0.159957	0.202126
C	-0.641820	1.208622	-0.209032
C	0.727562	0.794265	0.295776
C	1.075979	-0.600850	-0.228127
O	0.069722	-1.516355	0.194660
H	-1.704772	0.119342	1.303310
O	-0.925526	2.479722	0.338718
H	-0.615047	1.266285	-1.309670
H	0.695536	0.752295	1.396789
O	1.725404	1.702311	-0.128737
H	1.125775	-0.574297	-1.328885
C	2.411675	-1.110707	0.304032
H	-1.212418	-1.218633	-1.408326
O	-2.098066	-2.205067	0.097564
O	-2.901571	0.530541	-0.345097

```
H      -1.884695  -2.434583  1.012904
H      -3.534796  -0.177579  -0.167625
H      -1.814894  2.738358  0.064538
H      1.416320  2.595903  0.074513
H      2.490268  -2.176328  0.074668
O      3.503627  -0.469381  -0.310506
H      2.430923  -0.995053  1.398742
H      3.381097  0.486557  -0.226831
```

```
-----
E + ZPE = -686.757161 a.u.
H(298K) = -686.744235 a.u.
G(298K) = -686.794218 a.u.
```

In Figure 13.

RC-1(12T) [RC-1(12T), n = 1]

```
-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
  8      -0.905000  0.115999  -1.846962
 13      -0.267444  1.585017  -0.819654
 14      -0.071847  -1.322673  -1.487674
  1      -1.877787  -0.085565  -1.918133
  8      -3.307530  -0.965114  -1.683948
  1      -3.213426  -1.883542  -1.977098
  6      -3.813321  -0.959077  -0.319693
  8      -5.187174  -1.142149  -0.328502
  6      -6.063005  -0.042865  -0.657806
  6      -5.342346  1.297313  -0.595456
  6      -4.414634  1.328358  0.612185
  6      -3.297312  0.324532  0.375652
  6      -6.726541  -0.307590  -1.999813
  8      -5.834968  -0.215026  -3.090571
  1      -4.994360  -0.620619  -2.839917
  1      -7.201369  -1.298083  -1.960977
  1      -7.501577  0.447987  -2.154946
  1      -4.739789  1.442679  -1.510270
  8      -6.327725  2.299043  -0.506946
  1      -5.874039  3.093184  -0.188200
  1      -4.974132  1.058162  1.516733
  8      -3.925241  2.638881  0.798678
  1      -3.089766  2.763488  0.305798
  1      -3.391509  -1.817527  0.206526
  1      -2.626548  0.830736  -0.331098
  8      -2.614489  0.000913  1.547158
  1      -1.654615  0.150243  1.384597
  8      -0.118926  0.802582  0.759194
  8      1.259864  2.029257  -1.467433
  8      -1.278643  2.998830  -0.551805
  8      1.486162  -0.898854  -1.500850
  8      -0.578921  -1.862926  -0.035918
  8      -0.379442  -2.489744  -2.599114
  1      -6.835649  -0.036411  0.119982
 14      -0.474086  4.202014  0.462185
 14      2.293092  2.998839  -0.463915
 14      0.767368  1.713644  1.962668
 14      2.748313  -2.040102  -1.070117
 14      0.355068  -3.146193  0.735955
 14      0.539848  -3.991068  -2.351793
  8      0.163468  -4.171357  -0.660583
```

```
  8      1.967647  -2.619142  0.367360
  8      2.103067  -3.262589  -2.133205
  1      0.360849  -5.082819  -3.253680
  8      1.156207  4.284691  -0.170668
  8      2.182841  2.191158  1.077956
  8      -0.113673  3.207905  1.855903
  1      -1.162389  5.440133  0.668397
  8      3.871042  3.172878  -1.051403
 14      5.293081  2.615271  -1.829318
  8      5.518607  0.965411  -1.405499
 14      5.804707  -0.636009  -0.905112
  8      4.344675  -1.549683  -1.054760
  8      0.000862  -3.517585  2.328780
 14      -0.293308  -3.170880  3.999429
  8      0.473898  -1.685930  4.330857
 14      1.203274  -0.183846  4.727477
  8      0.980639  0.901201  3.426282
  1      6.419523  3.374587  -1.334013
  1      5.175394  2.723439  -3.265125
  1      6.221856  -0.679338  0.476955
  1      6.777446  -1.250721  -1.779676
  1      0.324035  -4.226170  4.770679
  1      -1.716981  -3.105691  4.226014
  1      0.563373  0.340554  5.912328
  1      2.616078  -0.403140  4.941209
```

```
-----
E + ZPE = -1751.230285 a.u.
H(298K) = -1751.179727 a.u.
G(298K) = -1751.315185 a.u.
```

TS-1(12T) [TS-n(12T), n = 1]

```
-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
  8      -0.914702  0.158407  -1.807761
 13      -0.193265  1.574365  -0.949315
 14      -0.189551  -1.242015  -1.404503
  1      -2.438002  -0.407618  -2.122074
  8      -3.206069  -1.037400  -1.986772
  1      -2.810171  -1.908523  -2.173146
  6      -3.749850  -0.833766  -0.016522
  8      -5.003277  -1.074359  -0.123961
  6      -5.970335  -0.014846  -0.471196
  6      -5.271427  1.318138  -0.687865
  6      -4.265270  1.586181  0.424581
  6      -3.171607  0.530452  0.331561
  6      -6.734632  -0.519066  -1.683769
  8      -5.974665  -0.508046  -2.864512
  1      -5.108891  -0.917115  -2.718488
  1      -7.127596  -1.520593  -1.458557
  1      -7.577658  0.159367  -1.839132
  1      -4.742187  1.301340  -1.655393
  8      -6.285601  2.290415  -0.700391
  1      -5.838944  3.145187  -0.602593
  1      -4.766218  1.504626  1.400080
  8      -3.779623  2.894977  0.292213
  1      -2.874069  2.926144  -0.098420
  1      -3.136601  -1.687153  0.268885
  1      -2.522581  0.825461  -0.498371
  8      -2.467082  0.342807  1.506892
  1      -1.477314  0.490936  1.297789
  8      -0.094562  0.954486  0.754336
```

8	1.392602	1.945347	-1.523004
8	-1.130881	3.070757	-0.744883
8	1.437152	-1.097714	-1.446509
8	-0.662090	-1.754516	0.100013
8	-0.622680	-2.508078	-2.405752
1	-6.635136	0.051517	0.395097
14	-0.259341	4.299763	0.178274
14	2.466031	2.925086	-0.591435
14	0.852754	1.903037	1.881344
14	2.603190	-2.319277	-0.995653
14	0.199958	-3.070175	0.899067
14	0.196970	-4.059148	-2.104415
8	-0.148224	-4.190805	-0.394770
8	1.866977	-2.771002	0.517641
8	1.863339	-3.564745	-1.975042
1	-0.137564	-5.158601	-2.955569
8	1.388642	4.285739	-0.412822
8	2.309648	2.252307	1.012144
8	0.026015	3.417221	1.664111
1	-0.897237	5.578968	0.280805
8	4.057235	2.948967	-1.176904
14	5.400437	2.202442	-1.938867
8	5.500162	0.561351	-1.440453
14	5.711978	-1.045868	-0.915270
8	4.230403	-1.922468	-1.041417
8	-0.194762	-3.292302	2.517702
14	-0.429957	-2.811681	4.158789
8	0.422027	-1.357659	4.409531
14	1.246499	0.116438	4.717964
8	1.004439	1.176433	3.401521
1	6.601652	2.880588	-1.501908
1	5.272367	2.253608	-3.377615
1	6.138917	-1.072893	0.465105
1	6.666480	-1.706999	-1.777435
1	0.108524	-3.849821	5.008702
1	-1.847287	-2.635035	4.381796
1	0.685820	0.704788	5.914155
1	2.653929	-0.168871	4.883286

 E + ZPE = -1751.205283 a.u.

H(298K) = -1751.155302 a.u.

G(298K) = -1751.287656 a.u.

PC-1(12T) [PC-n(12T), n = 1]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.959597	0.247922	-1.785669
13	-0.114792	1.584207	-0.939077
14	-0.340584	-1.200697	-1.408606
1	-2.737306	-0.401418	-2.485346
8	-3.334025	-1.137621	-2.260438
1	-2.808718	-1.925192	-2.480565
6	-3.797722	-0.685253	0.250283
8	-5.018318	-0.889747	0.016575
6	-5.948949	0.204685	-0.368144
6	-5.174790	1.471740	-0.690910
6	-4.139102	1.785598	0.386014
6	-3.131390	0.642416	0.408142
6	-6.764198	-0.347933	-1.526658
8	-6.044989	-0.431187	-2.724021

1	-5.206763	-0.910564	-2.606554
1	-7.184650	-1.317783	-1.223740
1	-7.589109	0.350556	-1.691867
1	-4.660875	1.342566	-1.657873
8	-6.135163	2.492850	-0.775124
1	-5.640425	3.326818	-0.772064
1	-4.638824	1.833535	1.366175
8	-3.588887	3.038777	0.106681
1	-2.639146	3.014440	-0.192866
1	-3.193292	-1.569603	0.458926
1	-2.501088	0.718364	-0.495480
8	-2.385266	0.536936	1.569403
1	-1.388400	0.636699	1.318975
8	-0.013288	0.954186	0.770512
8	1.477512	1.915275	-1.522870
8	-0.983150	3.121630	-0.684713
8	1.299514	-1.124623	-1.422760
8	-0.832374	-1.719656	0.091716
8	-0.765192	-2.453481	-2.434575
1	-6.580173	0.351517	0.513474
14	-0.052533	4.304337	0.242648
14	2.603042	2.844400	-0.602874
14	1.005509	1.843142	1.886398
14	2.453756	-2.361304	-0.991482
14	0.021806	-3.055367	0.868974
14	0.027076	-4.020993	-2.142058
8	-0.337001	-4.158402	-0.435999
8	1.703088	-2.807401	0.517786
8	1.708158	-3.586293	-1.993457
1	-0.328263	-5.103563	-3.006772
8	1.581108	4.240750	-0.382505
8	2.455821	2.150195	0.993330
8	0.231373	3.390143	1.709077
1	-0.641463	5.603694	0.378138
8	4.184345	2.821307	-1.213677
14	5.492534	2.018750	-1.980352
8	5.514218	0.378240	-1.473519
14	5.622138	-1.225815	-0.907700
8	4.092182	-2.012225	-1.029208
8	-0.387829	-3.275265	2.486346
14	-0.562766	-2.794028	4.133972
8	0.396671	-1.409165	4.388225
14	1.348572	-0.011671	4.685841
8	1.152970	1.084832	3.391501
1	6.723949	2.645255	-1.550665
1	5.360062	2.071608	-3.418565
1	6.037085	-1.245380	0.476460
1	6.543767	-1.960901	-1.745531
1	-0.098037	-3.876572	4.971816
1	-1.960972	-2.512063	4.372694
1	0.874241	0.602472	5.906287
1	2.732839	-0.411073	4.803000

 E + ZPE = -1751.210065 a.u.

H(298K) = -1751.159045 a.u.

G(298K) = -1751.293341 a.u.

PC'-1 (12T)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z

8	-1.637179	-2.541595	-3.569201
6	-3.713287	-1.686442	-1.383716
8	-4.952323	-1.866989	-0.811522
6	-5.548797	-0.720890	-0.201863
6	-5.466821	0.458584	-1.168228
6	-4.022303	0.877485	-1.355429
6	-3.200408	-0.349201	-1.709269
6	-6.984932	-1.112144	0.130898
8	-7.580957	-0.222211	1.046154
1	-7.564752	-1.188744	-0.801325
1	-6.969570	-2.098798	0.600922
1	-1.252509	-1.655387	-3.565988
1	-0.898268	-3.106149	-3.305435
1	-3.405107	-2.555799	-1.953067
1	-2.492818	-0.234616	-2.528181
8	-2.706199	-1.095317	-0.580958
1	-1.042720	-0.215998	0.275907
1	-3.072780	2.204256	-2.395342
8	-3.986323	1.855164	-2.368182
1	-3.652605	1.286202	-0.400096
1	-5.862332	0.131233	-2.143187
8	-6.243038	1.528892	-0.658888
1	-6.049839	2.303494	-1.204511
1	-5.024958	-0.476139	0.732850
1	-7.523972	0.666344	0.668596
8	-0.097370	-0.371990	-2.270418
14	0.853354	-1.471859	-1.555571
13	-0.160647	1.209717	-1.514938
8	-0.799124	0.722456	0.261976
8	-1.277795	2.520941	-1.883337
8	1.385613	1.899479	-1.186750
8	0.305152	-1.768334	-0.005340
8	2.399412	-0.925141	-1.419508
8	0.956469	-2.963095	-2.287320
14	1.203671	-2.773972	1.129204
14	2.018352	-4.194367	-1.568286
14	3.670237	-1.715700	-0.509017
14	-1.185280	3.973356	-0.901400
14	-0.687471	1.997966	1.528510
14	1.765058	3.165493	-0.088413
8	2.788005	-2.079135	0.947432
8	1.411847	-4.139472	0.069208
8	3.469098	-3.260668	-1.297428
1	2.125034	-5.457966	-2.227623
1	-2.002900	5.083075	-1.281713
8	-1.529664	3.203330	0.646343
8	0.511851	4.256958	-0.619093
8	-1.180368	1.355822	2.993332
14	-1.473675	0.480443	4.445488
1	-2.899797	0.388475	4.650653
1	-0.812183	1.159175	5.535987
8	-0.803866	-1.078304	4.248061
14	-0.249589	-2.696610	4.171335
1	-1.373252	-3.601586	4.233730
1	0.686607	-2.926968	5.247543
8	0.565450	-2.900984	2.676088
8	5.130737	-0.892941	-0.397444
14	6.286153	0.378000	-0.493617
1	6.731757	0.518536	-1.860808
1	7.379530	0.040663	0.390072
8	5.578299	1.841375	0.041527
14	5.055396	3.407151	0.493391
1	5.268512	3.588331	1.911411

1	5.771762	4.394018	-0.282660
8	3.378457	3.572221	0.155290
8	0.921057	2.540172	1.319898

E + ZPE = -1751.249260 a.u.
 H(298K) = -1751.197449 a.u.
 G(298K) = -1751.336106 a.u.

