Supporting Information for

Catalytic Roles of the Metal Ion in the Substrate-Binding Site of Coenzyme B_{12}-Dependent Diol Dehydratase

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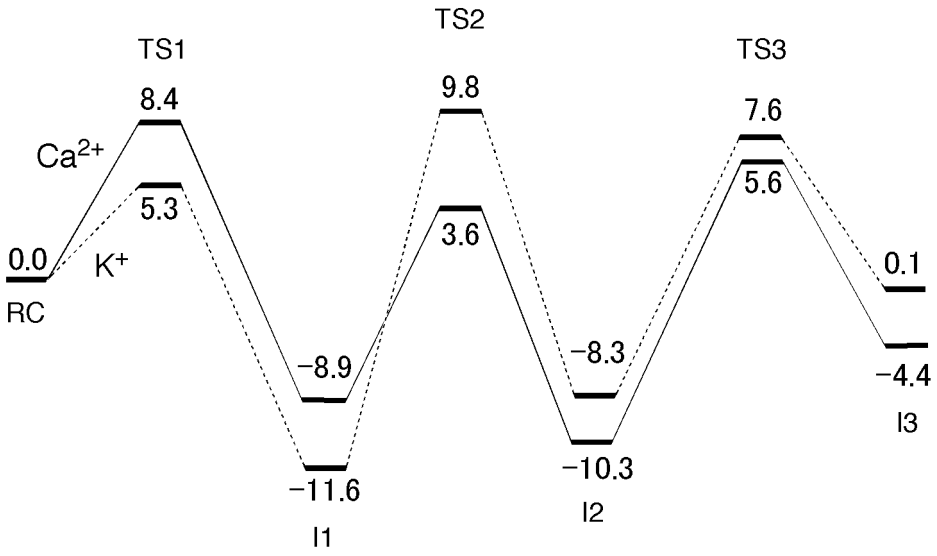

Figure S1. Computed energy diagram for the hydrogen abstractions and the OH migration in the Ca- and K-containing models.

Table S1. MM contribution (E(TS1) – E(RC)) of various residues for the K-model relative to the Ca-model. Top 15 residues are listed. Unit in kcal/mol.

	MM total	bonding[a]	nonbonding[b]	vdW	coulombic
SER333	-0.8	0.0	-0.8	-0.6	-0.2
LYS255	-0.8	0.0	-0.8	0.4	-1.2
GLN200	-0.7	0.0	-0.7	-0.1	-0.6
SER361	0.6	0.1	0.5	0.6	-0.1
GLU168	-0.6	0.0	-0.5	0.8	-1.3
ARG257	0.5	0.1	0.4	-0.1	0.5
PHE359	-0.4	0.0	-0.4	-0.1	-0.3
ILE360	0.4	0.2	0.2	0.1	0.2
TYR219	-0.4	-0.1	-0.3	0.3	-0.6
THR221	-0.4	0.0	-0.3	-0.3	0.0
TYR364	-0.4	-0.1	-0.2	-0.2	-0.1
GLN169	-0.3	-0.1	-0.3	0.0	-0.2
SER224	0.3	0.0	0.2	0.3	0.0
SER377	0.3	0.0	0.3	0.0	0.3
ALA331	-0.2	-0.1	-0.1	-0.1	-0.1
sum	-2.8	-0.1	-2.7	1.1	-3.8

[a]bonding = bond + angle + dihedral angle + improper torsion angle energy terms

[b]nonbonding = van der Waals (vdw) + coulomb energy terms

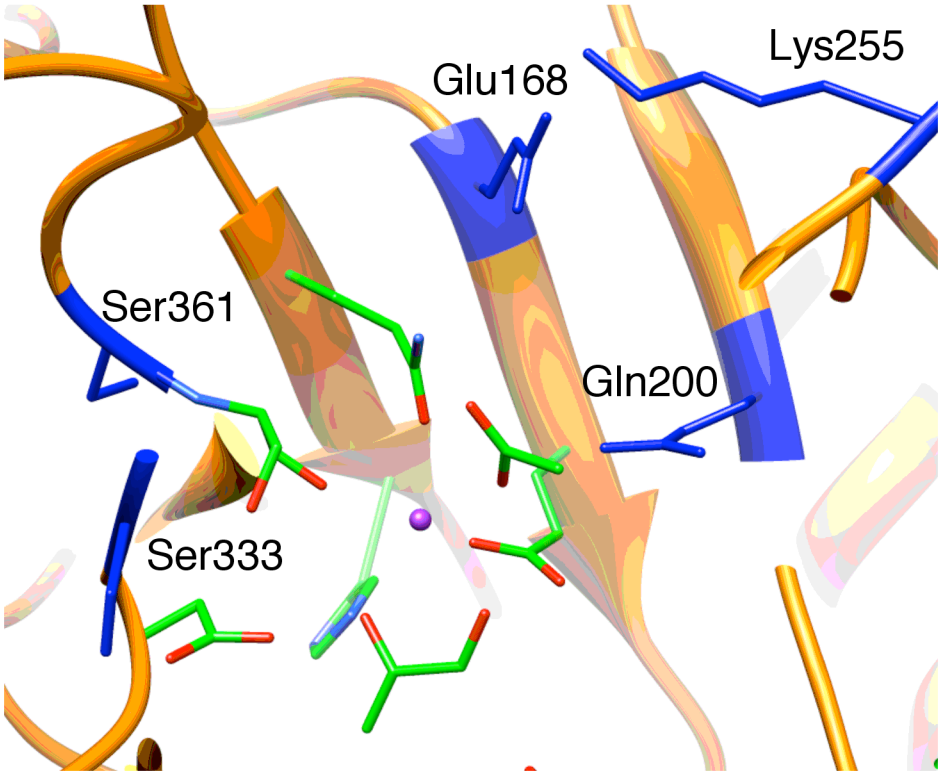

Figure S2. Key residues in the MM region to reduce the barrier for **TS1-K**. Top 5 residues are displayed in blue color.

Table S2. MM contribution (E(TS3) – E(RC)) of various residues for the K-model relative to the Ca-model. Top 15 residues are listed. Unit in kcal/mol.

	MM total	bonding[a]	nonbonding[b]	vdW	coulombic
GLN200	1.8	0.0	1.8	0.4	1.4
SER333	-1.6	0.0	-1.6	-1.3	-0.3
SER202	-1.5	0.0	-1.5	-0.1	-1.5
LYS255	-0.9	0.0	-0.9	0.3	-1.1
GLU208	0.9	0.0	0.9	-0.2	1.1
THR222	-0.8	0.0	-0.7	0.3	-1.0
THR171	-0.7	0.1	-0.8	0.1	-0.9
ALA220	-0.7	-0.5	-0.2	-0.1	-0.2
TYR219	0.6	-0.2	0.8	0.6	0.2
TIP77	0.5	0.0	0.5	0.0	0.5
TYR364	-0.5	-0.1	-0.4	-0.3	-0.1
GLY298	-0.5	0.0	-0.4	-0.2	-0.2
ALA331	-0.4	-0.1	-0.3	-0.2	-0.1
ARG257	-0.4	0.0	-0.4	0.0	-0.4
CYS201	0.4	-0.2	0.6	0.1	0.5
sum	-3.8	-1.1	-2.7	-0.6	-2.0