In Figure 15

RC-Iso(12T)

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	1.308137	0.645279	-0.579319
14	0.195982	1.809488	-0.100552
13	0.534650	-1.058861	-0.566801
1	2.334684	0.695034	-0.637042
8	3.797721	0.475694	-0.568857
6	4.508164	0.733278	0.640812
6	5.950342	1.098363	0.274494
6	6.536948	-0.020806	-0.570544
6	5.687459	-0.344437	-1.789777
6	4.266252	-0.677815	-1.357094
6	3.739267	1.860853	1.316697
8	4.507476	2.317726	2.422391
1	4.009952	2.984159	2.906591
1	3.584563	2.666985	0.586642
1	2.759856	1.491951	1.648860
1	4.512309	-0.162186	1.280521
1	5.941604	2.031758	-0.312362
8	6.798374	1.211796	1.397946
1	6.389974	1.821316	2.028985
1	6.585852	-0.923371	0.061967
8	7.830408	0.306420	-1.037272
1	8.367946	0.541051	-0.269222
1	5.635622	0.531880	-2.454041
8	3.436305	-0.816891	-2.411797
1	4.252438	-1.548375	-0.680843
1	2.686536	-1.458461	-2.183388
8	6.211712	-1.463586	-2.460797
1	7.155197	-1.300620	-2.590383
8	-0.989517	-0.800894	-1.350208
8	0.339956	-1.748497	1.008910
8	1.508836	-2.206072	-1.533961
8	0.830641	3.226139	0.437309
8	-0.846756	2.111223	-1.304078
8	-0.538944	1.057460	1.145583
14	-1.952533	1.703042	1.959929
14	-2.389889	2.879904	-0.953129
14	-0.396157	4.352918	1.071697
14	-2.025367	-2.177440	-1.551997
14	-0.644884	-3.178013	1.088010
14	0.698918	-3.770343	-1.696695
8	-0.883709	-3.289801	-2.257651
8	0.263338	-4.143598	-0.044029
8	-2.011191	-2.810584	0.069903
1	1.394827	-4.779958	-2.436286
8	-2.855093	2.107972	0.532675
8	-1.562213	4.228041	-0.213765


```

8      -1.187792  3.260966  2.171517
1      0.041435  5.632999  1.530485
8      -2.674570  0.856336  3.207759
14     -3.357672  -0.344379  4.243444
8      -2.371202  -1.732211  4.263407
14     -1.474777  -3.197952  4.290143
8      -1.048308  -3.601396  2.679982
8      -3.525666  2.906636  -2.185299
14     -4.442342  2.211023  -3.476876
8      -4.675149  0.561211  -3.116353
14     -4.955450  -1.107286  -2.826293
8      -3.517355  -1.847802  -2.274547
1      -0.294587  -3.013922  5.104155
1      -2.319097  -4.243358  4.824750
1      -4.678970  -0.664434  3.754840
1      -3.403310  0.226074  5.571308
1      -5.355854  -1.721671  -4.072434
1      -5.987308  -1.232608  -1.821395
1      -5.718229  2.890151  -3.507028
1      -3.721613  2.378206  -4.716939
    
```

 E + ZPE = -1751.238512 a.u.
 H(298K) = -1751.188502 a.u.
 G(298K) = -1751.321484 a.u.

TS-Iso(12T)

```

-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
8          1.404348  0.650864  -0.461060
14         0.271584  1.754318  0.028326
13         0.564859  -0.982441  -0.565378
1          2.698643  0.739551  -0.665997
8          3.809300  0.707876  -0.780295
6          4.482453  1.208402  0.387665
6          5.992556  1.098001  0.161083
6          6.374645  -0.308352  -0.258477
6          5.651900  -0.753936  -1.516567
6          4.149278  -0.814353  -1.288403
6          4.035645  2.658336  0.533049
8          4.795849  3.243557  1.585329
1          4.399093  4.081492  1.841904
1          4.230215  3.170845  -0.418772
1          2.966127  2.711838  0.753318
1          4.197968  0.619861  1.271287
1          6.284038  1.798810  -0.638742
8          6.725822  1.346620  1.342188
1          6.453658  2.203714  1.700450
1          6.111136  -0.995860  0.562966
8          7.759756  -0.391572  -0.527322
1          8.228152  -0.042786  0.242848
1          5.844518  -0.050109  -2.339984
8          3.427633  -1.023251  -2.338111
1          3.884737  -1.399254  -0.388264
1          2.462268  -1.653421  -2.085786
8          6.045987  -2.061135  -1.859131
1          7.010590  -2.090073  -1.800419
8          -0.967905  -0.736139  -1.342562
8          0.395886  -1.831238  0.934248
8          1.472397  -2.167243  -1.656072
8          0.829128  3.173930  0.678761
    
```

```

8      -0.760192  2.160541  -1.170337
8      -0.545432  0.973936  1.221823
14     -1.986368  1.578889  2.015696
14     -2.312978  2.909468  -0.827632
14     -0.427441  4.253551  1.335698
14     -2.059262  -2.054455  -1.587985
14     -0.645881  -3.216059  0.977430
14     0.608520  -3.719057  -1.867111
8      -0.950297  -3.155424  -2.374538
8      0.225574  -4.139954  -0.226188
8      -2.016106  -2.779933  -0.006366
1      1.286179  -4.688173  -2.672592
8      -2.855626  2.051807  0.586198
8      -1.561182  4.245277  0.011256
8      -1.274417  3.136107  2.370601
1      0.010024  5.503928  1.874336
8      -2.746440  0.650798  3.185212
14     -3.454322  -0.590677  4.146214
8      -2.437421  -1.959650  4.170988
14     -1.499892  -3.396078  4.165617
8      -1.044733  -3.723252  2.542830
8      -3.408304  3.008443  -2.097319
14     -4.305844  2.394246  -3.436803
8      -4.638222  0.750285  -3.120962
14     -4.982758  -0.896632  -2.799561
8      -3.551988  -1.678326  -2.277766
1      -0.331348  -3.212540  4.995934
1      -2.314754  -4.490070  4.645818
1      -4.741813  -0.931722  3.586198
1      -3.580194  -0.076247  5.491731
1      -5.434551  -1.518208  -4.024369
1      -5.988407  -0.979330  -1.764610
1      -5.546028  3.134072  -3.507790
1      -3.534588  2.538227  -4.649323
    
```

 E + ZPE = -1751.235234 a.u.
 H(298K) = -1751.184968 a.u.
 G(298K) = -1751.319687 a.u.

PC-Iso(12T)

```

-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
8          0.678398  0.507502  -2.058701
14         -0.105975  1.633408  -1.181562
13         0.261297  -1.113047  -1.483834
1          2.426439  1.114699  -2.401905
8          3.305964  1.530632  -2.344116
6          3.503701  2.084460  -1.061259
6          4.526235  1.258405  -0.266144
6          4.117707  -0.220927  -0.289664
6          4.665802  -0.944094  -1.558325
6          3.601114  -1.884462  -2.061733
6          3.953194  3.519706  -1.291895
8          4.278202  4.112557  -0.032508
1          4.650013  4.988979  -0.169572
1          4.830348  3.506565  -1.952294
1          3.138144  4.059946  -1.784543
1          2.578147  2.085065  -0.468864
1          5.536055  1.373854  -0.695021
8          4.531317  1.637635  1.100764
    
```

1	4.580113	2.604245	1.144757
1	3.018714	-0.285998	-0.254640
8	4.644834	-0.916365	0.825807
1	4.676501	-0.285007	1.560186
1	4.851582	-0.209945	-2.345107
8	2.871896	-1.606537	-2.998109
1	3.503993	-2.845775	-1.522803
1	1.366788	-2.564399	-3.081785
8	5.842060	-1.663938	-1.287834
1	5.899578	-1.749520	-0.321867
8	-1.453470	-1.253556	-1.277574
8	1.124989	-1.666299	-0.076091
8	0.542145	-2.705096	-2.587472
8	0.454917	3.192619	-1.275956
8	-1.721911	1.711344	-1.483669
8	0.091840	1.177790	0.406602
14	-0.662841	1.984260	1.767306
14	-2.838079	2.561729	-0.429406
14	-0.293608	4.411355	-0.223686
14	-2.353876	-2.472117	-0.469365
14	0.468314	-2.936015	0.904543
14	-0.188228	-4.237831	-1.905057
8	-1.789936	-3.771888	-1.519383
8	0.569809	-4.160237	-0.360772
8	-1.264095	-2.772335	0.850881
1	0.047651	-5.354337	-2.764902
8	-2.287885	2.060476	1.144963
8	-1.985985	4.081627	-0.511724
8	-0.165759	3.595427	1.315551
1	0.167747	5.760899	-0.328103
8	-0.419048	1.350738	3.303200
14	-0.202972	0.358690	4.688887
8	0.735922	-1.008856	4.279890
14	1.681158	-2.396021	3.941578
8	1.119081	-3.059133	2.456000
8	-4.475541	2.340102	-0.752017
14	-5.880695	1.452997	-1.196059
8	-5.723630	-0.115493	-0.531941
14	-5.566324	-1.665494	0.168516
8	-3.993168	-2.265192	-0.169084
1	3.075667	-2.032633	3.843660
1	1.465109	-3.380734	4.978537
1	-1.499065	-0.068189	5.165224
1	0.500590	1.130069	5.688915
1	-6.531546	-2.555436	-0.436660
1	-5.746121	-1.581463	1.599656
1	-7.029038	2.105724	-0.608437
1	-5.994609	1.376864	-2.633870

E + ZPE = -1751.245473 a.u.
H(298K) = -1751.193175 a.u.
G(298K) = -1751.333404 a.u.

In the supporting information

In Figure 3S

RC-1-BP-1W

C 1.605318 -0.821294 -0.066769

C	1.673569	0.685785	-0.264605
C	0.426116	1.306656	0.340493
C	-0.801042	0.797641	-0.421394
O	-0.582553	-0.360784	-1.150762
C	0.259776	-1.386212	-0.584466
O	2.783982	1.244898	0.407662
O	0.415646	2.713972	0.234974
O	-1.883472	0.607226	0.531391
C	-0.490928	-2.208421	0.446885
O	-0.802068	-1.362529	1.568239
O	2.710665	-1.376245	-0.760845
H	3.591346	0.893642	0.006637
H	1.720990	0.914303	-1.338989
H	0.365664	1.004907	1.395757
H	-1.619164	-0.209202	1.115612
H	-1.157260	1.554829	-1.120009
H	1.167293	3.057146	0.739121
H	0.477702	-2.042215	-1.430103
H	2.916810	-2.245829	-0.393131
H	1.703916	-1.023888	1.007504
H	0.146792	-3.031630	0.779974
H	-1.413866	-2.604685	0.014050
H	-1.189048	-1.883305	2.287039
H	-2.830707	0.470777	0.037494
O	-4.001918	0.360485	-0.672130
H	-4.293944	-0.555417	-0.793228
H	-4.745637	0.839451	-0.276809

E + ZPE = -763.591254 a.u.
H(298K) = -763.575304 a.u.
G(298K) = -763.632643 a.u.

TS-1-BP-1W

O -0.565722 0.247012 1.184589
C 0.503846 1.219936 0.861136
C 1.489994 0.662845 -0.164661
C 1.762116 -0.811263 0.096297
C 0.465387 -1.577048 -0.104255
C -0.662123 -0.888612 0.642458
C -0.214484 2.483921 0.419234
O -0.780731 2.377816 -0.869676
O 2.712756 1.357637 -0.033494
O 2.701846 -1.325137 -0.816618
O 0.590025 -2.871706 0.428282
O -1.922785 -0.257726 -1.018431
O -4.394948 -0.433783 -0.001619
H 3.518890 -0.814379 -0.718615
H 2.108724 -0.945389 1.132100
H 0.227247 -1.594772 -1.172931
H -1.871181 -0.713942 -1.870693
H -1.494119 -1.492512 0.997661
H 0.025792 -3.484190 -0.063808
H 1.005370 1.380389 1.818025
H 2.733373 2.099812 -0.651902
H 1.085642 0.776014 -1.177510
H 0.526974 3.286831 0.384789
H -0.966764 2.740439 1.174328
H -1.358523 1.594639 -0.920662
H -2.857874 -0.354829 -0.701525
H -5.066346 -0.857276 -0.552874
H -4.409167 -0.912406 0.838093

E + ZPE = -763.561363 a.u.
H(298K) = -763.544140 a.u.
G(298K) = -763.605143 a.u.

PC-1-BP-1W

O 0.536871 0.259029 -1.196404
C -0.547752 1.223622 -0.866630
C -1.527771 0.650492 0.157010
C -1.784711 -0.829329 -0.091775
C -0.470617 -1.574193 0.077387
C 0.612069 -0.898202 -0.724903
C 0.171826 2.481983 -0.410528
O 0.748942 2.352295 0.869539
O -2.758623 1.329373 0.023328
O -2.689804 -1.349732 0.850878
O -0.588734 -2.894933 -0.383939
O 2.035492 -0.154424 1.078707
O 4.508849 -0.444977 -0.045126
H -3.520132 -0.858299 0.766175
H -2.158312 -0.974437 -1.116225
H -0.167301 -1.529933 1.131738
H 2.010385 -0.523556 1.971540
H 1.473505 -1.477052 -1.054193
H -0.054146 -3.484160 0.166116
H -1.043637 1.385665 -1.825925
H -2.786927 2.075258 0.637201
H -1.124559 0.773002 1.168953
H -0.573842 3.280045 -0.356770
H 0.915166 2.754611 -1.168793
H 1.347801 1.580424 0.899773
H 2.954166 -0.282577 0.749172
H 5.198689 -0.870083 0.481090
H 4.466926 -0.948200 -0.869090

E + ZPE = -763.562285 a.u.
H(298K) = -763.543940 a.u.
G(298K) = -763.607530 a.u.

RC-2-BP-1W

O 0.342213 -1.446549 0.205559
C -0.868674 -1.006559 -0.377231
C -1.151428 0.403640 0.124449
C 0.000457 1.332402 -0.233549
C 1.309548 0.753254 0.294350
C 1.471757 -0.684187 -0.210395
O -1.891035 -1.846433 0.056871
O -0.256690 2.645877 0.226234
O 2.423026 1.498895 -0.166680
C 2.705051 -1.375010 0.362860
O 3.902811 -0.877905 -0.210033
O -2.355069 0.881686 -0.499974
O -4.219342 -0.414335 0.336084
H -1.298049 0.366919 1.212194
H 0.068881 1.411343 -1.325561
H 1.286957 0.738218 1.394762
H 1.540994 -0.678199 -1.309678
H -0.780665 -1.019528 -1.473118

H -1.847525 -2.682775 -0.429703
H -3.428166 0.247256 -0.070585
H -0.286252 2.649741 1.195335
H 2.401793 2.379538 0.232849
H 2.651360 -2.439335 0.122080
H 2.710787 -1.263114 1.455467
H 3.901996 0.085988 -0.105170
H -2.416770 1.845696 -0.369888
H -3.838264 -1.315884 0.317814
H -5.034656 -0.397010 -0.194204

E + ZPE = -763.592349 a.u.
H(298K) = -763.576869 a.u.
G(298K) = -763.632606 a.u.

TS-2-BP-1W

O 0.273004 -1.168564 0.327363
C -0.900550 -1.039180 -0.595592
C -0.875023 0.172171 0.205109
C 0.045500 1.310649 -0.176690
C 1.468316 0.838684 0.193792
C 1.527158 -0.639894 -0.175161
O -1.859291 -1.934204 -0.296209
O -0.314783 2.522442 0.429467
O 2.480293 1.534598 -0.484978
C 2.656497 -1.408709 0.499525
O 3.901447 -1.008670 -0.041960
O -2.630223 1.228884 -0.588718
O -4.307506 -0.584090 0.579358
H -1.378355 0.154898 1.167063
H -0.004505 1.470887 -1.258018
H 1.587031 0.934679 1.283215
H 1.576063 -0.770822 -1.262296
H -0.572279 -1.005817 -1.633397
H -1.802255 -2.708000 -0.879049
H -3.382619 0.739982 -0.188941
H -0.171591 2.470636 1.386742
H 2.613405 2.396639 -0.066216
H 2.543136 -2.474800 0.294271
H 2.614742 -1.246466 1.583434
H 3.997471 -0.050107 0.062126
H -2.597976 2.097135 -0.161606
H -3.725484 -1.328818 0.362464
H -5.171690 -0.805533 0.209716

E + ZPE = -763.529243 a.u.
H(298K) = -763.512145 a.u.
G(298K) = -763.571307 a.u.