[a]bonding = bond + angle + dihedral angle + improper torsion angle energy terms

[b]nonbonding = van der Waals (vdw) + coulomb energy terms

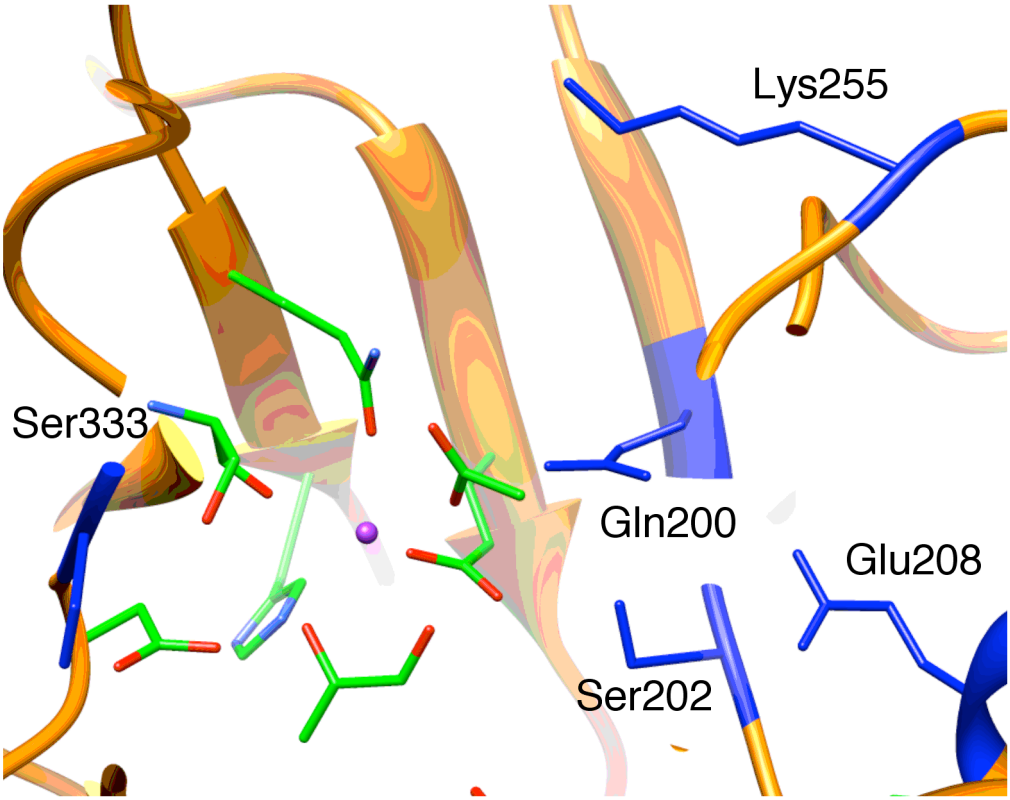

Figure S3. Key residues in the MM region to reduce the barrier for **TS3-K**. Top 5 residues are displayed in blue color.

Table S3. Convergence of QM/MM energies (a.u.). We repeat optimizations iterating back and forth between all stationary points with convergence criteria of 1 kcal/mol.

K							
Iteration	RC	TS1	I1	TS2	I2	TS3	I3
1	-2876.311130	-2876.305640	-2876.331395	-2876.292711	-2876.326754	-2876.302937	-2876.313997
2	-2876.311480	-2876.306346	-2876.331512	-2876.293183	-2876.328913	-2876.304509	-2876.314121
3	-2876.312029	-2876.307889	-2876.333088	-2876.293413	-2876.327757	-2876.303267	-2876.315661
4	-2876.314423	-2876.306698	-2876.332062	-2876.294000	-2876.329530	-2876.304860	
5	-2876.314797	-2876.308651	-2876.333830	-2876.294088	-2876.329719	-2876.305328	
6		-2876.309287	-2876.334470				
7		-2876.309294					
Ca							
	RC	TS1	I1	TS2	I2	TS3	I3
1	-2954.07642	-2954.063556	-2954.090593	-2954.063529	-2954.092069	-2954.067272	-2954.083431
2	-2954.076617	-2954.063905	-2954.089943	-2954.06371	-2954.092007	-2954.067636	-2954.08402
3		-2954.063991	-2954.09098	-2954.06407	-2954.09268	-2954.067695	

Table S4. The QM/MM energies (kcal/mol) of the Ca-containing model. 2810 atoms within a distance of 15 Å around any atom of substrate were allowed to move in the QM/MM optimization. All energies are measured from RC-Ca.

RC-Ca	I1-Ca	I2-Ca	I3-Ca
0.0	-9.0	-10.0	-4.2

The QM region of QM/MM optimized structures.
Units in Å

K-RC E =-2879.100267 (a.u.)

C	69.7137080	4.2135110	168.5269850
H	68.8867480	4.3373480	167.8170200
H	69.9526790	3.1419890	168.6146560
C	70.9782490	4.9265190	168.0717660
O	72.0277490	4.7636210	168.6898420
N	70.8923910	5.7623000	167.0081720
H	71.8052310	6.1841620	166.7458620
H	70.1681690	5.6159890	166.3053030
C	72.5939860	-2.8470790	168.7228990
H	72.9477100	-3.5547420	167.9415100
H	72.4599670	-3.4652610	169.6263590
C	73.6506400	-1.8131070	168.9819520
N	74.7681630	-2.1530190	169.7241710
C	75.5660620	-1.1020790	169.6346360
H	76.5670600	-1.0120390	170.0527910
N	75.0335610	-0.1091250	168.8916580
H	75.5193890	0.7922590	168.6906250
C	73.8072390	-0.5398200	168.4608730
H	73.2164990	0.0714280	167.7798150
C	72.8843170	0.9660540	164.2241750
H	72.8906330	1.2608770	163.1600340
H	73.0883510	-0.1198650	164.2465200
C	74.0322200	1.6423740	165.0159910
O	73.9926000	1.5791470	166.2604920
O	74.9516160	2.1660780	164.3192840
C	74.8674610	7.3675250	164.8031270
H	75.0774420	8.3755880	165.1992960
H	75.8153530	6.8353560	164.6222350
C	74.0266170	6.5177510	165.7750000

O	73.3550710	7.1464250	166.6427450
O	74.0411870	5.2883120	165.5929940
C	77.0239960	7.5151620	168.9260950
H	76.3804450	7.5197850	169.8185210
H	78.0661520	7.6361290	169.2727020
C	76.8940550	6.1358550	168.2797370
O	76.4655780	5.2087130	168.9538050
N	77.3281950	5.9686560	167.0028740
H	77.1812530	5.0465520	166.5598990
H	77.6032250	6.7582080	166.4214280
C	76.1925870	1.9836260	172.3936280
H	75.4481600	2.7613810	172.6417150
H	75.8122020	1.4442460	171.5128770
C	77.5450620	2.6766920	172.0677770
O	77.9415790	2.6175400	170.8752030
O	78.1579480	3.2601390	172.9937710
C	72.9981260	5.0381170	171.4878610
H	72.1312840	5.4089280	170.9243850
C	73.1947490	3.5429700	171.1826910
O	73.8635420	3.1985040	170.2215390
N	72.6064090	2.6173200	172.0010680
H	72.0364550	2.8439740	172.8145350
K	74.4842210	3.7570980	167.7472870
C	77.3365680	2.0359130	166.3898160
C	77.7949710	2.1425550	167.8365740
C	78.7852960	1.0414950	168.2344180
O	76.7119010	3.2204160	165.9565670
O	76.6559310	2.1063690	168.6825500
H	76.6403750	1.1808840	166.3039890
H	78.2270580	1.8076310	165.7607620
H	78.2963870	3.1215320	167.9591140
H	79.7296500	1.1177400	167.6700430
H	78.3442390	0.0400920	168.0677470

H	79.0034780	1.1670130	169.3064680
H	76.0192590	2.9475670	165.2679720
H	76.9827870	2.3668630	169.6043850
C	81.1406450	4.3705310	164.5409180
O	80.2110380	3.3676570	164.9305880
C	80.2575680	2.2437410	164.0602080
C	81.6604130	2.3134260	163.4158860
C	81.8850460	3.8272980	163.2896480
O	81.7233880	1.6470590	162.1880080
O	81.2509370	4.2785040	162.0991870
C	80.0493530	0.9660950	164.7765240
H	81.3912440	0.7356630	162.3006860
H	81.7469830	5.0371310	161.7467000
H	80.5961970	5.2899750	164.2326480
H	79.5133840	2.3551650	163.2432950
H	82.4038380	1.9184290	164.1386420
H	82.9647820	4.0669150	163.2730880
H	80.5519490	0.8098220	165.7361040
H	79.6473730	0.1136810	164.2240310

K-TS1 E =-2879.091743 (a.u.)