PC-2-BP-1W

O 0.503609 -1.188526 -0.442707
C -1.739678 -0.454940 -0.869447
C -0.477852 -0.241220 -0.059647
C 0.174346 1.115694 -0.324359
C 1.602787 0.843815 0.133218
C 1.813714 -0.593014 -0.361601
O -2.323234 -1.655102 -0.524439
O -0.506607 2.201246 0.272848
O 2.578114 1.691149 -0.431231

C	2.678341	-1.450880	0.550561
O	4.005339	-0.952283	0.613984
O	-2.683906	0.603032	-0.508473
O	-4.029977	-0.153276	1.336066
H	-0.730501	-0.342377	1.009125
H	0.186888	1.323151	-1.401343
H	1.644775	0.883534	1.233075
H	2.250681	-0.558282	-1.367549
H	-1.556472	-0.369723	-1.943544
H	-2.867607	-1.986051	-1.253180
H	-3.395210	0.241446	0.437341
H	-0.459089	2.132376	1.239381
H	2.529865	2.553841	0.002477
H	2.740824	-2.463510	0.145291
H	2.220459	-1.498507	1.547250
H	4.003052	-0.099971	1.070538
H	-2.213389	1.439889	-0.291226
H	-4.068820	-1.125235	1.303809
H	-4.942097	0.182776	1.327814

E + ZPE = -763.583024 a.u.
H(298K) = -763.566844 a.u.
G(298K) = -763.625462 a.u.

RC-3-BP-1W

C	0.335849	-1.587654	0.299209
C	-0.816787	-0.687739	-0.108595
C	-0.474001	0.768557	0.138665
C	0.839871	1.084291	-0.595893
O	1.864193	0.204550	-0.141420
C	1.606949	-1.157687	-0.437040
O	2.712449	-1.905815	-0.061338
O	-0.054168	-2.905271	-0.028909
O	-1.532660	1.574887	-0.368078
C	1.309293	2.505833	-0.372043
O	1.382270	2.747105	1.026014
O	-1.975317	-1.051083	0.669786
O	-3.852075	0.245253	-0.130317
H	0.507679	-1.486445	1.380594
H	-1.048800	-0.840969	-1.171826
H	-0.347455	0.935691	1.214053
H	0.681125	0.943781	-1.676532
H	1.484113	-1.295789	-1.519921
H	2.830537	-1.842953	0.899111
H	0.467153	-3.534538	0.487530
H	-2.062840	-2.021854	0.653589
H	-1.521154	2.433376	0.078144
H	0.605135	3.193955	-0.854054
H	2.290485	2.624189	-0.844832
H	1.713386	3.642554	1.168836
H	-3.070540	-0.441768	0.243969
H	-4.367821	-0.143593	-0.857379
H	-3.325576	1.003755	-0.473000

E + ZPE = -763.594474 a.u.
H(298K) = -763.578790 a.u.
G(298K) = -763.635264 a.u.

TS-3-BP-1W

C	-0.124195	1.647425	0.457240
C	0.664343	0.628552	-0.055800
C	0.320606	-0.786333	0.179169
C	-1.020835	-1.056694	-0.606510
O	-1.951514	-0.033538	-0.304488
C	-1.550179	1.204982	-0.663418
O	-2.441518	2.163762	-0.373851
O	0.246161	2.926693	0.156350
O	1.314948	-1.628219	-0.354919
C	-1.629525	-2.385905	-0.216001
O	-1.856799	-2.379158	1.181869
O	2.661409	0.590910	1.296851
O	3.946836	-0.635924	-0.833780
H	-0.630672	1.494252	1.410746
H	1.352190	0.860073	-0.868598
H	0.140296	-0.982452	1.239296
H	-0.787073	-1.056901	-1.677306
H	-1.170859	1.328871	-1.677636
H	-2.888434	1.981056	0.471339
H	-0.398206	3.546858	0.527508
H	2.864672	1.515059	1.492377
H	1.418437	-2.403068	0.214211
H	-0.934059	-3.180429	-0.508594
H	-2.564901	-2.514163	-0.771481
H	-2.239004	-3.227796	1.438998
H	3.301533	0.311099	0.611846
H	4.129934	-0.148516	-1.646731
H	3.088686	-1.072317	-0.968316

E + ZPE = -763.535781 a.u.
H(298K) = -763.517681 a.u.
G(298K) = -763.579449 a.u.

PC-3-BP-1W

C	1.212360	1.269719	0.717919
C	0.793511	0.374876	-0.180442
C	-0.200072	-0.680930	0.175782
C	-1.508812	-0.506503	-0.620007
O	-2.174466	0.662894	-0.013965
C	-1.972028	1.813876	-0.495969
O	-2.450081	2.846013	0.072228
O	2.113659	2.230603	0.385140
O	0.339486	-1.960848	-0.139861
C	-2.460804	-1.674140	-0.504369
O	-2.439427	-2.130098	0.838443
O	4.248446	0.480272	-0.648395
O	3.136354	-1.943740	0.272403
H	0.866010	1.274786	1.749020
H	1.162378	0.403692	-1.204944
H	-0.446663	-0.626197	1.242021
H	-1.320190	-0.278088	-1.672089
H	-1.412704	1.976411	-1.416472
H	-2.940773	2.645945	0.897054
H	2.315102	2.786926	1.150325
H	3.654319	1.184239	-0.348849
H	-0.181584	-2.633293	0.327394
H	-2.111694	-2.451354	-1.192746
H	-3.463151	-1.359511	-0.812211
H	-3.051264	-2.872339	0.926838
H	3.839139	-0.350846	-0.340161
H	3.538272	-2.733175	-0.111305

H 2.176103 -2.029348 0.120681

E + ZPE = -763.566529 a.u.

H(298K) = -763.547566 a.u.

G(298K) = -763.612528 a.u.

RC-4-BP-1W

O 0.518188 -1.602559 -0.196301
C 1.647223 -1.067355 0.482956
C 1.980428 0.297132 -0.119511
C 0.774343 1.224902 -0.041541
C -0.435739 0.548586 -0.661632
C -0.657928 -0.827913 -0.014397
O 2.694775 -1.968683 0.367971
O 3.029408 0.932115 0.583141
O 1.020395 2.430673 -0.735966
C -1.787471 -1.642583 -0.630137
O -3.031753 -1.049921 -0.263841
O -1.567301 1.420217 -0.464554
H 2.246972 0.152810 -1.177434
H 0.556508 1.432596 1.018366
H -0.285283 0.428102 -1.739743
H -0.849127 -0.700482 1.063457
H 1.426381 -0.972997 1.554853
H 2.981592 -2.018355 -0.557253
H 3.870593 0.525237 0.336014
H 1.811379 2.836065 -0.352199
H -2.147646 1.397194 -1.241764
H -1.718326 -2.662380 -0.239620
H -1.681058 -1.664549 -1.720677
H -3.756651 -1.579231 -0.621149
H -2.319133 1.244491 0.632270
O -2.947267 0.928868 1.474095
H -3.347271 0.085086 1.153880
H -3.645630 1.574120 1.680217

E + ZPE = -763.591047 a.u.

H(298K) = -763.575398 a.u.

G(298K) = -763.631437 a.u.

TS-4-BP-1W

O -0.480072 -1.596551 0.017206
C -1.572568 -1.010161 -0.684090
C -2.119181 0.141894 0.168373
C -0.991268 1.128598 0.472549
C 0.307832 0.584580 0.670239
C 0.647331 -0.763884 0.148964
O -2.518494 -1.986652 -0.916160
O -3.107206 0.877321 -0.507185
O -1.329175 2.201654 1.269556
C 1.619874 -1.467378 1.108569
O 2.796269 -0.683930 1.150832
O 1.547055 1.861768 -1.127416
H -2.492420 -0.258195 1.119859
H -0.597642 1.488681 -0.546207
H 1.072692 1.160052 1.186520
H 1.159784 -0.613650 -0.817622
H -1.239563 -0.642795 -1.663626

H -2.898133 -2.286360 -0.075171
H -3.967694 0.457311 -0.374464
H -2.138697 2.598754 0.911281
H 1.771137 2.765372 -0.868658
H 1.805666 -2.464584 0.699491
H 1.164492 -1.558293 2.098798
H 3.321715 -0.931730 1.923566
H 2.401132 1.404340 -1.284721
O 3.717536 0.186888 -1.350718
H 3.657304 -0.197907 -0.457327
H 4.620809 0.513122 -1.448254

E + ZPE = -763.526452 a.u.

H(298K) = -763.508409 a.u.

G(298K) = -763.570093 a.u.

PC-4-BP-1W

C 0.893934 -0.823510 0.042172
O -0.215908 -1.700209 -0.083544
C -1.354748 -1.055204 -0.623542
C -1.847313 -0.016751 0.408615
C -0.721403 0.824320 0.916175
C 0.608034 0.232274 1.126764
O -2.326132 -1.996237 -0.898862
O -2.844267 0.837888 -0.070616
O -0.967081 2.002640 1.306314
C 2.118154 -1.649741 0.387169
O 3.203676 -0.729011 0.438265
O -0.112206 1.645191 -1.353859
O 2.701149 1.628728 -1.113679
H -2.169829 -0.577108 1.302822
H 1.364804 1.017053 1.180865
H 0.559420 -0.274291 2.103356
H 1.069591 -0.331765 -0.920493
H -1.109227 -0.553811 -1.564599
H -2.604595 -2.442472 -0.083956
H -3.717031 0.504074 0.178418
H -1.899817 2.246682 1.096088
H -0.509131 2.523911 -1.421950
H 2.273125 -2.400825 -0.393059
H 1.982579 -2.148231 1.354056
H 4.036613 -1.214195 0.499351
H 0.855849 1.788472 -1.316345
H 3.051405 0.869645 -0.611741
H 3.122456 2.412605 -0.739082

E + ZPE = -763.589142 a.u.

H(298K) = -763.571880 a.u.

G(298K) = -763.630868 a.u.

RC-6-BP-1W

C -0.520277 -0.767916 0.729879
O 0.455125 -1.545334 0.044333
C 1.779608 -1.060763 0.235106
C 1.901029 0.355965 -0.336604
C 0.841407 1.259022 0.280094
C -0.524840 0.624488 0.094381
O 2.659923 -1.948032 -0.365999

O	3.161469	0.916294	-0.033382
O	0.789395	2.531101	-0.338794
O	-1.536466	1.439066	0.697549
C	-1.844199	-1.506692	0.666456
O	-2.480428	-1.450423	-0.619697
O	-3.515083	0.774395	-0.702202
H	1.741431	0.309737	-1.424630
H	1.044865	1.370308	1.355536
H	-0.726875	0.531922	-0.982126
H	-0.251153	-0.681926	1.793800
H	2.018327	-1.055673	1.307160
H	2.531546	-1.929413	-1.327056
H	3.839584	0.471059	-0.559633
H	1.545796	3.056099	-0.043758
H	-1.270768	2.369662	0.590426
H	-2.552654	-1.056883	1.364588
H	-1.684525	-2.550685	0.944944
H	-1.904902	-1.788502	-1.323038
H	-3.177278	-0.225925	-0.790267
H	-4.400776	0.806700	-0.302621
H	-2.820460	1.212370	-0.073661

E + ZPE = -763.598960 a.u.
H(298K) = -763.583785 a.u.
G(298K) = -763.638575 a.u.

TS-6-BP-1W

C	-0.525509	-0.692768	0.562799
O	0.390476	-1.553442	0.063392
C	1.782070	-1.147267	0.198678
C	1.975725	0.252817	-0.388101
C	1.017444	1.233701	0.274998
C	-0.412396	0.746877	0.098002
O	2.543939	-2.110340	-0.417578
O	3.283581	0.710201	-0.128732
O	1.071781	2.514403	-0.313146
O	-1.338183	1.538799	0.802888
C	-1.703417	-1.215862	1.093851
O	-3.108428	-1.650247	-0.560787
O	-3.612431	1.021465	-0.872897
H	1.772209	0.219532	-1.468400
H	1.246844	1.292394	1.349689
H	-0.654877	0.729238	-0.976558
H	-0.546965	-0.711483	1.815358
H	2.032565	-1.161165	1.264894
H	2.443710	-2.049810	-1.380927
H	3.900420	0.283911	-0.738969
H	1.904273	2.937904	-0.062327
H	-1.071540	2.467000	0.703365
H	-2.457152	-0.527872	1.458396
H	-1.736363	-2.266332	1.359158
H	-2.623881	-2.019064	-1.311831
H	-3.356487	-0.731625	-0.810448
H	-4.498926	1.299291	-0.609043
H	-3.003219	1.406398	-0.218831

E + ZPE = -763.536163 a.u.
H(298K) = -763.519264 a.u.
G(298K) = -763.577893 a.u.

PC-6-BP-1W

C	-0.553068	0.719786	0.248133
C	-0.600105	-0.666644	0.825063
O	0.405486	-1.425731	0.770668
C	1.796168	-1.023782	0.310549
C	1.775811	0.321130	-0.412034
C	0.855550	1.291383	0.317198
C	-1.786670	-1.161653	1.535576
O	2.282040	-2.068966	-0.401368
O	3.077928	0.852774	-0.396654
O	0.797453	2.540464	-0.326643
O	-1.518012	1.514629	0.888267
O	-1.771096	-1.658876	-1.358663
O	-3.434517	0.604841	-1.115491
H	1.413579	0.189165	-1.440557
H	1.173269	1.403593	1.363041
H	-0.809761	0.580251	-0.816090
H	-1.770097	-0.667091	2.517577
H	2.332815	-0.958460	1.257699
H	1.947804	-2.056723	-1.312591
H	3.573406	0.518360	-1.156619
H	1.617842	3.022689	-0.151584
H	-1.356951	2.433980	0.620351
H	-2.700093	-0.846011	1.029987
H	-1.735921	-2.241335	1.662394
H	-1.365313	-1.741582	-2.230679
H	-2.446781	-0.959284	-1.443976
H	-4.383984	0.476411	-0.994384
H	-3.130188	1.091625	-0.332426

E + ZPE = -763.585578 a.u.
H(298K) = -763.566900 a.u.
G(298K) = -763.629828 a.u.

In Figure 4S

RC-5-BP-1W

C	-0.495559	1.327670	-0.274486
O	-0.935184	0.023449	-0.789555
C	-0.544860	-1.224047	-0.122594
C	0.992461	-1.281008	-0.003061
C	1.638286	0.019019	-0.467926
C	0.955072	1.202311	0.201074
C	-1.284232	-1.408459	1.186405
O	-0.828771	-0.432584	2.116996
H	-1.194959	-0.626504	2.990245
H	-1.064707	-2.419552	1.546218
H	-2.363176	-1.312936	1.020629
H	-0.874768	-1.995123	-0.822014
O	1.540455	-2.315548	-0.800646
H	1.484224	-3.153224	-0.322244
H	1.261469	-1.434049	1.048999
H	1.538416	0.103842	-1.559412
O	2.999503	0.071114	-0.092473
H	3.484302	-0.602121	-0.589851
H	0.975675	1.056943	1.289539
O	1.574550	2.425025	-0.140884
H	2.492890	2.384912	0.162786
H	-0.541142	1.971232	-1.153883

O	-1.377852	1.810449	0.658568
H	-1.295927	1.262855	1.465636
H	-2.032957	0.037906	-1.131506
O	-3.232429	0.093300	-1.494164
H	-3.526687	-0.689848	-1.986453
H	-3.831843	0.201106	-0.737899

E + ZPE = -763.586375 a.u.

H(298K) = -763.570385 a.u.

G(298K) = -763.627206 a.u.

TS-5-BP-Iso-1-1W

C	-1.277897	-0.701680	-0.551817
C	-2.636526	-0.596427	0.049595
O	-2.721791	-1.104139	1.353676
C	-0.200492	-1.490965	0.024279
O	-0.816089	-2.474091	-0.849695
C	1.213378	-1.165643	-0.378493
O	2.006905	-2.268855	0.000822
C	1.692318	0.105494	0.327471
O	3.051523	0.235355	-0.038474
C	0.919835	1.360937	-0.081162
O	1.471513	2.499464	0.520154
O	-0.425540	1.189433	0.303531
O	-1.843291	3.194011	-0.720333
H	1.592861	-0.027581	1.415529
H	1.258549	-1.011355	-1.466676
H	-0.306382	-1.753064	1.076605
H	-1.134582	-0.308154	-1.554215
H	1.001738	1.526385	-1.162010
H	1.410248	2.403961	1.483901
H	3.462138	0.917986	0.509874
H	2.934188	-2.018424	-0.127711
H	-3.323824	-1.162381	-0.587987
H	-2.931058	0.457368	-0.022186
H	-2.336203	-0.467243	1.971919
H	-1.374351	-3.080171	-0.328553
H	-1.746654	3.270926	-1.679320
H	-1.604140	4.061130	-0.365837
H	-0.952056	1.950899	-0.060009

E + ZPE = -763.535147 a.u.

H(298K) = -763.517741 a.u.

G(298K) = -763.579273 a.u.

PC-5-BP-Iso-1-1W

C	-1.608506	-0.044905	-0.556570
C	-2.759121	0.642107	0.137215
O	-3.407757	-0.274000	0.996994
C	-0.783477	-1.023995	0.129765
O	-1.881530	-1.513109	-0.784632
C	0.567017	-1.428904	-0.383913
O	0.694348	-2.809521	-0.115056
C	1.687882	-0.646374	0.307281
O	2.876028	-1.207914	-0.213666
C	1.631558	0.857102	0.034335
O	2.832251	1.469305	0.447265
O	0.525981	1.360686	0.718585
O	-0.429438	3.455450	-0.735137

H	1.626608	-0.804060	1.395399
H	0.619172	-1.237214	-1.465271
H	-1.009372	-1.266118	1.165198
H	-1.230367	0.396802	-1.473781
H	1.563528	1.050706	-1.043711
H	2.879904	1.427095	1.415267
H	3.629203	-0.728186	0.160614
H	1.611351	-3.061676	-0.302602
H	-3.478915	0.970603	-0.614918
H	-2.365555	1.515598	0.664018
H	-3.093728	-0.164889	1.904938
H	-2.665754	-1.764027	-0.236139
H	-0.446002	3.220522	-1.672632
H	0.054328	4.290560	-0.687483
H	0.214403	2.176918	0.267604

E + ZPE = -763.544636 a.u.

H(298K) = -763.527008 a.u.

G(298K) = -763.588863 a.u.

TS-5-BP-Iso-2-1W

C	2.067052	1.392274	-0.188746
O	1.706921	2.472769	0.329552
C	1.908626	0.037310	0.433617
O	3.252652	-0.363814	0.574491
C	1.073903	-0.911247	-0.482876
O	1.838889	-2.092018	-0.595259
C	-0.302776	-1.232298	0.107954
O	-0.766582	-2.358074	-0.621015
C	-1.273587	-0.060867	-0.043232
C	-2.544435	-0.259251	0.774878
O	-3.179325	-1.451575	0.318724
O	-0.614480	1.116520	0.391240
O	-1.951639	3.155127	-0.815267
H	1.455750	0.127432	1.424654
H	0.935895	-0.462739	-1.478173
H	-0.183241	-1.492821	1.171525
H	-1.530284	0.019923	-1.109991
H	2.632703	1.488181	-1.116422
H	1.149443	2.345003	1.131249
H	3.405748	-1.132265	-0.002280
H	1.295810	-2.754916	-1.048432
H	-3.201745	0.608214	0.638858
H	-2.276059	-0.341516	1.835176
H	-3.895664	-1.684541	0.922595
H	-1.689887	-2.514241	-0.360191
H	-2.861527	3.257348	-0.506191
H	-2.017186	3.022784	-1.770411
H	-1.083944	1.887143	-0.001278

E + ZPE = -763.547138 a.u.

H(298K) = -763.529719 a.u.

G(298K) = -763.591357 a.u.

PC-5-BP-Iso-2-1W

C	-3.272183	-0.847580	-0.463532
O	-4.549943	-0.223381	-0.396261
C	-2.282607	0.174575	0.069538
O	-2.637449	0.569986	1.383405

C	-0.874158	-0.407040	0.154449
C	0.121568	0.617171	0.685433
C	1.568811	0.158796	0.895907
C	2.045849	1.264545	-0.063541
O	2.735868	0.851089	-1.120789
O	-0.492552	-0.793363	-1.154345
O	0.510079	1.541355	-0.430506
O	1.759495	-1.131790	0.397674
H	-3.018050	-1.117296	-1.492879
H	-3.245968	-1.744879	0.167838
H	-2.279378	1.047953	-0.600989
H	-0.876820	-1.258823	0.846039
H	-0.281414	1.235243	1.485063
H	1.952936	0.280156	1.910962
H	2.348024	2.212708	0.376443
H	-5.233909	-0.880070	-0.577917
H	2.727697	-1.319453	0.390114
H	0.281657	1.098905	-1.285740
H	0.319980	-1.321985	-1.077974
H	-3.587701	0.758423	1.379317
H	3.177166	1.590618	-1.567979
O	4.450266	-1.241737	0.371037
H	4.923931	-2.081521	0.435114
H	4.742054	-0.840047	-0.458649

E + ZPE = -763.552217 a.u.
H(298K) = -763.535037 a.u.
G(298K) = -763.596009 a.u.

In Figure 5S

RC-1-BP-2W

C	1.747081	-0.956862	-0.077688
C	1.923788	0.488921	-0.515807
C	0.915914	1.343734	0.232521
C	-0.503878	0.944442	-0.184479
O	-0.559572	-0.344980	-0.748282
C	0.267154	-1.392760	-0.200762
O	3.210308	0.976371	-0.186776
O	1.053824	2.718284	-0.065200
O	-1.408105	1.088014	0.900282
C	-0.312854	-1.949401	1.085593
O	-0.225988	-0.951961	2.106003
O	2.599561	-1.743889	-0.895077
H	3.865272	0.479139	-0.696174
H	1.750686	0.570066	-1.598617
H	1.045641	1.174993	1.311220
H	-1.137092	0.440192	1.597311
H	-0.858684	1.622427	-0.963497
H	1.942262	2.993566	0.202769
H	0.214998	-2.183470	-0.953288
H	2.786609	-2.580304	-0.448805
H	2.069023	-1.030578	0.969006
H	0.266549	-2.833094	1.372569
H	-1.357447	-2.236199	0.921392
H	-0.509489	-1.328508	2.950168
H	-2.794260	0.965882	0.522079
O	-3.754972	0.767817	0.148133
H	-4.176013	1.588583	-0.154429
H	-3.612419	0.092421	-0.667082

O	-3.164048	-0.771870	-1.669247
H	-3.526585	-1.667831	-1.615124
H	-2.200362	-0.838013	-1.504448

E + ZPE = -839.989581 a.u.
H(298K) = -839.971771 a.u.
G(298K) = -840.033088 a.u.

TS-1-BP-2W

C	-0.440946	1.358066	0.637970
O	0.116385	0.390774	1.219664
C	-0.194314	-1.029425	0.928688
C	-1.285415	-1.171608	-0.133954
C	-2.358480	-0.108611	0.055388
C	-1.723945	1.255193	-0.160009
C	1.131964	-1.674984	0.569561
O	1.586206	-1.359810	-0.736413
O	-1.895080	-2.435184	0.020212
O	-3.389128	-0.251542	-0.891226
O	-2.587347	2.261102	0.306676
O	1.029655	1.397935	-1.040446
O	3.292369	1.756199	0.266922
O	4.311115	-0.723820	-0.369428
H	-3.780472	-1.129525	-0.771744
H	-2.756823	-0.166134	1.079434
H	-1.481888	1.377557	-1.221942
H	0.905241	1.891277	-1.863018
H	-0.090951	2.340297	0.948951
H	-2.468966	3.065699	-0.217025
H	-0.551149	-1.416799	1.885440
H	-1.471223	-3.073543	-0.568215
H	-0.859709	-1.068431	-1.139345
H	0.992196	-2.758108	0.611301
H	1.873490	-1.390120	1.326160
H	1.447884	-0.411751	-0.936823
H	1.889914	1.693612	-0.634497
H	3.900121	2.472305	0.042718
H	3.771225	0.917245	0.086304
H	4.732095	-1.232694	0.334855
H	3.462436	-1.167913	-0.556098

E + ZPE = -839.955909 a.u.
H(298K) = -839.936217 a.u.
G(298K) = -840.002466 a.u.

PC-1-BP-2W

C	-0.527739	1.360754	0.738090
O	0.061227	0.386116	1.256106
C	-0.246056	-1.035936	0.943535
C	-1.329857	-1.166185	-0.128170
C	-2.402199	-0.097381	0.039320
C	-1.745858	1.262609	-0.139647
C	1.086810	-1.662047	0.575756
O	1.542187	-1.299450	-0.715495
O	-1.948596	-2.426078	0.017971
O	-3.395645	-0.220620	-0.947708
O	-2.628513	2.291411	0.221052
O	1.179885	1.455481	-1.011815
O	3.514319	1.701033	0.308398

O	4.307561	-0.836855	-0.437200
H	-3.801795	-1.094770	-0.852437
H	-2.838089	-0.164019	1.046993
H	-1.397182	1.359232	-1.177344
H	1.152634	1.834261	-1.900299
H	-0.175048	2.338603	1.063422
H	-2.488291	3.059161	-0.350411
H	-0.602239	-1.432641	1.896563
H	-1.523015	-3.065787	-0.567823
H	-0.888937	-1.065488	-1.126930
H	0.950271	-2.746537	0.581803
H	1.821655	-1.399410	1.346565
H	1.444010	-0.333624	-0.865282
H	2.041193	1.722304	-0.607552
H	4.162345	2.378911	0.079376
H	3.925969	0.837612	0.087253
H	4.728487	-1.396099	0.227670
H	3.418035	-1.210907	-0.585338

E + ZPE = -839.955944 a.u.
H(298K) = -839.935435 a.u.
G(298K) = -840.003525 a.u.

RC-2-BP-2W

O	0.553763	1.353890	-0.628377
C	-0.709637	0.767642	-0.388362
C	-0.652147	-0.707316	-0.797327
C	0.433500	-1.417862	0.000631
C	1.752934	-0.678093	-0.167730
C	1.581784	0.799213	0.188130
O	-1.673970	1.491364	-1.085062
O	0.630799	-2.743678	-0.450584
O	2.753742	-1.218077	0.679537
C	2.842404	1.617785	-0.070236
O	3.854530	1.340500	0.882948
O	-1.891633	-1.370105	-0.539726
O	-3.339218	-0.657616	1.424851
O	-3.849835	1.588426	0.628626
H	-0.424244	-0.776387	-1.868132
H	0.155867	-1.414231	1.065647
H	2.065989	-0.751388	-1.220258
H	1.305320	0.889123	1.250778
H	-0.965751	0.864820	0.676890
H	-1.580359	1.362159	-2.042131
H	-2.745773	-1.032757	0.678173
H	-0.119688	-3.285813	-0.172122
H	2.912561	-2.136460	0.419091
H	2.595173	2.677968	0.022481
H	3.197435	1.429129	-1.092614
H	3.998446	0.381587	0.890433
H	-2.455563	-1.335681	-1.327055
H	-3.645503	0.338636	1.102907
H	-4.108333	-1.236186	1.551867
H	-4.748449	1.736845	0.299098
H	-3.235581	1.722795	-0.123386

E + ZPE = -839.992729 a.u.
H(298K) = -839.974705 a.u.
G(298K) = -840.036335 a.u.

TS-2-BP-2W

O	-0.615283	-0.988719	-0.910601
C	0.804010	-0.826202	-0.479836
C	0.381651	0.490084	-0.943212
C	-0.397806	1.382937	-0.007533
C	-1.810900	0.777254	0.067068
C	-1.617664	-0.736216	0.108130
O	1.652991	-1.603611	-1.176503
O	-0.485877	2.693194	-0.492334
O	-2.534442	1.183708	1.199353
C	-2.863149	-1.533510	-0.258402
O	-3.823609	-1.426959	0.776100
O	2.138014	1.763174	-0.687624
O	3.192129	0.675042	1.488068
O	3.631696	-1.977944	0.898892
H	0.441089	0.724054	-2.001646
H	0.055362	1.347262	0.992315
H	-2.337715	1.048069	-0.858728
H	-1.239629	-1.057612	1.085350
H	0.905495	-0.995706	0.591118
H	1.752119	-1.315298	-2.098414
H	2.625313	1.396029	0.097965
H	0.415286	3.053355	-0.512189
H	-2.888137	2.071986	1.051992
H	-2.604097	-2.590007	-0.349240
H	-3.259046	-1.178071	-1.217650
H	-4.003696	-0.489966	0.944694
H	2.725312	1.679137	-1.451152
H	3.435579	-0.262570	1.326272
H	3.973988	1.099631	1.863436
H	4.542009	-2.293514	0.833926
H	3.238972	-2.105962	0.021836

E + ZPE = -839.923006 a.u.
H(298K) = -839.903046 a.u.
G(298K) = -839.969422 a.u.

PC-2-BP-2W

O	-0.826838	-1.051996	-0.577575
C	1.355913	-0.119023	-0.176880
C	-0.034695	0.125348	-0.742130
C	-0.775049	1.262734	-0.015170
C	-2.201602	0.735082	0.004289
C	-1.974411	-0.755695	0.221484
O	2.004102	-1.200374	-0.783957
O	-0.709268	2.508098	-0.673002
O	-3.025534	1.255508	1.026472
C	-3.131653	-1.633206	-0.222795
O	-4.262130	-1.426866	0.611683
O	2.115077	1.081311	-0.280975
O	4.333276	0.750913	0.939616
O	4.369583	-1.652288	0.573531
H	0.044826	0.359535	-1.814098
H	-0.418277	1.352611	1.020085
H	-2.655452	0.901910	-0.983824
H	-1.759188	-0.937690	1.285386
H	1.309024	-0.347361	0.890412
H	1.951176	-1.136485	-1.750621
H	3.480829	1.002168	0.436305
H	0.144396	2.919239	-0.481318

H	-3.298096	2.151300	0.785130
H	-2.857436	-2.687281	-0.134347
H	-3.366868	-1.417296	-1.273511
H	-4.436171	-0.475159	0.667541
H	2.188813	1.361577	-1.208684
H	4.462364	-0.325989	0.791115
H	5.084036	1.247523	0.575138
H	5.126990	-2.027153	0.100881
H	3.581851	-1.747336	-0.004714

E + ZPE = -839.983600 a.u.