C	69.7138620	4.2122280	168.5274830
H	68.8857020	4.3368050	167.8190950
H	69.9509850	3.1402500	168.6152340
C	70.9788660	4.9221370	168.0688380
O	72.0277110	4.7636190	168.6897530
N	70.8948040	5.7474510	166.9977590
H	71.8067590	6.1699560	166.7302270
H	70.1638380	5.6051760	166.3014310
C	72.6017710	-2.8408520	168.7290240
H	72.9539350	-3.5527540	167.9508950
H	72.4679130	-3.4540210	169.6357730
C	73.6616190	-1.8083660	168.9813600

N	74.7780050	-2.1473420	169.7256270
C	75.5817430	-1.1020020	169.6264070
H	76.5836220	-1.0141250	170.0425570
N	75.0539850	-0.1126820	168.8749520
H	75.5464270	0.7811300	168.6620240
C	73.8243790	-0.5405020	168.4494550
H	73.2342690	0.0682300	167.7660590
C	72.9064890	0.9648590	164.2105670
H	72.9105870	1.2822900	163.1532800
H	73.1032410	-0.1225140	164.2025560
C	74.0677930	1.6092630	165.0052470
O	74.0232790	1.5677050	166.2486790
O	75.0143110	2.0876730	164.3067270
C	74.8821010	7.3660380	164.7960410
H	75.0788330	8.3746820	165.1972190
H	75.8364510	6.8470910	164.6115990
C	74.0498170	6.5027000	165.7622570
O	73.3403400	7.1223440	166.6056520
O	74.1058920	5.2715000	165.5975460
C	77.0179680	7.5033550	168.9124620
H	76.3628490	7.4994930	169.7964690
H	78.0547620	7.6257450	169.2740560
C	76.9056440	6.1265810	168.2575070
O	76.4771310	5.1916070	168.9201610
N	77.3560400	5.9694650	166.9850100
H	77.2446340	5.0477590	166.5418890
H	77.6412330	6.7586140	166.4078170
C	76.1989890	1.9833140	172.3717450
H	75.4560810	2.7624770	172.6195870
H	75.8161450	1.4415410	171.4933870
C	77.5507270	2.6747280	172.0416730
O	77.9530240	2.6014790	170.8508900
O	78.1590670	3.2702630	172.9626390

C	73.0071790	5.0350410	171.4773490
H	72.1419680	5.4070820	170.9120720
C	73.1999900	3.5396050	171.1714950
O	73.8687500	3.1936350	170.2103510
N	72.6082460	2.6157670	171.9886990
H	72.0385250	2.8445070	172.8019270
K	74.5116030	3.7317120	167.7385230
C	77.4066050	1.9326050	166.3616280
C	77.8648240	2.0734160	167.8018250
C	78.8187120	0.9642950	168.2578130
O	76.8050380	3.0693760	165.8748570
O	76.7120880	2.0899180	168.6355540
H	76.7740650	1.0349980	166.2284940
H	78.4472330	1.6636210	165.6828130
H	78.3841560	3.0469580	167.8916460
H	79.7632460	0.9704030	167.6913520
H	78.3390010	-0.0268550	168.1503530
H	79.0378140	1.1456580	169.3212930
H	76.0858350	2.7769130	165.1980660
H	77.0344360	2.3500850	169.5622470
C	81.1292880	4.5521030	164.4912180
O	80.0577180	3.6977170	164.8507240
C	80.0653750	2.4848160	164.0833950
C	81.4944910	2.4080770	163.5020860
C	81.8416650	3.8834250	163.2884920
O	81.5842910	1.6679020	162.3142580
O	81.2467800	4.3019640	162.0658390
C	79.6889960	1.3047110	164.9155740
H	81.2002510	0.7816980	162.4621870
H	81.7292170	5.0812140	161.7402390
H	80.7273960	5.5319130	164.1463990
H	79.3682060	2.5785570	163.2265840
H	82.1734470	2.0081050	164.2839330

H	82.9365650	4.0460190	163.2688680
H	80.4108800	1.0747590	165.7138630
H	79.4001230	0.4273160	164.3201990

K-I1 E =-2879.11881 (a.u.)

C	69.7124680	4.2125880	168.5308570
H	68.8873220	4.3312200	167.8178530
H	69.9574570	3.1425870	168.6209970
C	70.9743300	4.9320880	168.0789040
O	72.0275390	4.7636070	168.6893520
N	70.8848990	5.7796250	167.0241200
H	71.7983060	6.1974570	166.7618020
H	70.1607930	5.6384690	166.3199720
C	72.5350190	-2.8932570	168.7037340
H	72.8992830	-3.5746190	167.9042380
H	72.4020730	-3.5395580	169.5874770
C	73.5681560	-1.8443650	168.9892980
N	74.7034690	-2.1654230	169.7108170
C	75.4611310	-1.0822050	169.6477930
H	76.4614380	-0.9708510	170.0618310
N	74.8835890	-0.0866720	168.9435640
H	75.3284030	0.8378400	168.7379940
C	73.6727830	-0.5501990	168.5092180
H	73.0504040	0.0626610	167.8593140
C	72.9782920	0.9706630	164.3144070
H	73.0302410	1.2876550	163.2569060
H	73.1599530	-0.1197600	164.3083950
C	74.1182330	1.5936580	165.1692650
O	73.9669730	1.6188120	166.4059590
O	75.1515520	1.9764470	164.5406140
C	74.8677650	7.3950760	164.8293130
H	75.0730090	8.4041050	165.2239670
H	75.8191440	6.8675980	164.6516860

C	74.0324370	6.5378230	165.7977370
O	73.3784220	7.1520170	166.6889070
O	74.0344840	5.3117260	165.5895790
C	77.0177610	7.5234480	168.9806970
H	76.3774050	7.5453350	169.8750810
H	78.0619660	7.6510200	169.3187570
C	76.8872210	6.1319440	168.3627840
O	76.4323050	5.2226960	169.0429850
N	77.3498070	5.9305680	167.1006450
H	77.2470480	4.9831890	166.7070120
H	77.6454290	6.6981810	166.4993090
C	76.2194500	1.9741460	172.2567680
H	75.4859270	2.7663960	172.4909800
H	75.8148990	1.4064320	171.4049370
C	77.5631290	2.6508980	171.8595480
O	77.9229770	2.5330850	170.6596030
O	78.1951920	3.2756140	172.7504920
C	72.9568140	5.0542940	171.5193720
H	72.0884830	5.4310570	170.9626620
C	73.1564810	3.5607750	171.2059550
O	73.8160110	3.2259440	170.2362490
N	72.5823850	2.6278460	172.0263380
H	72.0220110	2.8447280	172.8490430
K	74.3973380	3.8716190	167.7772650
C	77.1664980	2.0180270	167.2602360
C	78.6240960	2.0404580	167.5780700
C	79.2468040	0.9447860	168.3672510
O	76.8448260	3.0249550	166.3393760
O	76.4057010	2.1096090	168.4643730
H	76.8776130	1.0416590	166.8145220
H	78.5691040	1.3269090	165.0261990
H	79.2192880	2.8722910	167.1947110
H	79.8941780	0.2839800	167.7461530

H	78.4722510	0.3134240	168.8368790
H	79.8697040	1.3664780	169.1766730
H	76.1899830	2.6630620	165.6510450
H	76.9498830	2.4206710	169.2554460
C	81.1298900	4.4712060	164.4640240
O	80.0745360	3.5822340	164.8007460
C	80.0842330	2.4285720	163.9608070
C	81.5215720	2.3434090	163.4351890
C	81.8681770	3.8289700	163.2644960
O	81.6456430	1.6378040	162.2295940
O	81.2805520	4.2710280	162.0457180
C	79.6108190	1.1972920	164.6980310
H	81.2770050	0.7402960	162.3331440
H	81.7774920	5.0424480	161.7233350
H	80.7060600	5.4408930	164.1189030
H	79.4285900	2.5878400	163.0819990
H	82.1762460	1.9219380	164.2272880
H	82.9612710	3.9991300	163.2614660
H	80.2425380	1.0071570	165.5812450
H	79.6682930	0.3290580	164.0162950

K-TS2 E =-2879.08469 (a.u.)

C	69.7142600	4.1984800	168.5403670
H	68.8849830	4.3139400	167.8316110
H	69.9581150	3.1285730	168.6345560
C	70.9747580	4.9104730	168.0727550
O	72.0276350	4.7636130	168.6895750
N	70.8817560	5.7195600	166.9889890
H	71.7892540	6.1433590	166.7077410
H	70.1436620	5.5709610	166.3019410
C	72.5487250	-2.8948380	168.6872830
H	72.8999500	-3.5709570	167.8770560
H	72.4027020	-3.5535290	169.5605140

C	73.6140260	-1.8852400	168.9993440
N	74.7287580	-2.2776450	169.7140180
C	75.5331970	-1.2263920	169.6866980
H	76.5388240	-1.1838420	170.1018190
N	75.0129110	-0.1826750	169.0134980
H	75.5140180	0.7712630	168.8883010
C	73.7828710	-0.5800910	168.5636290
H	73.1802970	0.0741300	167.9350170
C	72.9072050	0.9820930	164.2195070
H	72.9206490	1.3330530	163.1733940
H	73.1162050	-0.1025350	164.1756530
C	74.0493780	1.6070520	165.0478760
O	73.9693750	1.6061130	166.2817280
O	75.0494060	2.0367210	164.3706030
C	74.8936430	7.3629530	164.7963920
H	75.0657920	8.3741880	165.2018330
H	75.8600690	6.8641610	164.6205430
C	74.0684120	6.4787580	165.7484160
O	73.3088930	7.0812510	166.5594420
O	74.1779990	5.2490960	165.5973460
C	77.0413890	7.5315510	168.9328790
H	76.4165970	7.5420750	169.8381790
H	78.0926350	7.6484590	169.2508980
C	76.8783750	6.1588760	168.2849770
O	76.3718260	5.2537700	168.9270580
N	77.3752520	5.9732360	167.0288900
H	77.2018720	5.0671450	166.5810980
H	77.6745870	6.7526600	166.4449920
C	76.2548970	1.9904050	172.3229030
H	75.5133850	2.7773290	172.5510060
H	75.8853800	1.4449730	171.4416780
C	77.6167570	2.6728620	172.0047540
O	78.0547200	2.5613920	170.8329560

O	78.1852200	3.3048470	172.9319440
C	72.9495830	5.0530280	171.5554100
H	72.0848540	5.4347290	170.9960340
C	73.1312220	3.5553470	171.2522500
O	73.7426980	3.2165730	170.2543330
N	72.5993700	2.6227570	172.1024050
H	72.0730680	2.8316600	172.9493370
K	74.4092560	3.7662010	167.8078900
C	77.2140890	1.9681830	166.6082210
C	78.2529830	2.0423940	167.5024290
C	78.8122660	0.8666680	168.2390170
O	76.7869800	2.9750740	165.8833010
O	76.2481410	2.0978480	168.7915570
H	76.7043700	1.0063960	166.4473110
H	79.0591570	0.9188290	165.3111570
H	78.7355670	3.0161400	167.6341590
H	79.8183400	0.5924570	167.8609290
H	78.1558000	-0.0155740	168.1404190
H	78.8952300	1.1276420	169.3083460
H	76.0051760	2.6287930	165.2143970
H	76.8890200	2.3547790	169.5122170
C	81.1203010	4.3772600	164.5155950
O	80.1540680	3.4016960	164.8797200
C	80.2456160	2.2390190	164.0640690
C	81.6303100	2.3070250	163.4103160
C	81.8686760	3.8192390	163.2761410
O	81.6919300	1.6426260	162.1765070
O	81.2471650	4.2694800	162.0782460
C	80.0647090	0.9696420	164.8739490
H	81.3503630	0.7345330	162.2797200
H	81.7396120	5.0378770	161.7420610
H	80.6071710	5.3134280	164.2031090
H	79.4830100	2.2892430	163.2582060

H	82.3847030	1.9086430	164.1213930
H	82.9499920	4.0522240	163.2660760
H	80.8005120	0.9381220	165.6972540
H	80.2153340	0.0937640	164.2145770

K-I2 E =-2879.113493 (a.u.)

C	69.7124680	4.2125880	168.5308570
H	68.8873220	4.3312200	167.8178530
H	69.9574570	3.1425870	168.6209970
C	70.9743300	4.9320880	168.0789040
O	72.0275390	4.7636070	168.6893520
N	70.8848990	5.7796250	167.0241200
H	71.7983060	6.1974570	166.7618020
H	70.1607930	5.6384690	166.3199720
C	72.5350190	-2.8932570	168.7037340
H	72.8992830	-3.5746190	167.9042380
H	72.4020730	-3.5395580	169.5874770
C	73.5681560	-1.8443650	168.9892980
N	74.7034690	-2.1654230	169.7108170
C	75.4611310	-1.0822050	169.6477930
H	76.4614380	-0.9708510	170.0618310
N	74.8835890	-0.0866720	168.9435640
H	75.3284030	0.8378400	168.7379940
C	73.6727830	-0.5501990	168.5092180
H	73.0504040	0.0626610	167.8593140
C	72.9782920	0.9706630	164.3144070
H	73.0302410	1.2876550	163.2569060
H	73.1599530	-0.1197600	164.3083950
C	74.1182330	1.5936580	165.1692650
O	73.9669730	1.6188120	166.4059590
O	75.1515520	1.9764470	164.5406140
C	74.8677650	7.3950760	164.8293130
H	75.0730090	8.4041050	165.2239670

H	75.8191440	6.8675980	164.6516860
C	74.0324370	6.5378230	165.7977370
O	73.3784220	7.1520170	166.6889070
O	74.0344840	5.3117260	165.5895790
C	77.0177610	7.5234480	168.9806970
H	76.3774050	7.5453350	169.8750810
H	78.0619660	7.6510200	169.3187570
C	76.8872210	6.1319440	168.3627840
O	76.4323050	5.2226960	169.0429850
N	77.3498070	5.9305680	167.1006450
H	77.2470480	4.9831890	166.7070120
H	77.6454290	6.6981810	166.4993090
C	76.2194500	1.9741460	172.2567680
H	75.4859270	2.7663960	172.4909800
H	75.8148990	1.4064320	171.4049370
C	77.5631290	2.6508980	171.8595480
O	77.9229770	2.5330850	170.6596030
O	78.1951920	3.2756140	172.7504920
C	72.9568140	5.0542940	171.5193720
H	72.0884830	5.4310570	170.9626620
C	73.1564810	3.5607750	171.2059550
O	73.8160110	3.2259440	170.2362490
N	72.5823850	2.6278460	172.0263380
H	72.0220110	2.8447280	172.8490430
K	74.3973380	3.8716190	167.7772650
C	77.1664980	2.0180270	167.2602360
C	78.6240960	2.0404580	167.5780700
C	79.2468040	0.9447860	168.3672510
O	76.8448260	3.0249550	166.3393760
O	76.4057010	2.1096090	168.4643730
H	76.8776130	1.0416590	166.8145220
H	78.5691040	1.3269090	165.0261990
H	79.2192880	2.8722910	167.1947110

H	79.8941780	0.2839800	167.7461530
H	78.4722510	0.3134240	168.8368790
H	79.8697040	1.3664780	169.1766730
H	76.1899830	2.6630620	165.6510450
H	76.9498830	2.4206710	169.2554460
C	81.1298900	4.4712060	164.4640240
O	80.0745360	3.5822340	164.8007460
C	80.0842330	2.4285720	163.9608070
C	81.5215720	2.3434090	163.4351890
C	81.8681770	3.8289700	163.2644960
O	81.6456430	1.6378040	162.2295940
O	81.2805520	4.2710280	162.0457180
C	79.6108190	1.1972920	164.6980310
H	81.2770050	0.7402960	162.3331440
H	81.7774920	5.0424480	161.7233350
H	80.7060600	5.4408930	164.1189030
H	79.4285900	2.5878400	163.0819990
H	82.1762460	1.9219380	164.2272880
H	82.9612710	3.9991300	163.2614660
H	80.2425380	1.0071570	165.5812450
H	79.6682930	0.3290580	164.0162950

K-TS3 E =-2879.088137 (a.u.)