H(298K) = -839.965476 a.u.

G(298K) = -840.028017 a.u.

RC-3-BP-2W

C	0.678252	-1.628253	0.319047
O	0.200830	-2.926888	0.032826
C	-0.518503	-0.697092	0.252292
C	-0.077963	0.734982	0.511918
O	-1.152747	1.648944	0.337519
C	1.017941	1.102866	-0.495618
C	1.575525	2.491979	-0.272330
O	2.038110	2.589762	1.067446
O	2.093777	0.173993	-0.389219
C	1.728535	-1.161748	-0.691358
O	2.873068	-1.946078	-0.661445
O	-1.501396	-1.083907	1.222533
O	-3.768959	-0.532083	0.259984
O	-3.112866	1.059018	-1.469553
H	1.119937	-1.586818	1.326282
H	-0.972231	-0.765155	-0.748426
H	0.322454	0.817739	1.528434
H	0.594219	1.064489	-1.512045
H	1.328137	-1.225557	-1.712319
H	3.239378	-1.946006	0.236559
H	0.866778	-3.577277	0.294347
H	-1.445446	-2.049171	1.336705
H	-1.651888	1.720479	1.163136
H	0.783379	3.222245	-0.468003
H	2.393433	2.655522	-0.983266
H	2.378794	3.481467	1.211404
H	-2.872483	-0.798576	0.704397
H	-4.209562	-1.329085	-0.076807
H	-3.562033	0.163405	-0.549274
H	-3.746066	1.759548	-1.683597
H	-2.348071	1.474259	-1.011947

E + ZPE = -839.994310 a.u.

H(298K) = -839.976380 a.u.

G(298K) = -840.037972 a.u.

TS-3-BP-2W

C	-0.226272	1.724171	0.552370
O	0.393897	2.900962	0.236529
C	0.467695	0.551310	0.268717
C	-0.154457	-0.764565	0.540269
O	0.740173	-1.831983	0.351073
C	-1.290590	-0.930402	-0.521232
C	-2.159332	-2.134133	-0.228445

O	-2.693760	-1.997556	1.075703
O	-2.098252	0.233533	-0.480980
C	-1.441337	1.382097	-0.784867
O	-2.234548	2.467468	-0.735057
O	2.173821	0.086160	1.776425
O	4.111946	0.037825	-0.124981
O	2.407541	-1.266802	-1.885668
H	-0.901677	1.742828	1.408747
H	1.283937	0.595588	-0.451446
H	-0.613084	-0.790269	1.533974
H	-0.830015	-1.044803	-1.510222
H	-0.864798	1.382556	-1.711261
H	-2.849196	2.410580	0.016856
H	-0.205493	3.640405	0.415279
H	2.212044	0.792991	2.434417
H	1.407969	-1.764939	1.053872
H	-1.536507	-3.030620	-0.316874
H	-2.952531	-2.176331	-0.982821
H	-3.263675	-2.755744	1.256703
H	2.971318	0.177551	1.203846
H	4.389750	0.889054	-0.486060
H	3.609586	-0.410778	-0.837507
H	2.763252	-1.974798	-2.437515
H	1.798341	-1.690988	-1.255187

E + ZPE = -839.929918 a.u.

H(298K) = -839.909537 a.u.

G(298K) = -839.977016 a.u.

PC-3-BP-2W

C	0.596848	1.833695	0.909320
O	1.190637	2.997476	0.550483
C	0.463297	0.823270	0.044521
C	-0.170590	-0.476284	0.437808
O	0.706340	-1.581791	0.260075
C	-1.381078	-0.798942	-0.450321
C	-2.049139	-2.121306	-0.159896
O	-2.320889	-2.188084	1.228375
O	-2.384658	0.239652	-0.163142
C	-2.355768	1.331462	-0.800140
O	-3.145159	2.278532	-0.486329
O	2.987343	-0.958929	1.584034
O	3.809786	0.379408	-0.678499
O	2.018203	-1.138261	-2.167328
H	0.243738	1.771793	1.937159
H	0.844709	0.918202	-0.972000
H	-0.515772	-0.426027	1.478414
H	-1.118479	-0.736781	-1.511187
H	-1.695681	1.503531	-1.648222
H	-3.715504	2.068752	0.283403
H	1.210282	3.609337	1.298006
H	2.823800	-0.369483	2.331540
H	1.506834	-1.418757	0.816559
H	-1.359747	-2.910877	-0.476082
H	-2.968171	-2.193480	-0.751890
H	-2.781677	-3.015697	1.415243
H	3.361424	-0.397320	0.868914
H	3.517773	1.300235	-0.685434
H	3.216063	-0.093727	-1.299895
H	2.407529	-1.913083	-2.592205
H	1.508630	-1.472015	-1.401427

E + ZPE = -839.962111 a.u.
H(298K) = -839.940357 a.u.
G(298K) = -840.012069 a.u.

RC-4-BP-2W

C -0.366122 -0.903461 -0.155207
O 0.827279 -1.662098 -0.039230
C 1.843577 -1.001520 0.700746
C 2.254119 0.260592 -0.055790
C 1.047526 1.167684 -0.257625
C -0.084561 0.400777 -0.919253
O 2.900851 -1.883009 0.873346
O 3.208683 1.012283 0.666827
O 1.372759 2.276264 -1.073221
C -1.345010 -1.819700 -0.876191
O -2.581636 -1.117211 -1.033679
O -1.232285 1.257418 -0.925379
O -2.255564 1.772611 1.327232
H 2.652014 -0.038633 -1.037275
H 0.708415 1.512114 0.733029
H 0.188778 0.166596 -1.956560
H -0.753157 -0.654920 0.846814
H 1.473369 -0.749116 1.703501
H 3.301691 -2.074268 0.011220
H 4.063513 0.562829 0.626007
H 2.116557 2.738908 -0.661022
H -1.962747 0.772313 -1.350365
H -1.492227 -2.727959 -0.284242
H -0.936554 -2.084367 -1.857060
H -3.158909 -1.615271 -1.628985
H -1.783961 1.677352 0.414906
H -2.924604 0.911688 1.396186
H -2.752047 2.606663 1.355645
O -3.601516 -0.256365 1.352564
H -3.382727 -0.678391 0.487986
H -4.563150 -0.150914 1.392458

E + ZPE = -839.995961 a.u.
H(298K) = -839.978190 a.u.
G(298K) = -840.039038 a.u.

TS-4-BP-2W

C -0.258883 -0.966438 -0.208168
O 0.936709 -1.725972 -0.045379
C 1.930526 -1.003933 0.649684
C 2.226490 0.268246 -0.143232
C 0.690246 1.350421 -0.165597
C 0.149460 0.316100 -0.905594
O 3.059867 -1.791148 0.760942
O 3.060839 1.105457 0.514850
O 1.030935 2.490468 -0.803901
C -1.199478 -1.862116 -1.005389
O -2.532621 -1.386095 -0.851527
O -1.996666 1.276337 -1.382488
O -2.000295 1.940428 1.309287
H 2.523731 0.068010 -1.175412
H 0.483895 1.421163 0.901755
H 0.261125 0.321911 -1.987350

H -0.696379 -0.737133 0.773724
H 1.601025 -0.758878 1.666682
H 3.395354 -2.016850 -0.121347
H 3.601111 1.614971 -0.108225
H 1.399474 3.128436 -0.174708
H -2.512846 0.452428 -1.369854
H -1.104693 -2.869471 -0.590243
H -0.910426 -1.874959 -2.061430
H -3.134624 -1.975217 -1.327324
H -2.092921 1.649297 -0.480908
H -2.427619 1.111105 1.612727
H -2.549689 2.661958 1.640488
O -3.062257 -0.564289 1.802430
H -3.070244 -0.949962 0.907042
H -3.968528 -0.621967 2.130442

E + ZPE = -839.915512 a.u.
H(298K) = -839.895558 a.u.
G(298K) = -839.961685 a.u.

PC-4-BP-2W

C -0.153508 -1.068499 -0.404303
O -1.483815 -1.473195 -0.740601
C -2.411162 -0.433368 -0.446435
C -1.725528 0.371062 0.657513
C 0.164513 1.439198 -0.732232
C -0.243096 0.333780 0.236100
O -3.635771 -0.982348 -0.095369
O -2.334205 1.622949 0.859594
O -0.004850 2.665058 -0.072634
C 0.402421 -2.130506 0.535647
O 1.789070 -1.820713 0.791913
O 2.976227 1.004727 1.578601
O 1.544050 1.260384 -1.054922
H -1.820447 -0.209886 1.585570
H -0.416183 1.419151 -1.660809
H 0.407154 0.413410 1.113233
H 0.436087 -1.046796 -1.328995
H -2.597782 0.180393 -1.335913
H -3.536877 -1.473845 0.734564
H -1.714060 2.323567 0.598797
H -0.003026 3.389512 -0.715611
H 2.661942 0.091602 1.638150
H 0.325326 -3.113709 0.066658
H -0.136122 -2.124150 1.486925
H 2.202385 -2.531617 1.306518
H 2.603868 1.339050 0.748569
H 2.510532 -0.058476 -1.227114
H 1.784814 1.868538 -1.771914
O 2.977993 -0.942119 -1.144769
H 2.531630 -1.423160 -0.285800
H 3.929325 -0.791513 -1.005069

E + ZPE = -839.986450 a.u.
H(298K) = -839.968092 a.u.
G(298K) = -840.030950 a.u.

RC-6-BP-2W

O	-0.542643	0.510536	-0.357895
C	0.507399	1.467311	-0.486072
C	1.689430	1.030537	0.378583
C	2.132877	-0.364090	-0.039605
C	0.960928	-1.331920	0.015700
C	-0.194143	-0.792322	-0.825962
O	-0.008942	2.704005	-0.128037
O	2.795138	1.893697	0.203196
O	3.136216	-0.874875	0.820102
O	1.315790	-2.596424	-0.509835
C	-1.434130	-1.656459	-0.761478
O	-1.855972	-1.800957	0.607097
H	1.368988	1.009501	1.431210
H	2.508258	-0.319815	-1.073683
H	0.629169	-1.426194	1.059432
H	0.119397	-0.736261	-1.879454
H	0.810167	1.541792	-1.538604
H	-0.182668	2.720525	0.826053
H	2.628839	2.724929	0.667675
H	3.941205	-0.352320	0.702048
H	2.089503	-2.915266	-0.023381
H	-1.215935	-2.638605	-1.181961
H	-2.239213	-1.184906	-1.334012
H	-2.123823	-2.715115	0.777894
H	-2.888759	-0.868450	0.963383
O	-3.624062	-0.133357	1.111864
H	-3.584652	0.191093	2.025786
H	-3.445700	0.669251	0.424313
O	-3.095103	1.577678	-0.564549
H	-3.220074	2.504055	-0.312714
H	-2.132241	1.435007	-0.676521

E + ZPE = -839.996889 a.u.
H(298K) = -839.978739 a.u.
G(298K) = -840.040667 a.u.

TS-6-BP-2W

O	0.348488	-0.685035	-0.042047
C	-0.841442	-1.506038	-0.236952
C	-2.038222	-0.821406	0.421720
C	-2.213451	0.576691	-0.157986
C	-0.944524	1.390055	0.056195
C	0.258539	0.607927	-0.436865
O	-0.552248	-2.747997	0.272351
O	-3.221463	-1.537797	0.148621
O	-3.254524	1.280177	0.482004
O	-0.971320	2.620526	-0.616876
C	1.414947	1.234449	-0.893946
O	2.537330	1.782831	0.937578
H	-1.858823	-0.745789	1.504212
H	-2.406731	0.497441	-1.238678
H	-0.785234	1.528657	1.136631
H	0.313706	0.719992	-1.686567
H	-0.995476	-1.618984	-1.315282
H	-0.544522	-2.719895	1.241946
H	-3.287398	-2.295113	0.746016
H	-4.094615	0.852749	0.263699
H	-1.700501	3.146923	-0.258610
H	1.360949	2.283848	-1.157173
H	2.255436	0.619225	-1.200472
H	2.927340	2.660951	0.831049
H	3.289667	1.143444	0.948521

O	4.426686	-0.136339	0.728894
H	4.684886	-0.584015	1.544197
H	3.962101	-0.803339	0.180719
O	2.919403	-1.723044	-0.951610
H	3.190670	-2.634980	-1.118123
H	2.014627	-1.767765	-0.606401

E + ZPE = -839.927617 a.u.
H(298K) = -839.907044 a.u.
G(298K) = -839.974667 a.u.

PC-6-BP-2W

O	0.606447	-0.131301	-0.824604
C	-0.296647	-1.365525	-0.734914
C	-1.587099	-1.061575	0.030941
C	-2.080388	0.350004	-0.248782
C	-1.004895	1.329960	0.203821
C	0.306491	1.035672	-0.460170
O	0.477420	-2.340690	-0.208457
O	-2.576363	-1.964412	-0.410956
O	-3.231066	0.648202	0.504740
O	-1.332632	2.668909	-0.041671
C	1.288737	2.102244	-0.690630
O	0.839513	-0.845510	1.972982
H	-1.408946	-1.170047	1.106512
H	-2.270408	0.481080	-1.323417
H	-0.800422	1.155484	1.276922
H	0.843790	2.794159	-1.416799
H	-0.499138	-1.570413	-1.786431
H	0.657953	-2.097873	0.732212
H	-2.510024	-2.786794	0.092703
H	-3.980499	0.160639	0.135121
H	-2.068196	2.909059	0.539746
H	1.419856	2.667932	0.236916
H	2.226970	1.693436	-1.060871
H	0.730962	-1.061682	2.907474
H	1.718599	-0.409677	1.876423
O	3.149280	0.418712	1.352870
H	3.919103	0.242867	1.908539
H	3.382945	0.105510	0.453612
O	3.536770	-0.400049	-1.261892
H	4.331866	-0.915386	-1.451751
H	2.793445	-0.973853	-1.492615

E + ZPE = -839.982486 a.u.
H(298K) = -839.960735 a.u.
G(298K) = -840.030642 a.u.

In Figure 6S

RC-5-BP-2W

C	-0.454095	1.139174	-0.480712
O	0.590568	0.450976	0.236495
C	0.645005	-0.956453	-0.031425
C	-0.672881	-1.597286	0.389244
C	-1.840935	-0.936533	-0.329088
C	-1.822393	0.563385	-0.093365
O	1.732948	-1.481321	0.655491

O	-0.694163	-2.966272	0.040087
O	-3.069160	-1.455196	0.142411
C	-0.319797	2.614501	-0.143491
O	-0.514460	2.870260	1.237322
O	-2.823738	1.150742	-0.905500
H	-0.795709	-1.465410	1.474211
H	-1.738816	-1.123347	-1.410052
H	-2.014962	0.760869	0.968316
H	-0.299206	1.001060	-1.560464
H	0.837509	-1.116120	-1.099679
H	1.577453	-1.442974	1.612703
H	-0.172568	-3.469578	0.679219
H	-3.062089	-2.411907	-0.004273
H	-1.089950	3.168681	-0.684465
H	0.658356	2.979453	-0.478009
H	0.202808	2.454208	1.734905
H	-3.213894	1.904418	-0.445123
O	3.003223	1.334756	-0.291177
H	3.579673	0.397140	-0.439028
H	3.382004	1.868281	0.427049
H	2.060655	1.073218	-0.040774
O	4.076152	-0.806167	-0.636415
H	4.979672	-0.925023	-0.307641
H	3.488678	-1.395922	-0.123599

E + ZPE = -839.991962 a.u.
H(298K) = -839.973359 a.u.
G(298K) = -840.036892 a.u.