C	69.7111480	4.2222470	168.5277410
H	68.8870950	4.3448270	167.8142330
H	69.9530530	3.1514010	168.6150010
C	70.9755470	4.9387130	168.0789520
O	72.0276150	4.7636120	168.6895300
N	70.8899430	5.7906320	167.0272990
H	71.8049060	6.2052780	166.7668760
H	70.1663210	5.6539370	166.3217110
C	72.5572450	-2.8787550	168.7161150
H	72.9177490	-3.5725530	167.9255520

H	72.4237940	-3.5111120	169.6098470
C	73.5972930	-1.8317680	168.9854620
N	74.7366280	-2.1538100	169.7011440
C	75.5010470	-1.0762400	169.6230120
H	76.5062850	-0.9655960	170.0254980
N	74.9234020	-0.0830870	168.9145270
H	75.3679020	0.8360150	168.6943770
C	73.7061100	-0.5426830	168.4934230
H	73.0834910	0.0674570	167.8413090
C	72.9466250	0.9852810	164.2935050
H	72.9888640	1.2943400	163.2335040
H	73.1387790	-0.1031490	164.2982670
C	74.0815600	1.6284400	165.1365510
O	73.9565330	1.6218520	166.3767360
O	75.0852040	2.0601850	164.4931450
C	74.8662290	7.3943170	164.8268380
H	75.0757990	8.4037010	165.2184010
H	75.8159520	6.8619400	164.6542570
C	74.0266640	6.5444100	165.7978770
O	73.3909930	7.1618270	166.7001540
O	74.0091580	5.3193160	165.5843330
C	77.0200210	7.5153620	168.9647440
H	76.3756750	7.5331320	169.8562920
H	78.0626700	7.6412850	169.3081460
C	76.8919730	6.1268110	168.3398030
O	76.4318880	5.2147380	169.0142180
N	77.3622250	5.9306270	167.0804490
H	77.2570270	4.9872360	166.6766730
H	77.6681480	6.7001830	166.4870810
C	76.2379110	1.9682820	172.2091740
H	75.5041200	2.7618220	172.4377690
H	75.8351460	1.3953960	171.3603290
C	77.5787450	2.6453940	171.8067150

O	77.9463080	2.5111960	170.6083000
O	78.2016790	3.2870850	172.6911540
C	72.9624980	5.0488870	171.5108510
H	72.0932220	5.4220720	170.9533460
C	73.1633640	3.5553170	171.1990110
O	73.8139910	3.2199940	170.2231850
N	72.5999090	2.6225140	172.0268700
H	72.0442240	2.8398560	172.8526430
K	74.3926060	3.8706830	167.7634940
C	77.0994320	1.9979960	167.0922900
C	78.5893370	1.8403400	167.2942000
C	78.9925100	0.7013940	168.2057660
O	76.8188500	3.0716490	166.2398120
O	76.4413960	2.1141680	168.3494020
H	76.6874230	1.0782550	166.6374140
H	79.1006310	1.5897450	166.1166450
H	79.0783980	2.7998990	167.5279420
H	79.9954490	0.3128710	167.9505520
H	78.2777100	-0.1371690	168.1231600
H	78.9820370	1.0567220	169.2512920
H	76.1468640	2.7580510	165.5413120
H	77.0100360	2.4274310	169.1158480
C	81.1769110	4.5370400	164.5152540
O	80.1338190	3.6597110	164.9003970
C	80.1703030	2.4238020	164.1730990
C	81.5619710	2.4004330	163.5049410
C	81.8720830	3.8856320	163.2920640
O	81.6016490	1.6741490	162.3051790
O	81.2485900	4.3030530	162.0843060
C	79.9408390	1.2373640	165.0648900
H	81.2361440	0.7816510	162.4607520
H	81.7193010	5.0865700	161.7513720
H	80.7419870	5.5057170	164.1811440

H	79.4043940	2.4538350	163.3729680
H	82.2985640	2.0089760	164.2370480
H	82.9638200	4.0633630	163.2516740
H	80.8268410	0.9398050	165.6504170
H	79.4630900	0.3918070	164.5535880

K-I3 E =-2879.100163 (a.u.)

C	69.7109650	4.2211400	168.5283810
H	68.8871190	4.3432310	167.8145360
H	69.9540280	3.1505780	168.6155630
C	70.9745010	4.9392390	168.0804350
O	72.0274440	4.7636010	168.6891290
N	70.8871910	5.7943820	167.0308880
H	71.8020570	6.2074210	166.7710070
H	70.1674130	5.6535770	166.3219370
C	72.5386120	-2.8907130	168.7100070
H	72.9057560	-3.5729280	167.9124160
H	72.4028140	-3.5358680	169.5942420
C	73.5710640	-1.8420800	168.9991170
N	74.7120250	-2.1698160	169.7088690
C	75.4682490	-1.0850090	169.6521610
H	76.4748890	-0.9793560	170.0518550
N	74.8835570	-0.0819580	168.9646380
H	75.3185970	0.8502460	168.7683040
C	73.6706460	-0.5421910	168.5332910
H	73.0444190	0.0754660	167.8914750
C	72.9359060	0.9868300	164.3011600
H	72.9843160	1.2929850	163.2403910
H	73.1301240	-0.1010390	164.3112870
C	74.0623450	1.6356230	165.1523810
O	73.9239430	1.6326560	166.3912010
O	75.0706170	2.0683850	164.5168010
C	74.8569630	7.3968010	164.8281980

H	75.0741670	8.4056440	165.2170280
H	75.8031210	6.8568710	164.6585280
C	74.0116380	6.5550790	165.8017390
O	73.4011450	7.1748790	166.7193920
O	73.9667190	5.3327680	165.5764340
C	77.0257400	7.5287940	168.9785600
H	76.3904090	7.5541550	169.8762540
H	78.0726660	7.6525910	169.3096490
C	76.8832230	6.1391510	168.3611680
O	76.4188410	5.2337980	169.0410860
N	77.3461860	5.9332090	167.1001100
H	77.2192010	4.9878000	166.7048430
H	77.6467350	6.6995410	166.4997950
C	76.2205790	1.9738690	172.2538580
H	75.4787530	2.7584360	172.4885620
H	75.8232480	1.4053380	171.3996570
C	77.5545700	2.6679220	171.8568780
O	77.9025800	2.5767700	170.6497910
O	78.1908450	3.2830950	172.7506710
C	72.9538200	5.0541860	171.5213630
H	72.0845810	5.4292310	170.9650290
C	73.1553750	3.5607420	171.2086750
O	73.8057220	3.2269600	170.2326690
N	72.5930730	2.6265590	172.0363050
H	72.0392080	2.8416000	172.8638640
K	74.3619720	3.9002690	167.7692870
C	77.0110070	2.0369810	167.2095120
C	78.5106870	1.9131350	167.4138690
C	78.8858380	0.7076560	168.2726540
O	76.7216250	3.1095610	166.3472590
O	76.3373410	2.1420140	168.4504920
H	76.6253750	1.1142070	166.7380890
H	78.9597020	1.8434820	166.4119210

H	78.8870400	2.8494030	167.8594920
H	79.9468220	0.4353450	168.1365300
H	78.2774330	-0.1715950	167.9937660
H	78.6965200	0.9380740	169.3330630
H	76.0962730	2.7777480	165.6185850
H	76.9048750	2.4622760	169.2153490
C	81.1741910	4.3769670	164.5192700
O	80.2360560	3.3823090	164.9066220
C	80.3016620	2.2339090	164.0638050
C	81.6965820	2.3136540	163.4077140
C	81.9130620	3.8269830	163.2687380
O	81.7506920	1.6318180	162.1870660
O	81.2661540	4.2664550	162.0807260
C	80.1457270	0.9588290	164.8020210
H	81.4107930	0.7249740	162.3151340
H	81.7406880	5.0419080	161.7346070
H	80.6357760	5.2986690	164.2063690
H	79.5418470	2.3110700	163.2595800
H	82.4500890	1.9306510	164.1269480
H	82.9911570	4.0733490	163.2429460
H	80.7784540	0.7672630	165.6759370
H	79.5605220	0.1510390	164.3602170

Ca-RC E =-2956.835156 (a.u.)

C	69.7716400	4.3032410	168.6520190
H	68.9670950	4.6250530	167.9764250
H	69.8599780	3.2116660	168.5832280
C	71.0833900	4.9015840	168.1853910
O	72.0105730	4.1694560	167.8293920
N	71.2030710	6.2489720	168.1956640
H	72.0750900	6.6675390	167.8060440
H	70.3825240	6.8230750	168.3675810
C	72.5122580	-2.8725500	168.6668430

H	72.8770010	-3.5522930	167.8678520
H	72.3852340	-3.5145010	169.5537910
C	73.5493250	-1.8287400	168.9530430
N	74.6735900	-2.1626110	169.6840990
C	75.4418540	-1.0905820	169.6460560
H	76.4387790	-1.0003570	170.0729610
N	74.8817310	-0.0799060	168.9429850
H	75.3150480	0.8508850	168.7817850
C	73.6682930	-0.5304070	168.4879750
H	73.0393480	0.0944810	167.8549750
C	72.8031240	1.0298260	164.4024920
H	72.7970560	1.2681880	163.3278130
H	73.1038230	-0.0307660	164.4952080
C	73.8641290	1.8665730	165.1196470
O	73.7983750	1.9782290	166.3770320
O	74.7759270	2.3683980	164.4074070
C	74.8383250	7.4227520	165.0206740
H	75.0126120	8.4718980	165.3050360
H	75.8093680	6.9233310	164.8753620
C	74.0777750	6.6639750	166.1151140
O	73.4700480	7.3495180	166.9803040
O	74.1298700	5.4114170	166.0603450
C	76.9529760	7.4952360	168.8883540
H	76.3323830	7.5083000	169.7955410
H	78.0143600	7.5418360	169.1877550
C	76.6838210	6.2018760	168.1338060
O	75.8825580	5.3806290	168.5902450
N	77.3523140	5.9739160	166.9860570
H	77.1080530	5.1116870	166.4693950
H	77.8834430	6.7090900	166.5211780
C	76.0648000	1.9202920	172.4108090
H	75.2407950	2.6220390	172.6406190
H	75.7314260	1.3273960	171.5424520

C	77.3019650	2.7737540	172.0154380
O	77.3523220	3.1024970	170.7941740
O	78.1341660	3.1383870	172.8719420
C	72.9215340	5.2050310	171.4819960
H	72.0726380	5.6921450	170.9748580
C	73.0400660	3.7349280	171.0515500
O	73.5761550	3.4759490	169.9711720
N	72.5578290	2.7600360	171.8593980
H	72.1118000	2.9308630	172.7626230
Ca	74.3692360	3.7757340	167.7153620
C	77.1288310	2.2731920	166.4727140
C	77.4467390	2.3079330	167.9565990
C	78.3057100	1.1192210	168.3951720
O	76.3719350	3.4152140	166.1092890
O	76.2173140	2.3577430	168.6927590
H	76.5592310	1.3533630	166.2396440
H	78.0800530	2.2415080	165.9078910
H	78.0004900	3.2387480	168.1751210
H	79.2990240	1.1498650	167.9142350
H	77.8216590	0.1589460	168.1388700
H	78.4468570	1.1772290	169.4860030
H	75.7666760	3.1337530	165.3284790
H	76.5051010	2.6658510	169.6481230
C	81.1864300	4.4902120	164.5259950
O	80.1689650	3.5666980	164.9016490
C	80.2513410	2.3531490	164.1530690
C	81.6605600	2.3678570	163.5038540
C	81.9116790	3.8693750	163.3058980
O	81.7144610	1.6598600	162.3002770
O	81.2750730	4.2698350	162.1023230
C	80.0459820	1.1595000	165.0036200
H	81.4106270	0.7435430	162.4453870
H	81.7405520	5.0479360	161.7476700

H	80.7130910	5.4388080	164.1930420
H	79.5160880	2.3692570	163.3230260
H	82.4007120	1.9900140	164.2384760
H	82.9958400	4.0858140	163.2729270
H	80.5074100	1.1276920	165.9968230
H	79.7086910	0.2354610	164.5267140

Ca-TS1 E =-2956.821908 (a.u.)

C	69.7750800	4.2531170	168.6111620
H	68.9450850	4.4962730	167.9363670
H	69.9385770	3.1671040	168.5994290
C	71.0495540	4.9287010	168.1462550
O	72.1337540	4.3314690	168.2135720
N	70.9655970	6.1990420	167.7151850
H	71.8549930	6.6534750	167.4232760
H	70.0616180	6.6474810	167.5734770
C	72.5283540	-2.8660570	168.6811650
H	72.8843820	-3.5582730	167.8889640
H	72.4022550	-3.4956710	169.5769420
C	73.5759980	-1.8277050	168.9481170
N	74.6994920	-2.1646720	169.6781330
C	75.4800260	-1.1024380	169.6236690
H	76.4792870	-1.0181800	170.0457390
N	74.9290040	-0.0943020	168.9101460
H	75.3740830	0.8293660	168.7406070
C	73.7079730	-0.5365840	168.4662420
H	73.0792460	0.0887580	167.8338080
C	72.8206860	1.0613830	164.4247680
H	72.8045060	1.3159460	163.3537270
H	73.1348910	0.0028730	164.4915370
C	73.8884920	1.8932860	165.1369360
O	73.7989200	2.0681200	166.3851140
O	74.8348300	2.3237540	164.4225970

C	74.8681330	7.3704580	164.9940720
H	75.0498140	8.4164520	165.2897080
H	75.8323950	6.8618900	164.8371390
C	74.0831940	6.6231590	166.0795730
O	73.3900110	7.3205420	166.8647870
O	74.1842300	5.3703520	166.0893010
C	77.0114780	7.4824360	168.8484300
H	76.3932040	7.4745860	169.7575190
H	78.0706670	7.5551210	169.1485910
C	76.7770000	6.1805430	168.0963690
O	76.0003780	5.3417180	168.5651110
N	77.4444730	5.9590010	166.9493350
H	77.2510550	5.0792870	166.4464180
H	77.9687270	6.6957250	166.4792310
C	76.0921490	1.9405340	172.3908670
H	75.2988240	2.6697270	172.6389370
H	75.7272400	1.3611460	171.5276400
C	77.3606110	2.7422600	171.9907220
O	77.5149380	2.9353410	170.7490380
O	78.1293060	3.1886760	172.8673080
C	72.9917100	5.1182170	171.4068450
H	72.1174920	5.5397830	170.8871820
C	73.1761570	3.6366240	171.0431260
O	73.8516500	3.3306970	170.0566350
N	72.5832640	2.6950160	171.8146340
H	72.0529610	2.9052890	172.6619270
Ca	74.4355390	3.7811640	167.7850640
C	77.2055280	2.1347890	166.4176210
C	77.5544170	2.1865530	167.8870160
C	78.3541100	0.9720510	168.3644190
O	76.5648930	3.2900830	166.0030210
O	76.3289290	2.3105180	168.6311060
H	76.6293980	1.2271510	166.1567930

H	78.3321400	1.9445330	165.7828930
H	78.1502010	3.0989070	168.0734140
H	79.3654930	0.9582730	167.9245250
H	77.8426860	0.0281300	168.1041340
H	78.4519730	1.0440270	169.4583480
H	75.8839130	3.0228000	165.2706460
H	76.6373420	2.5801010	169.5912700
C	81.1716490	4.6709240	164.4836160
O	80.0127400	3.9278080	164.8314030
C	80.0029130	2.6380480	164.1963910
C	81.4309160	2.4570100	163.6219900
C	81.8456900	3.9017440	163.3259710
O	81.4891050	1.6672430	162.4666030
O	81.2628640	4.2778050	162.0869450
C	79.5856610	1.5709340	165.1572500
H	81.1079000	0.7864980	162.6469630
H	81.7383340	5.0594250	161.7528640
H	80.8578550	5.6676270	164.1030390
H	79.3167340	2.6528290	163.3286690
H	82.0954000	2.0643600	164.4194470
H	82.9466260	4.0113140	163.2966490
H	80.2691580	1.4510420	166.0127220
H	79.3506350	0.6170510	164.6624140

Ca-I1 E =-2956.849183 (a.u.)