TS-5-BP-Iso-1-2W

C	1.236871	-1.162962	-0.568298
O	-0.681096	-0.592465	0.458121
C	-1.064391	0.706576	0.086581
C	0.089298	1.658854	0.405640
C	1.351402	1.371674	-0.411582
C	1.915028	0.020129	-0.060246
O	-2.229619	1.108330	0.768597
O	-0.270389	2.983680	0.071573
O	2.356740	2.316113	-0.115811
C	1.382744	-2.516761	0.036142
O	1.978918	-2.509968	1.304955
O	2.885761	-0.443088	-1.035890
H	0.324217	1.575608	1.478292
H	1.098796	1.394980	-1.482145
H	2.293838	-0.046671	0.959106
H	0.737960	-1.082702	-1.530192
H	-1.322182	0.756446	-0.978806
H	-2.091026	1.013353	1.724721
H	-0.988385	3.270485	0.653074
H	1.973161	3.198486	-0.229907
H	2.006850	-3.113272	-0.637642
H	0.385966	-2.973956	0.030230
H	1.323542	-2.242016	1.964449
H	3.620654	-0.900239	-0.588121
O	-2.497543	-2.163101	-0.571369
H	-3.298331	-1.592691	-0.602035
H	-2.726672	-2.931003	-0.031536
H	-1.371480	-1.235272	0.112449
O	-4.347085	-0.164073	-0.582451
H	-5.202112	-0.243025	-0.141212
H	-3.796007	0.403002	-0.011962

E + ZPE = -839.929456 a.u.
H(298K) = -839.909851 a.u.
G(298K) = -839.975781 a.u.

PC-5-BP-Iso-1-2W

C	1.614471	-0.936261	-0.589877
O	-0.788975	-0.584991	0.850681
C	-1.335315	0.504379	0.182108
C	-0.390694	1.690803	0.372690
C	0.918910	1.544763	-0.409995
C	1.703206	0.357530	0.064494
O	-2.622570	0.834153	0.677120
O	-0.967169	2.879112	-0.128676
O	1.740825	2.674776	-0.209804
C	2.067645	-2.198919	0.102703
O	3.227042	-1.926729	0.865853
O	2.776662	-0.029670	-0.924966
H	-0.166815	1.786364	1.446592
H	0.678551	1.423156	-1.476102
H	2.111687	0.410281	1.070665
H	0.969379	-1.032394	-1.458328
H	-1.488124	0.296752	-0.885174
H	-2.577907	0.883218	1.645444
H	-1.807630	3.028069	0.327948
H	1.204655	3.462112	-0.388814
H	2.325295	-2.943577	-0.652680
H	1.236617	-2.569634	0.708938
H	2.992326	-1.770695	1.790553
H	3.565021	-0.362357	-0.426499
O	-1.892592	-2.632142	-0.507510
H	-2.806510	-2.280134	-0.573625
H	-1.957819	-3.485025	-0.059505
H	-1.154329	-1.411888	0.451657
O	-4.192647	-1.136595	-0.581173
H	-4.995828	-1.434346	-0.136322
H	-3.842504	-0.396984	-0.049691

E + ZPE = -839.938838 a.u.
H(298K) = -839.919000 a.u.
G(298K) = -839.985648 a.u.

TS-5-BP-Iso-2-2W

C	2.622400	0.638879	-0.027866
O	3.473973	0.687203	-1.116384
C	1.154434	0.581062	-0.480611
O	0.871633	1.781972	-1.170119
C	0.172843	0.427592	0.677914
O	0.530004	1.392023	1.659420
C	-1.323025	0.604179	0.329246
O	-1.955753	0.567383	1.607450
C	-1.917043	-0.482023	-0.591247
C	-3.422232	-0.361993	-0.821274
O	-4.120665	-0.560651	0.405057
O	-1.270349	-0.304627	-1.830752
O	2.633135	-0.836438	1.241017
O	2.057708	-2.961714	0.185715
H	1.042675	-0.285228	-1.145710
H	0.292229	-0.585144	1.092824
H	-1.464083	1.587952	-0.143346

H	-1.700136	-1.469425	-0.161194
H	2.831031	1.538533	0.551581
H	3.303522	-0.052818	-1.721243
H	1.514975	1.884925	-1.885795
H	-0.194085	1.430505	2.301893
H	-3.715431	-1.111872	-1.562973
H	-3.634380	0.635722	-1.227250
H	-5.071311	-0.557004	0.234334
H	-2.913040	0.450039	1.484815
H	3.527898	-0.815943	1.623464
H	2.338057	-1.992070	0.634468
H	-0.848878	-1.118493	-2.119603
H	2.054337	-2.905782	-0.786945
H	1.154869	-3.201282	0.462471

 E + ZPE = -839.939197 a.u.
 H(298K) = -839.919115 a.u.
 G(298K) = -839.986518 a.u.

PC-5-BP-Iso-2-2W

C	3.632842	0.769407	-0.759499
O	4.945609	0.278091	-0.508109
C	2.698256	-0.094993	0.070121
O	3.049807	-0.022746	1.440976
C	1.253306	0.385485	-0.040628
C	0.321384	-0.415479	0.855694
C	-1.157117	-0.002228	0.892540
C	-1.539597	-1.441107	0.491682
O	-2.277215	-1.578286	-0.612145
O	0.853566	0.227461	-1.390738
O	-0.002398	-1.726838	0.197347
O	-1.449394	0.948871	-0.081089
H	3.378469	0.693612	-1.821193
H	3.543665	1.813800	-0.435144
H	2.765357	-1.135443	-0.285071
H	1.193906	1.432890	0.282250
H	0.752149	-0.650178	1.826861
H	-1.532779	0.277319	1.878512
H	-1.751535	-2.139609	1.298627
H	5.591162	0.937017	-0.792113
H	-2.265799	1.446819	0.183652
H	0.178304	-1.636125	-0.771630
H	0.019048	0.711588	-1.508787
H	4.011472	-0.128380	1.495011
H	-2.610811	-2.486867	-0.696855
O	-4.803663	-0.004925	-0.721668
H	-5.117306	0.162947	-1.619561
H	-3.965184	-0.482903	-0.820440
O	-3.720422	2.070030	0.694229
H	-4.311861	1.475103	0.186325
H	-3.899814	2.968628	0.389679

 E + ZPE = -839.943928 a.u.
 H(298K) = -839.924118 a.u.
 G(298K) = -839.991401 a.u.

In Figure 8S

RC-2(12T) [RC-n(12T), n = 2]

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

8	-0.332397	-0.149269	-2.307754
14	0.121666	1.342497	-1.651990
13	0.320753	-1.575956	-1.258539
8	-0.083947	-0.959124	0.327289
8	2.015592	-1.815023	-1.452652
8	-0.502239	-3.147517	-1.397408
8	0.002228	2.571627	-2.733877
8	-0.810362	1.717168	-0.366653
8	1.673714	1.108190	-1.244190
14	0.618237	4.134800	-2.156838
14	-0.271626	3.014070	0.700663
14	2.625879	2.333316	-0.425407
14	0.487755	-1.861493	1.698304
14	2.815013	-2.742005	-0.220725
14	0.092561	-4.328373	-0.225050
8	-0.129263	-3.430754	1.259932
8	1.830795	-4.175850	-0.338068
8	2.153798	-2.106711	1.263026
1	-0.461584	-5.646790	-0.295637
8	-0.210851	4.146225	-0.622754
8	1.435349	2.706268	0.783540
8	-1.081298	3.190885	2.157872
1	0.549895	5.274029	-3.014847
14	-1.724593	2.661517	3.672277
8	-0.884491	1.242511	4.103387
8	4.505558	-2.682257	-0.314244
14	5.991089	-1.883083	-0.617327
8	5.833295	-0.254248	-0.094245
8	0.156522	-1.184051	3.211455
1	-1.472865	3.702022	4.643443
1	-3.136833	2.399881	3.523971
1	7.027248	-2.518522	0.166334
1	6.315492	-1.900032	-2.025177
8	4.211533	2.029154	0.004650
14	5.704029	1.328613	0.518170
1	-0.841861	-0.866291	5.562195
14	-0.041208	-0.175751	4.575807
1	6.764903	2.144451	-0.028333
1	1.246057	0.205310	5.111365
1	5.725557	1.323343	1.962635
8	2.152198	3.578352	-1.552321
1	-1.271813	-0.115590	-2.695842
8	-2.723368	0.307602	-3.037470
1	-2.944041	1.236036	-3.212201
6	-3.747625	-0.252973	-2.215896
6	-4.228720	0.773585	-1.212159
6	-5.270052	0.144222	-0.304679
6	-4.666024	-1.105714	0.348989
8	-4.239928	-1.997849	-0.670319
6	-3.184302	-1.463717	-1.476214
6	-5.667813	-1.877304	1.189513
8	-6.779652	-2.284718	0.418567
1	-5.158757	-2.739458	1.639599
1	-6.049060	-1.246112	1.997893
1	-6.434702	-2.788403	-0.331456
1	-4.572002	-0.588326	-2.856994
1	-2.376024	-1.149414	-0.786179
8	-2.761623	-2.391215	-2.381107
1	-1.972686	-2.879378	-2.009655
1	-3.369712	1.097457	-0.599744

8	-4.738366	1.870930	-1.948301
1	-5.045876	2.530905	-1.313922
1	-3.813230	-0.802342	0.979452
1	-6.140458	-0.151438	-0.904795
8	-5.630422	1.132053	0.648659
1	-6.512455	0.940939	0.985099

 E + ZPE = -1751.242959 a.u.

H(298K) = -1751.192280 a.u.

G(298K) = -1751.328108 a.u.

TS-2(12T) [TS-n(12T), n = 2]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.267438	-0.141551	-2.357905
14	-0.086302	1.293050	-1.616809
13	0.557265	-1.451560	-1.441362
8	-0.010617	-1.147776	0.216040
8	2.284277	-1.495905	-1.499126
8	-0.047581	-3.138169	-1.746602
8	-0.398419	2.619442	-2.567572
8	-1.104027	1.467131	-0.313812
8	1.464080	1.425159	-1.087731
14	-0.079347	4.211992	-1.847451
14	-0.828555	2.759730	0.854639
14	2.146897	2.731997	-0.151168
14	0.641903	-2.095443	1.511530
14	3.162444	-2.402308	-0.319352
14	0.714110	-4.340551	-0.683425
8	0.272299	-3.678243	0.871651
8	2.411058	-3.943320	-0.665313
8	2.348851	-2.066509	1.186925
1	0.361413	-5.704612	-0.944293
8	-0.968351	4.012742	-0.352544
8	0.894436	2.808973	1.059770
8	-1.741010	2.619028	2.264679
1	-0.344282	5.367951	-2.646846
14	-2.454981	1.744460	3.564868
8	-1.388278	0.490703	4.008562
8	4.822360	-2.057357	-0.297029
14	6.132613	-0.958967	-0.442688
8	5.660207	0.564457	0.193374
8	0.117520	-1.639454	3.058395
1	-2.655245	2.654482	4.669080
1	-3.711776	1.166093	3.126831
1	7.234073	-1.461629	0.349776
1	6.522390	-0.799660	-1.825272
8	3.749208	2.635201	0.333073
14	5.276016	2.068525	0.898162
1	-0.876065	-1.575728	5.426323
14	-0.247192	-0.715033	4.448157
1	6.265751	3.044122	0.497561
1	0.936205	-0.082510	4.984184
1	5.212460	1.943221	2.336738
8	1.522956	3.988595	-1.195251
1	-1.511537	-0.053476	-3.510078
8	-2.404707	0.126596	-3.900653
1	-2.528156	1.086451	-3.874825
6	-3.663641	-0.764905	-2.266848
6	-3.983504	0.475369	-1.536405
6	-4.730454	0.029028	-0.252010
6	-3.933975	-1.112204	0.381382

8	-3.806192	-2.094640	-0.647718
6	-2.744453	-1.738585	-1.616069
6	-4.657526	-1.762255	1.547322
8	-5.958818	-2.181710	1.192497
1	-4.051412	-2.596324	1.920559
1	-4.765320	-1.029672	2.354425
1	-5.878934	-2.880678	0.530678
1	-4.318333	-1.135203	-3.051369
1	-1.938828	-1.269136	-1.037828
8	-2.388085	-2.761932	-2.384430
1	-1.400058	-3.053141	-2.130660
1	-3.049774	0.960256	-1.205248
8	-4.772543	1.321619	-2.329715
1	-5.008401	2.084410	-1.784670
1	-2.941679	-0.757367	0.699305
1	-5.716946	-0.354512	-0.543934
8	-4.850242	1.179937	0.546970
1	-5.612680	1.089790	1.130274

 E + ZPE = -1751.172245 a.u.

H(298K) = -1751.121179 a.u.

G(298K) = -1751.255925 a.u.

PC-2(12T) [PC-n(12T), n = 2]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-0.489697	0.196116	-2.150199
14	0.413373	1.441873	-1.654442
13	-0.209939	-1.243427	-1.194309
8	-0.605135	-0.821376	0.477399
8	1.297234	-2.072219	-1.274526
8	-1.414658	-2.760886	-1.393982
8	0.525451	2.796659	-2.611581
8	-0.112458	2.015128	-0.181572
8	1.959795	0.895899	-1.423702
14	1.617732	4.104299	-2.102927
14	0.848159	3.115692	0.799907
14	3.272449	1.807166	-0.709091
14	-0.207788	-1.856624	1.809164
14	1.924378	-3.183097	-0.118686
14	-1.085066	-4.126960	-0.223302
8	-1.160091	-3.220026	1.233481
8	0.613573	-4.335336	-0.359284
8	1.343619	-2.508223	1.375521
1	-1.963290	-5.231213	-0.444581
8	1.044166	4.303424	-0.462677
8	2.429794	2.398823	0.695796
8	0.244526	3.413166	2.341580
1	1.721094	5.256400	-2.942952
14	-0.585865	3.111897	3.817106
8	-0.410810	1.452913	4.202210
8	3.560938	-3.559898	-0.231821
14	5.216387	-3.279132	-0.608630
8	5.559590	-1.628997	-0.313779
8	-0.384195	-1.199970	3.348296
1	0.040456	3.904808	4.851071
1	-1.985609	3.436953	3.672374
1	6.017796	-4.095120	0.275689
1	5.465521	-3.599446	-1.995078
8	4.752358	1.049319	-0.475358
14	6.038661	-0.007921	-0.055545

```

1      -1.369950  -0.481585  5.605733
14     -0.271120  -0.171020  4.719307
1      7.166129  0.292465  -0.908743
1      1.007051  -0.368221  5.363849
1      6.362724  0.176627  1.340672
8      3.069172  3.209226  -1.728773
1      -1.654054  3.096759  -2.409875
8      -2.484813  2.702282  -2.117085
1      -2.347844  2.417623  -1.197219
6      -4.148431  0.276077  -1.736335
6      -3.581620  0.027980  -0.320664
6      -4.879670  -0.092720  0.467294
6      -5.736567  -0.924004  -0.471025
8      -5.331805  -0.520706  -1.788988
6      -3.199220  -0.170609  -2.833406
6      -7.232909  -0.694055  -0.354015
8      -7.569770  0.642373  -0.656225
1      -7.762066  -1.392762  -1.016514
1      -7.546470  -0.886595  0.676305
1      -7.218570  0.825750  -1.537690
1      -4.386322  1.337283  -1.869733
1      -2.737589  0.614571  -3.446221
8      -2.942795  -1.346057  -3.015468
1      -2.143949  -2.558976  -2.002414
1      -3.080159  -0.951213  -0.292557
8      -2.743861  1.027409  0.181913
1      -1.844051  0.663311  0.321145
1      -5.507091  -1.988936  -0.318518
1      -5.315767  0.909584  0.590783
8      -4.739586  -0.744068  1.707549
1      -4.140799  -0.215725  2.249521
    
```

 E + ZPE = -1751.256732 a.u.
 H(298K) = -1751.204291 a.u.
 G(298K) = -1751.343492 a.u.