C	69.7707340	4.3032390	168.6522100
H	68.9663680	4.6246920	167.9764190
H	69.8597560	3.2117770	168.5829870
C	71.0815290	4.9022220	168.1858690
O	72.0087870	4.1700470	167.8287620
N	71.2028600	6.2487150	168.1968170
H	72.0751770	6.6650090	167.8050130
H	70.3829010	6.8234190	168.3699170

C	72.5061930	-2.8755870	168.6531970
H	72.8700160	-3.5509590	167.8502540
H	72.3794990	-3.5224910	169.5369080
C	73.5443950	-1.8345700	168.9451410
N	74.6734260	-2.1780510	169.6631590
C	75.4367080	-1.1021650	169.6446880
H	76.4347740	-1.0183260	170.0699310
N	74.8694060	-0.0786190	168.9664400
H	75.2958360	0.8617120	168.8308260
C	73.6560930	-0.5261200	168.5070490
H	73.0181270	0.1069440	167.8916650
C	72.8024930	1.0335080	164.3923440
H	72.7963980	1.2786710	163.3193170
H	73.1087650	-0.0263380	164.4747670
C	73.8602810	1.8660340	165.1138970
O	73.7784050	2.0127990	166.3622790
O	74.7993200	2.3340620	164.4041850
C	74.8420280	7.4157850	165.0199930
H	75.0153770	8.4649630	165.3049120
H	75.8132860	6.9171650	164.8732490
C	74.0822510	6.6564620	166.1139420
O	73.4686920	7.3409080	166.9756080
O	74.1402800	5.4032930	166.0636070
C	76.9582960	7.4888350	168.8773190
H	76.3371130	7.4965550	169.7841850
H	78.0191640	7.5373320	169.1776670
C	76.6936380	6.1971150	168.1189660
O	75.8847380	5.3776570	168.5645480
N	77.3752750	5.9687720	166.9788850
H	77.1490380	5.1091460	166.4589010
H	77.9173680	6.7003220	166.5206750
C	76.0737020	1.9238010	172.4109190
H	75.2447090	2.6215120	172.6351620

H	75.7499020	1.3320560	171.5379150
C	77.3083620	2.7872130	172.0283310
O	77.3455160	3.1531390	170.8167720
O	78.1494700	3.1269250	172.8855270
C	72.9208110	5.2060970	171.4841500
H	72.0722950	5.6922430	170.9756480
C	73.0368940	3.7362940	171.0552390
O	73.5697820	3.4789360	169.9728460
N	72.5568230	2.7598570	171.8611480
H	72.1122480	2.9301060	172.7648730
Ca	74.3506830	3.7814800	167.7355140
C	77.0119310	2.2311100	166.5244530
C	77.3976610	2.2782540	167.9593660
C	78.2458060	1.0849500	168.4019640
O	76.3821710	3.3391480	166.0533660
O	76.1772540	2.3674330	168.7497000
H	76.6898820	1.2770780	166.0851690
H	78.9736230	1.2552790	165.5119940
H	77.9644540	3.2063660	168.1579200
H	79.2422770	1.1161830	167.9285020
H	77.7624730	0.1264080	168.1399420
H	78.3772830	1.1377100	169.4945110
H	75.7538540	3.0344570	165.2607750
H	76.4972860	2.7006880	169.6888170
C	81.1759200	4.5168790	164.5100770
O	80.1297430	3.6242570	164.8723200
C	80.2167810	2.3905840	164.1534130
C	81.6104360	2.3803360	163.5067840
C	81.8954540	3.8749540	163.2985650
O	81.6658260	1.6702220	162.2991230
O	81.2703220	4.2803240	162.0892520
C	79.9804400	1.2046440	165.0690820
H	81.3388450	0.7609770	162.4347880

H	81.7419320	5.0575230	161.7413500
H	80.7346300	5.4798920	164.1716730
H	79.4675160	2.3893140	163.3359430
H	82.3499220	1.9919900	164.2388420
H	82.9835430	4.0717730	163.2674320
H	80.7257790	1.1904940	165.8853910
H	80.0667940	0.2707850	164.4821790

Ca-TS2 E =-2956.829553 (a.u.)

C	69.7702200	4.2839810	168.6090230
H	68.9531460	4.5294120	167.9157180
H	69.8999640	3.1943090	168.5954860
C	71.0471720	4.8893720	168.0639410
O	71.8755580	4.1777730	167.4866280
N	71.2445400	6.2184560	168.2189960
H	72.1018420	6.6388470	167.8004980
H	70.5077340	6.7979730	168.6085870
C	72.5339010	-2.8799680	168.6618910
H	72.8914920	-3.5545200	167.8547080
H	72.3997340	-3.5338850	169.5397830
C	73.5799220	-1.8476300	168.9592380
N	74.7287680	-2.2040120	169.6340070
C	75.4815700	-1.1145220	169.6246470
H	76.4900900	-1.0378450	170.0293420
N	74.8959320	-0.0747950	168.9964810
H	75.2956930	0.9351300	168.8906660
C	73.6757750	-0.5231700	168.5635890
H	73.0008100	0.1205130	168.0000180
C	72.8502850	1.0758350	164.3623480
H	72.8480650	1.3651060	163.3012440
H	73.1644670	0.0161020	164.3986880
C	73.8865210	1.8751390	165.1247460
O	73.8116320	2.0688180	166.3362310

O	74.8895430	2.3013660	164.4011140
C	74.8795600	7.3952840	165.0096410
H	75.0498780	8.4406900	165.3108880
H	75.8513060	6.9026120	164.8473930
C	74.1303900	6.6161010	166.0971790
O	73.4816330	7.2881350	166.9438230
O	74.2336340	5.3656320	166.0581030
C	76.9415000	7.4908320	168.9035320
H	76.3266460	7.5133980	169.8145220
H	78.0050090	7.5331290	169.1952180
C	76.6562620	6.1956160	168.1588460
O	75.8225610	5.4026660	168.6053870
N	77.3469030	5.9374400	167.0301840
H	77.1233510	5.0682380	166.5202970
H	77.9013990	6.6564810	166.5660490
C	76.0917770	1.9479960	172.3917290
H	75.3181860	2.6948440	172.6548830
H	75.7065470	1.3742060	171.5337940
C	77.3885960	2.7099600	171.9782990
O	77.6182410	2.7628580	170.7414130
O	78.0949870	3.2427150	172.8666170
C	72.8594150	5.3111160	171.5991970
H	72.0601460	5.8855180	171.1034420
C	72.8332320	3.8624640	171.1038160
O	73.1122800	3.6757190	169.9154770
N	72.5360510	2.8422980	171.9366700
H	72.2428330	2.9594770	172.9081440
Ca	74.2462030	3.8207100	167.8491630
C	77.0661680	2.2493120	166.5473420
C	77.8999310	2.3001180	167.6655010
C	78.5131160	1.0999000	168.3014070
O	76.5898700	3.2594460	165.9280610
O	75.7595140	2.3636950	168.7745850

H	76.7606160	1.2430230	166.1942420
H	79.0156950	1.0526510	165.4312410
H	78.1964180	3.2832390	168.0387500
H	79.6026950	1.0658420	168.0947980
H	78.0577640	0.1614910	167.9390900
H	78.3810510	1.1882820	169.3941180
H	75.6255570	2.8015820	165.0207120
H	76.3632640	2.5810980	169.5376360
C	81.1369190	4.4452810	164.5261930
O	80.1243730	3.5122850	164.8873320
C	80.2238910	2.3079010	164.1285900
C	81.6121450	2.3388320	163.4727120
C	81.8738590	3.8439630	163.3025680
O	81.6651420	1.6575780	162.2486930
O	81.2567080	4.2729500	162.0971760
C	80.0278170	1.0837660	165.0041710
H	81.3500640	0.7419070	162.3678320
H	81.7482290	5.0384320	161.7510970
H	80.6609440	5.3952940	164.1997190
H	79.4684760	2.3205480	163.3160740
H	82.3624900	1.9427390	164.1892610
H	82.9585510	4.0585540	163.2865000
H	80.7569900	1.0838700	165.8343840
H	80.1752590	0.1751010	164.3907920

Ca-I2 E =-2956.851186 (a.u.)