In Figure 9S

RC-3(12T) [RC-n(12T), n = 3]

```

-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
8          -0.531338  -0.121011  -2.227583
14         -0.280434  1.400201  -1.536325
13         0.392831  -1.452427  -1.260891
8          0.066192  -0.987294  0.380975
8          2.077120  -1.482904  -1.620226
8          -0.287556  -3.086509  -1.477418
8          -0.657399  2.657678  -2.518260
8          -1.172801  1.527350  -0.180726
8          1.312533  1.367315  -1.241123
14         0.810151  -1.931271  1.637608
14         3.069292  -2.383106  -0.513281
14         0.558141  -4.270354  -0.466212
14        -0.238285  4.246821  -1.835931
14        -0.766328  2.797173  0.973502
14         2.122894  2.650786  -0.361340
1         -0.528727  5.422783  -2.591963
8          1.395393  3.880140  -1.365044
8          -0.955062  4.009888  -0.266791
    
```

```

8          0.969950  2.757691  0.931473
8          0.365435  -3.528711  1.102133
8          2.253878  -3.913607  -0.698245
1          0.149044  -5.634543  -0.620415
8          2.453627  -1.948651  1.056225
8          0.563204  -1.397022  3.219679
14         0.232025  -0.516899  4.645777
8          -0.871531  0.746854  4.285309
14        -2.045367  1.923541  3.908787
8          -1.501126  2.731873  2.477558
14         5.358239  2.015409  0.340582
8          5.668961  0.515670  -0.403065
14         6.037617  -1.031750  -1.053342
8          4.725809  -2.083772  -0.719053
1          6.254987  -0.907145  -2.476603
1          7.217855  -1.539248  -0.388875
1          6.268451  3.007477  -0.186472
1          5.462201  1.906942  1.777291
1         -0.371179  -1.388482  5.628707
1          1.453327  0.072112  5.147999
1         -2.108942  2.913654  4.959719
1         -3.328501  1.309714  3.660727
8          3.760923  2.548317  -0.045658
1         -1.419865  -0.366217  -2.662861
8         -2.727642  -0.884408  -3.231009
1         -2.549311  -1.794080  -3.524891
6         -3.755472  -0.992934  -2.233740
6         -4.146662  0.378371  -1.734278
6         -5.266490  0.176905  -0.709690
8         -4.837616  -0.653921  0.333393
6         -4.445676  -1.965309  -0.075254
6         -3.285457  -1.861642  -1.072983
6         -4.080717  -2.698130  1.204028
8         -3.114655  -1.990749  1.945864
1         -3.402274  -1.068754  1.993982
1         -4.996373  -2.852255  1.792087
1         -3.654124  -3.671495  0.948147
1         -5.290190  -2.481616  -0.562001
1         -6.132661  -0.289431  -1.217557
8         -5.633965  1.381613  -0.121661
1         -5.673890  2.040976  -0.828331
8         -4.684264  1.213756  -2.743273
1         -3.993883  1.426969  -3.382594
1         -3.303329  0.864585  -1.217348
1         -4.622457  -1.466775  -2.714836
1         -2.439111  -1.380359  -0.549977
8         -2.924538  -3.116693  -1.587064
1         -1.934484  -3.217699  -1.509679
    
```

 E + ZPE = -1751.236731 a.u.
 H(298K) = -1751.186054 a.u.
 G(298K) = -1751.321883 a.u.

TS-3(12T) [TS-n(12T), n = 3]

```

-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
8          -0.603079  -0.214358  -2.175868
14         -0.390845  1.258630  -1.500635
13         0.365682  -1.468001  -1.300617
8          0.076437  -1.089715  0.390693
8          2.054222  -1.470071  -1.676983
    
```


8	-0.217587	-3.188336	-1.435303
8	-0.826419	2.555068	-2.436194
8	-1.281015	1.410451	-0.114934
8	1.204947	1.426964	-1.148651
14	0.941458	-1.954974	1.617336
14	3.149201	-2.263696	-0.598968
14	0.776635	-4.303013	-0.464488
14	-0.504645	4.165426	-1.760308
14	-0.931442	2.715479	1.015692
14	1.929387	2.770521	-0.296478
1	-0.887697	5.304355	-2.536095
8	1.164168	3.996350	-1.281176
8	-1.226101	3.953565	-0.180253
8	0.803514	2.821836	1.031161
8	0.567825	-3.585661	1.110610
8	2.433469	-3.853011	-0.756955
1	0.440525	-5.688602	-0.613579
8	2.568365	-1.884168	0.998199
8	0.715323	-1.436527	3.211778
14	0.476714	-0.483429	4.609502
8	-0.800124	0.623433	4.312800
14	-2.120512	1.619877	3.900812
8	-1.671520	2.552929	2.520515
14	5.187433	2.241999	0.370120
8	5.562994	0.796153	-0.452103
14	5.993851	-0.693051	-1.188852
8	4.776123	-1.853090	-0.849911
1	6.140124	-0.496609	-2.613507
1	7.235050	-1.152365	-0.603586
1	6.072244	3.287448	-0.095492
1	5.303361	2.054418	1.798342
1	0.083119	-1.341214	5.705900
1	1.675071	0.257480	4.932373
1	-2.412003	2.533174	4.981841
1	-3.265263	0.796107	3.569991
8	3.578709	2.740621	0.007004
1	-1.626513	-0.352895	-3.255350
8	-2.476361	-0.445201	-3.810330
1	-2.328011	-1.142248	-4.459419
6	-3.711209	-1.129431	-2.022520
6	-4.120591	0.248381	-1.712457
6	-5.240665	0.103457	-0.629638
8	-4.754804	-0.706091	0.392964
6	-4.349001	-1.968712	-0.039307
6	-3.006313	-1.900654	-1.042540
6	-3.910063	-2.749756	1.198485
8	-2.989689	-2.034008	1.964989
1	-3.348520	-1.154777	2.148162
1	-4.827972	-2.975550	1.761804
1	-3.439652	-3.681478	0.881238
1	-5.147749	-2.512992	-0.562101
1	-6.123808	-0.358418	-1.104412
8	-5.547609	1.327434	-0.074037
1	-5.704498	1.951276	-0.797064
8	-4.702697	0.927041	-2.788707
1	-4.035154	0.962087	-3.493414
1	-3.300746	0.807492	-1.233808
1	-4.246671	-1.675499	-2.796263
1	-2.264893	-1.357136	-0.431268
8	-2.683627	-3.168086	-1.412346
1	-1.622188	-3.260694	-1.416376

E + ZPE = -1751.170958 a.u.
 H(298K) = -1751.120165 a.u.

G(298K) = -1751.254414 a.u.

PC-3(12T) [PC-n(12T), n = 3]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-1.274255	-0.048706	-0.829818
14	-0.395903	1.319690	-1.006965
13	-0.232773	-1.288410	-0.088341
8	0.551592	-0.649889	1.320841
8	0.875904	-2.175583	-1.077394
8	-1.228492	-2.754334	0.693823
8	-0.930144	2.446772	-2.088533
8	-0.159553	2.105044	0.417372
8	1.081908	0.794832	-1.548880
14	1.705404	-1.484825	2.286846
14	2.145939	-3.121417	-0.385590
14	-0.170488	-3.933058	1.594348
14	0.119027	3.849775	-2.373564
14	1.084907	3.329703	0.596610
14	2.478684	1.824860	-1.782916
1	-0.333245	4.858552	-3.280170
8	1.627888	3.035724	-2.709886
8	0.478539	4.298379	-0.722640
8	2.442856	2.632233	-0.241720
8	0.668039	-2.861579	2.643954
8	1.052841	-4.238523	0.423283
1	-0.920004	-5.022628	2.136102
8	2.643016	-2.258123	1.041572
8	2.487415	-0.618727	3.499442
14	3.214135	0.644303	4.408298
8	2.389044	2.111901	4.109867
14	1.596832	3.608708	3.867377
8	1.385395	3.837097	2.173785
14	5.297199	0.145546	-2.579023
8	4.838983	-1.498945	-2.660148
14	4.468751	-3.168690	-2.741691
8	3.385940	-3.533210	-1.455127
1	3.855378	-3.477916	-4.012912
1	5.678942	-3.934849	-2.543083
1	5.871806	0.530460	-3.848751
1	6.232687	0.334843	-1.493867
1	3.093057	0.316376	5.811331
1	4.598081	0.776568	4.013369
1	2.443396	4.675396	4.353718
1	0.314786	3.608330	4.532762
8	3.916064	1.129428	-2.303805
1	-2.406569	-0.433686	-2.099240
8	-3.165189	-0.739793	-2.641759
1	-2.802393	-1.313495	-3.323612
6	-5.539568	-1.085515	-0.690539
6	-5.729342	0.333802	-1.244688
6	-7.150938	0.678305	-0.812623
8	-7.289687	0.077671	0.447426
6	-6.669842	-1.204288	0.392592
6	-4.156962	-1.331176	-0.144802
6	-6.175415	-1.496542	1.794874
8	-5.207818	-0.537362	2.169125
1	-5.628678	0.331985	2.107475
1	-7.028752	-1.494964	2.484265
1	-5.690691	-2.475374	1.832573
1	-7.405183	-1.957751	0.080581

1	-7.867514	0.239215	-1.530117
8	-7.386982	2.038748	-0.643721
1	-7.219691	2.470037	-1.491553
8	-5.634630	0.477147	-2.632790
1	-4.731103	0.225327	-2.894232
1	-5.051563	1.028138	-0.718423
1	-5.704731	-1.824344	-1.480557
1	-3.505226	-0.460283	0.025904
8	-3.755440	-2.459692	0.092005
1	-2.203032	-2.706523	0.535570

 E + ZPE = -1751.256807 a.u.
 H(298K) = -1751.204256 a.u.
 G(298K) = -1751.346300 a.u.

In Figure 10S

RC-4(12T) [RC-n(12T), n = 4]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	2.708001	1.331804	-2.616711
6	3.336310	1.009280	-1.359117
6	4.151511	-0.259993	-1.540821
6	4.925652	-0.572841	-0.257394
6	5.763381	0.629800	0.145249
6	4.257764	2.146555	-0.907029
8	4.923732	1.774358	0.279706
6	3.495064	3.427098	-0.591248
1	2.552580	0.846711	-0.598419
1	1.322949	0.930102	-2.504700
1	2.762286	2.302029	-2.731739
1	2.810599	3.224102	0.242776
1	4.200936	4.203252	-0.282258
8	2.787849	3.869806	-1.744813
1	1.831128	3.752195	-1.588623
1	4.984141	2.347262	-1.715662
1	6.520513	0.833763	-0.633209
8	6.344384	0.388006	1.374042
1	6.932016	1.120490	1.592751
8	5.773161	-1.672835	-0.474831
1	5.273072	-2.299302	-1.018546
1	4.882866	-0.073636	-2.341748
8	3.398525	-1.365649	-1.946761
1	2.635586	-1.521106	-1.321971
1	4.217710	-0.770089	0.565111
8	0.351492	0.635787	-2.247044
13	0.070648	-1.205562	-1.903313
14	-0.420866	1.594492	-1.097092
8	1.182496	-1.562206	-0.559033
8	0.168884	-2.525522	-3.013877
8	-1.554727	-1.018139	-1.315133
8	-0.012256	1.027372	0.375910
8	-2.021471	1.724403	-1.307032
8	0.165044	3.169313	-1.167278
14	-0.564485	4.300418	0.015228
14	-3.092976	2.425599	-0.099329
14	-0.681707	1.697981	1.857838
14	-2.290926	-2.391205	-0.543757
14	0.643509	-2.910588	0.424369

14	-0.317481	-4.072866	-2.351055
8	0.576409	-4.101263	-0.841908
1	-0.246385	-5.227540	-3.193212
8	-1.874617	-3.651337	-1.667233
8	-1.065203	-2.684074	0.656953
8	-3.886989	-2.227349	-0.020163
14	-5.451627	-1.858946	0.553278
1	-6.407919	-2.794396	0.005954
1	-5.467943	-1.869647	1.998416
8	-5.861730	-0.286224	0.004862
14	-6.188139	1.290544	-0.549045
1	-6.504457	1.301700	-1.957569
1	-7.238472	1.890109	0.241755
8	-4.741841	2.198477	-0.276433
1	-0.119176	5.657741	-0.029940
8	-0.243385	3.332484	1.425361
8	-2.334514	1.810368	1.337977
14	2.138670	-2.578909	3.385667
1	3.488824	-2.092184	3.227093
8	1.146546	-1.305225	3.974213
14	0.103661	-0.110492	4.590125
8	-0.288456	0.995238	3.321309
1	0.781345	0.647014	5.617744
1	-1.123462	-0.694456	5.079607
1	2.069846	-3.683680	4.315839
8	1.502445	-3.071417	1.873796
8	-2.261525	3.958587	-0.147304

 E + ZPE = -1751.238524 a.u.
 H(298K) = -1751.188497 a.u.
 G(298K) = -1751.322723 a.u.

TS-4(12T) [TS-n(12T), n = 4]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	-2.928518	-0.012751	-3.100940
6	-3.680780	-0.039349	-1.164480
6	-3.724405	1.335749	-0.838874
6	-4.389994	0.665335	0.749781
6	-5.743549	0.013715	0.586622
6	-4.960184	-0.799118	-1.480926
8	-5.599729	-1.120536	-0.252934
6	-4.735703	-2.147239	-2.164465
1	-2.828649	-0.618444	-0.813638
1	-1.971444	-0.191363	-2.950709
1	-3.307112	-0.720546	-3.647865
1	-3.796903	-2.590384	-1.810880
1	-5.578294	-2.785333	-1.880234
8	-4.710589	-1.959248	-3.577157
1	-4.632236	-2.816732	-4.008732
1	-5.615095	-0.175571	-2.108827
1	-6.452985	0.724223	0.129031
8	-6.182423	-0.420405	1.824815
1	-7.068872	-0.789648	1.733562
8	-4.480500	1.864882	1.420456
1	-3.688897	2.381883	1.163191
1	-4.626062	1.856686	-1.202713
8	-2.710391	2.066439	-0.512671
1	-1.205845	1.949976	-0.625802
1	-3.677463	-0.024930	1.217672
8	-0.443327	-0.431087	-2.231539

```

13  0.615167  0.995157 -2.073013
14  -0.277025 -1.487711 -1.005004
8   -0.198722  2.053132 -0.722681
8   0.986244  2.171777 -3.293139
8   2.099870  0.451894 -1.346078
8   -0.464759 -0.649818  0.417547
8   1.161884 -2.273988 -0.977034
8   -1.443575 -2.683746 -0.943453
14  -1.341317 -3.828958  0.417509
14  1.745339 -3.204115  0.389822
14  -0.210244 -1.345388  2.009019
14  3.358853  1.488667 -0.791565
14  0.898242  3.265370  0.023224
14  2.081829  3.471493 -2.904888
8   1.308794  4.070870 -1.438744
1   2.410030  4.427733 -3.916078
8   3.392603  2.633869 -2.103488
8   2.366211  2.424975  0.309429
8   4.759918  0.784049 -0.174766
14  5.876446 -0.249622  0.613934
1   7.191933 -0.009004  0.064147
1   5.846979 -0.004412  2.037968
8   5.444889 -1.877399  0.307811
14  5.034802 -3.507942  0.007572
1   5.309536 -3.856559 -1.366972
1   5.758457 -4.361256  0.923371
8   3.352900 -3.693761  0.334527
1   -2.309965 -4.881404  0.445969
8   -1.291311 -2.690373  1.739103
8   1.284354 -2.186857  1.725259
14  -0.866906  3.883310  2.783645
1   -2.265544  3.902463  2.419439
8   -0.500857  2.433297  3.615649
14  -0.180446  0.977992  4.449301
8   -0.322165 -0.327634  3.338258
1   -1.164646  0.792440  5.490962
1   1.161321  1.003850  4.984629
1   -0.501315  5.014110  3.605773
8   0.111812  3.901529  1.367902
8   0.351083 -4.256946  0.404365
    
```

 E + ZPE = -1751.170971 a.u.
 H(298K) = -1751.119855 a.u.
 G(298K) = -1751.255163 a.u.

PC-4(12T) [PC-n(12T), n = 4]

```

-----
Atomic      Coordinates (Angstroms)
Number      X          Y          Z
-----
8   2.927145 -0.742381 -3.555200
6   4.002129 -0.472312 -0.758482
6   3.495690 -1.804661 -1.252631
6   4.535659 -0.619894  0.700796
6   5.961236 -0.067053  0.608231
6   5.190322  0.071376 -1.561867
8   6.341108 -0.143744 -0.738726
6   5.059002  1.555667 -1.919361
1   3.151739  0.215798 -0.769282
1   2.009419 -0.567974 -3.296857
1   3.328592  0.140320 -3.610851
1   4.925470  2.139715 -1.002090
1   5.988169  1.878412 -2.399187
    
```

```

8   3.995034  1.778464 -2.826608
1   3.204719  2.042194 -2.323910
1   5.343888 -0.502592 -2.482416
1   6.668920 -0.672545  1.181754
8   5.928124  1.263529  1.069882
1   6.807611  1.642051  0.950033
8   4.638567 -1.958980  1.141094
1   3.760528 -2.361244  1.131633
1   4.106576 -2.346741 -1.988968
8   2.489997 -2.317290 -0.795527
1   0.730712 -1.993835 -0.360504
1   3.947061 -0.020038  1.402790
8   0.520782  0.116822 -2.172091
13  -0.808655 -1.041732 -2.029006
14  0.556374  1.227368 -0.995573
8   -0.217808 -2.112302 -0.515892
8   -1.278604 -2.276960 -3.145661
8   -2.233484 -0.275805 -1.399618
8   0.655328  0.441281  0.468141
8   -0.759882  2.206042 -0.976230
8   1.865512  2.285373 -0.997865
14  1.917667  3.507030  0.305725
14  -1.222334  3.282364  0.326373
14  0.494688  1.262687  2.013822
14  -3.635397 -1.096219 -0.827249
14  -1.491719 -3.144037  0.229577
14  -2.557441 -3.387888 -2.743147
8   -1.926795 -3.976955 -1.202961
1   -2.970919 -4.364709 -3.700639
8   -3.764663 -2.327269 -2.052460
8   -2.821700 -2.079151  0.381163
8   -4.941557 -0.170980 -0.306162
14  -5.895450  1.068469  0.400202
1   -7.187608  1.075224 -0.247775
1   -6.015192  0.832788  1.821052
8   -5.130921  2.575209  0.133840
14  -4.418718  4.101438 -0.155936
1   -4.575529  4.477422 -1.541448
1   -5.010771  5.077800  0.730689
8   -2.745244  3.985970  0.235709
1   3.012091  4.427290  0.280662
8   1.729625  2.446046  1.680188
8   -0.888726  2.266270  1.702109
14  -0.034515 -3.971998  3.140052
1   1.293345 -4.495593  2.920094
8   0.060656 -2.409161  3.826086
14  0.148503 -0.881532  4.590914
8   0.489413  0.293966  3.386283
1   1.237483 -0.890214  5.540493
1   -1.114579 -0.579320  5.223145
1   -0.824313 -4.831218  3.991448
8   -0.830241 -3.803230  1.624745
8   0.294295  4.146887  0.290817
    
```

 E + ZPE = -1751.271442 a.u.
 H(298K) = -1751.219268 a.u.
 G(298K) = -1751.357989 a.u.

In Figure 11S

RC-6(12T) [RC-n(12T), n = 6]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	3.090830	-1.932866	0.864162
6	3.800072	-1.241652	1.900859
6	5.060211	-0.621990	1.319916
6	4.765104	0.576558	0.403682
6	6.043116	0.978524	-0.317948
6	6.628199	-0.213535	-1.042064
6	6.885125	-1.325890	-0.033305
8	7.354151	-2.480487	-0.647794
1	7.995142	-2.206239	-1.318778
1	5.712932	-0.281446	2.138552
1	4.020253	0.275582	-0.355354
1	3.748981	-2.420893	0.341348
1	2.041639	-1.203280	0.120682
1	4.051235	-1.958457	2.687596
1	3.130493	-0.472179	2.294679
8	5.675448	-1.684124	0.592550
8	7.866455	0.080293	-1.655324
1	7.756208	0.890114	-2.171089
8	5.811786	1.996655	-1.265796
1	5.282567	2.676748	-0.824793
8	4.336737	1.690678	1.131096
1	3.348287	1.654230	1.296772
1	7.596961	-0.971697	0.734621
1	6.765401	1.328097	0.439754
1	5.904769	-0.586171	-1.784385
8	1.304265	-0.698194	-0.390570
13	0.579738	0.817147	0.471122
14	0.049700	-1.589919	-1.090704
8	0.492846	-2.580177	-2.316757
8	-0.720932	-2.465611	0.039528
8	-0.875477	-0.378334	-1.659239
8	-0.679536	0.092507	1.426320
8	-0.014762	2.118331	-0.497317
8	1.783770	1.516209	1.603307
14	1.054888	2.733072	2.664341
14	-0.956670	3.325883	0.323548
14	-1.634366	1.112062	2.452203
14	-0.868958	-3.352840	-3.158375
14	-2.326163	-3.092131	-0.320352
14	-2.449764	-0.670961	-2.378580
8	-1.816612	-1.918297	-3.422599
8	-3.989981	-2.222075	3.113611
8	-3.040639	-1.738858	-1.141940
14	-3.776406	-3.826265	2.577920
8	-3.184082	-3.762024	0.955382
8	-1.734187	-3.899648	-1.748050
1	-0.603612	-4.254349	-4.233283
1	-2.821819	-4.525776	3.405969
1	-5.051169	-4.507049	2.544516
1	1.939255	3.355296	3.604277
8	-1.732236	4.393697	-0.739355
14	-2.511460	4.773810	-2.217451
1	-3.453696	5.846090	-1.985122
1	-1.549679	5.136178	-3.233242
8	-3.379951	3.383126	-2.728749
14	-4.305211	2.032014	-3.193809
1	-4.585050	2.107439	-4.610127
1	-5.519697	1.958312	-2.414579
8	-3.408462	0.581946	-2.929213
1	-5.451838	-0.105354	3.148174
8	-2.906021	0.352673	3.266277

14	-4.229612	-0.631859	3.712701
1	-4.300627	-0.698871	5.155449
8	0.218214	3.769529	1.531947
8	-0.332461	1.892265	3.310706
8	-2.022690	2.398852	1.346159

E + ZPE = -1751.241269 a.u.
 H(298K) = -1751.190766 a.u.
 G(298K) = -1751.327051 a.u.

TS-6(12T) [TS-n(12T), n = 6]

Atomic Number	Coordinates (Angstroms)		
	X	Y	Z
8	3.135869	-1.090344	-2.119766
6	2.827244	-0.632876	0.369568
6	4.152076	-0.148692	0.437682
6	4.194050	1.226297	-0.533586
6	5.685507	1.550428	-0.657372
6	6.513466	0.348484	-1.054478
6	6.413417	-0.691139	0.051718
8	7.170953	-1.818439	-0.218146
1	7.993399	-1.519887	-0.631480
1	4.311148	0.361089	1.407169
1	3.786733	0.949032	-1.510107
1	2.967520	-1.992106	-2.419019
1	2.328812	-0.585245	-2.337492
1	2.621134	-1.676315	0.158127
1	1.963213	0.012909	0.591348
8	5.079087	-1.136916	0.139070
8	7.880553	0.676068	-1.180769
1	7.952668	1.453315	-1.750913
8	5.869061	2.540753	-1.642242
1	5.325507	3.303963	-1.402820
8	3.574327	2.252519	0.088102
1	2.585701	2.518030	-0.220249
1	6.713149	-0.239544	1.016309
1	6.025606	1.921299	0.323677
1	6.118574	-0.094489	-1.981205
8	0.778650	0.139489	-1.746806
13	0.183461	1.519035	-0.780984
14	-0.103336	-1.208111	-1.527834
8	0.129058	-2.387739	-2.677529
8	0.253069	-1.958324	-0.087272
8	-1.707393	-0.844515	-1.524994
8	0.126197	0.808046	0.851365
8	-1.358379	2.148563	-1.243667
8	1.281512	2.937809	-0.511239
14	0.546434	4.155762	0.569301
14	-2.313533	3.094292	-0.162735
14	-0.664119	1.701704	2.113296
14	-0.864813	-3.853990	-2.558168
14	-0.773317	-3.248954	0.535190
14	-3.023303	-1.957104	-1.230495
8	-2.455729	-3.164585	-2.358728
8	-0.610187	-1.848025	4.207301
8	-2.384618	-2.685348	0.219845
14	-0.005828	-3.383138	3.772047
8	-0.406838	-3.675528	2.122822
8	-0.577482	-4.252207	-0.877368
1	-0.673195	-4.874493	-3.541393
1	1.435247	-3.390624	3.899744
1	-0.620259	-4.409315	4.582577

```

1      1.320623  5.350945  0.729829
8      -3.912100  3.351929 -0.655155
14     -5.369027  2.912116 -1.446723
1      -6.455903  3.642727 -0.832007
1      -5.288921  3.195041 -2.861721
8      -5.641820  1.234636 -1.213759
14     -6.004644 -0.414185 -0.972420
1      -6.987462 -0.831990 -1.947388
1      -6.477132 -0.624301  0.377243
8      -4.594952 -1.372334 -1.216654
1      -2.693186 -0.451903  4.821114
8      -0.816961  0.855809  3.573340
14     -1.256328 -0.340975  4.714088
1      -0.655997 -0.003148  5.986181
8      -1.108192  4.342146  0.067577
8      0.288391  3.159642  1.980663
8      -2.123471  2.276733  1.366062
    
```

 E + ZPE = -1751.156937 a.u.
 H(298K) = -1751.105439 a.u.
 G(298K) = -1751.242023 a.u.

PC-6(12T) [PC-n(12T), n = 6]

```

Atomic      Coordinates (Angstroms)
Number      X           Y           Z
-----
8      -2.473193 -2.288773 -2.919507
6      -2.484389  0.466033  2.895651
6      -3.644392  0.385305  2.253988
6      -3.153269 -2.934955  0.332128
6      -4.455552 -2.728629 -0.416303
6      -4.797643 -1.259229 -0.738419
6      -4.986837 -0.382968  0.493630
8      -5.639952  0.811917  0.178228
1      -6.300018  0.612902 -0.501461
1      -4.600324  0.694229  2.672588
1      -2.975947 -2.278055  1.199268
1      -2.630893 -1.391609 -3.244156
1      -1.829247 -2.170153 -2.200102
1      -1.552249  0.182576  2.410892
1      -2.472229  0.852290  3.907730
8      -3.707321 -0.095603  0.970304
8      -6.036820 -1.246338 -1.420920
1      -6.039182 -2.004568 -2.023962
8      -4.562861 -3.504737 -1.573577
1      -3.811701 -3.271685 -2.160658
8      -2.367534 -3.813818  0.032134
1      -0.835870 -3.789448  0.878109
1      -5.561631 -0.924817  1.267899
1      -5.234800 -3.086453  0.278641
1      -4.008093 -0.805610 -1.354084
8      -1.256044 -1.213998 -0.631756
13     0.221535 -1.688027  0.208956
14     -1.142774  0.341855 -1.094958
8      -2.208373  0.831910 -2.269564
8      -1.221768  1.420418  0.136018
8      0.375110  0.473343 -1.755757
8      0.507541 -0.616188  1.550277
8      1.681935 -2.006094 -0.653080
8      0.011933 -3.380637  1.141100
14     1.457336 -3.797041  2.173093
14     3.218607 -2.180558  0.109339
    
```

```

14     1.896860 -0.687446  2.566812
14     -1.975901  2.485159 -2.886165
14     -0.736758  3.096872 -0.036925
14     1.094636  1.964934 -2.321541
8      -0.278583  2.421870 -3.299088
8      0.876824  3.121887  3.601774
8      0.749593  2.957520 -0.933005
14     -0.426096  4.118517  3.108063
8      -0.652508  3.958078  1.409023
8      -1.790381  3.382686 -1.398163
1      -2.899813  2.959962 -3.868981
1      -1.626720  3.732887  3.814057
1      -0.081678  5.498264  3.371501
1      1.278806 -5.046846  2.842073
8      4.540383 -2.082611 -0.933890
14     5.329340 -1.525355 -2.359455
1      6.748953 -1.477958 -2.087367
1      5.035983 -2.408692 -3.464461
8      4.774686  0.056435 -2.708335
14     4.356635  1.663380 -3.118342
1      4.658031  1.880548 -4.515667
1      5.089101  2.576032 -2.269783
8      2.673989  1.926056 -2.894474
1      3.427003  2.811062  3.850570
8      2.113480  0.596939  3.634921
14     2.173207  2.205846  4.238775
1      2.038645  2.140618  5.677299
8      2.740038 -3.593183  1.047818
8      1.614980 -2.349417  3.084782
8      3.160485 -1.045257  1.426962
    
```

 E + ZPE = -1751.236349 a.u.
 H(298K) = -1751.182943 a.u.
 G(298K) = -1751.324581 a.u.