C	69.7422640	4.3276570	168.6403340
H	68.9243520	4.6067060	167.9628160
H	69.8689500	3.2388770	168.5858170
C	71.0268600	4.9581970	168.1454620
O	71.9381670	4.2474970	167.7141900
N	71.1505280	6.3043340	168.2029750
H	72.0136030	6.7208780	167.7960890

H	70.3429430	6.8782720	168.4277370
C	72.4887670	-2.9026680	168.6540680
H	72.8533050	-3.5746420	167.8485220
H	72.3596080	-3.5539250	169.5340870
C	73.5214490	-1.8572910	168.9474280
N	74.6616830	-2.1874810	169.6541100
C	75.4097110	-1.1001920	169.6321440
H	76.4108200	-1.0015100	170.0477950
N	74.8191950	-0.0832890	168.9644070
H	75.2245400	0.8630010	168.8093660
C	73.6101750	-0.5462940	168.5136970
H	72.9589650	0.0823360	167.9078680
C	72.8778150	1.0359420	164.4423730
H	72.8994600	1.3708290	163.3933270
H	73.1537410	-0.0347740	164.4252030
C	73.9618390	1.7661280	165.2433240
O	73.7645900	2.0014220	166.4690410
O	75.0275590	2.0626800	164.6349600
C	74.8533360	7.4450710	165.0095430
H	75.0469480	8.4822960	165.3243910
H	75.8146330	6.9330550	164.8440150
C	74.0907110	6.6658700	166.0880990
O	73.4528100	7.3319020	166.9459340
O	74.1769500	5.4143540	166.0286330
C	76.9313200	7.4928400	168.9222470
H	76.3102740	7.5205670	169.8289150
H	77.9929690	7.5400070	169.2207110
C	76.6579740	6.1882990	168.1883400
O	75.8325140	5.3897690	168.6442090
N	77.3484290	5.9248440	167.0625930
H	77.1516630	5.0262620	166.5961890
H	77.8995450	6.6383630	166.5866160
C	76.0955240	1.9384530	172.2763510

H	75.3132760	2.6822100	172.5208280
H	75.7105040	1.3305600	171.4416340
C	77.3662590	2.7111420	171.8231210
O	77.5582510	2.7744900	170.5724830
O	78.1006450	3.2489280	172.6797730
C	72.8808020	5.2465790	171.5251150
H	72.0435890	5.7592620	171.0236300
C	72.9620970	3.7837870	171.0684960
O	73.4271320	3.5496790	169.9496140
N	72.5368840	2.7914930	171.8838570
H	72.1329380	2.9431400	172.8097140
Ca	74.2703590	3.8422230	167.7448920
C	76.8518770	2.1832180	167.3315930
C	78.3155570	2.1826500	167.6103450
C	78.9579480	1.0825660	168.3810060
O	76.4804890	3.2023720	166.4367640
O	76.0750230	2.3172500	168.5379880
H	76.5492940	1.2089830	166.8924590
H	78.6794420	1.2738180	165.2042970
H	78.9123000	3.0180210	167.2339520
H	79.8068400	0.6343340	167.8281680
H	78.2391890	0.2755000	168.6143110
H	79.3460630	1.4746190	169.3402370
H	75.9614940	2.7884480	165.6450190
H	76.6516560	2.5445030	169.3777250
C	81.1126090	4.4927310	164.4802650
O	80.0512160	3.6057370	164.8197620
C	80.0919940	2.4187480	164.0225970
C	81.5175780	2.3641590	163.4560940
C	81.8423780	3.8537600	163.2743990
O	81.6208070	1.6618520	162.2487100
O	81.2417620	4.2867220	162.0616740
C	79.7129480	1.1976160	164.8320370

H 81.2826350 0.7534140 162.3608830
H 81.7319860 5.0601800 161.7309960
H 80.6873770 5.4634720 164.1436450
H 79.4004460 2.5174700 163.1627220
H 82.2024780 1.9544120 164.2289370
H 82.9339370 4.0318420 163.2633470
H 80.3914010 1.0848510 165.6952820
H 79.7930210 0.3021400 164.1891000

Ca-TS3 E =-2956.826465 (a.u.)
C 69.7210740 4.2931980 168.6010890
H 68.8904680 4.4791480 167.9112120
H 69.9394240 3.2164820 168.6140100
C 70.9701160 5.0187500 168.1479010
O 72.0820600 4.4978210 168.3221680
N 70.8454930 6.2420340 167.6111240
H 71.7322230 6.7077260 167.3322250
H 69.9338340 6.6442820 167.3967810
C 72.5101560 -2.8878970 168.6773590
H 72.8696760 -3.5743650 167.8818430
H 72.3828730 -3.5238270 169.5686380
C 73.5497610 -1.8428630 168.9476460
N 74.6975550 -2.1748180 169.6410610
C 75.4545200 -1.0942830 169.5965510
H 76.4635240 -0.9992420 169.9937320
N 74.8626290 -0.0796790 168.9270610
H 75.2752600 0.8600440 168.7599910
C 73.6424650 -0.5366480 168.4996450
H 72.9838810 0.0924100 167.9021720
C 72.8414850 1.0756310 164.4852890
H 72.8621100 1.3732970 163.4249100
H 73.1477070 0.0133250 164.5094900
C 73.9004770 1.8635690 165.2642640

O	73.6888350	2.1448490	166.4794470
O	74.9596660	2.1516210	164.6447080
C	74.8428440	7.3900660	164.9919410
H	75.0558320	8.4233880	165.3115420
H	75.7917710	6.8538330	164.8324340
C	74.0278510	6.6467140	166.0588780
O	73.3196730	7.3466050	166.8273640
O	74.1227930	5.3936510	166.0712390
C	77.0025030	7.5032180	168.8989790
H	76.3983410	7.5168950	169.8175120
H	78.0676500	7.5750700	169.1768330
C	76.7423040	6.1931380	168.1728140
O	75.9226690	5.3952000	168.6413900
N	77.4293190	5.9220650	167.0490140
H	77.2387730	5.0171450	166.5893110
H	77.9817980	6.6313470	166.5686020
C	76.1402330	1.9568830	172.2305340
H	75.3734260	2.7135890	172.4792440
H	75.7408730	1.3571340	171.3981200
C	77.4161890	2.7127140	171.7709350
O	77.6384220	2.7278280	170.5214750
O	78.1292110	3.2841050	172.6239230
C	72.9377210	5.1208900	171.4689060
H	72.0556820	5.5300580	170.9542960
C	73.1334970	3.6439760	171.0990670
O	73.7864680	3.3504470	170.0945320
N	72.5753680	2.6898430	171.8807340
H	72.0588460	2.8859260	172.7396420
Ca	74.3171270	3.8826640	167.8419410
C	76.8726190	2.1552640	167.1961560
C	78.3615170	2.0275500	167.4130460
C	78.7854750	0.8547250	168.2712460
O	76.5420590	3.2360950	166.3625800

O	76.1640880	2.2960480	168.4356870
H	76.4905740	1.2271050	166.7293500
H	78.9237420	1.8188770	166.2267070
H	78.8208920	2.9849450	167.7034420
H	79.8502370	0.6133620	168.1128550
H	78.1924770	-0.0469900	168.0322130
H	78.6317440	1.1055210	169.3354830
H	75.9512520	2.8826020	165.5964560
H	76.7447300	2.5150580	169.2669080
C	81.1661380	4.6283290	164.5118580
O	80.0484780	3.8380460	164.8876130
C	80.0633110	2.5499830	164.2503520
C	81.4532790	2.4440770	163.5708210
C	81.8264530	3.9087140	163.3121920
O	81.4613560	1.6994170	162.3837850
O	81.2181810	4.3153830	162.0961740
C	79.8120160	1.4409220	165.2330160
H	81.1236050	0.7994420	162.5557680
H	81.7013680	5.0908820	161.7589870
H	80.8024420	5.6184050	164.1604870
H	79.2976170	2.5353390	163.4522040
H	82.1786130	2.0381400	164.3058730
H	82.9248470	4.0358410	163.2664820
H	80.6818480	1.2051190	165.8688860
H	79.3750150	0.5456750	164.7700120

Ca-I3 E =-2956.841891 (a.u.)

C	69.7406220	4.3277440	168.6414650
H	68.9241300	4.6065610	167.9627520
H	69.8690470	3.2391070	168.5860600
C	71.0233890	4.9595400	168.1468160
O	71.9320970	4.2465570	167.7150260
N	71.1497160	6.3049230	168.2025120

H	72.0140550	6.7211250	167.7963320
H	70.3421940	6.8788220	168.4268200
C	72.4599800	-2.9259050	168.6542770
H	72.8214190	-3.6012320	167.8500450
H	72.3288000	-3.5751850	169.5352660
C	73.4953730	-1.8820590	168.9428900
N	74.6345520	-2.2086850	169.6525980
C	75.3870620	-1.1245460	169.6173800
H	76.3911340	-1.0281700	170.0270780
N	74.8001550	-0.1134510	168.9386050
H	75.2059730	0.8303060	168.7692510
C	73.5890810	-0.5762480	168.4950070
H	72.9398570	0.0490580	167.8834970
C	72.8553130	1.0286870	164.4295690
H	72.8803430	1.3561850	163.3784050
H	73.1305890	-0.0420760	164.4226000
C	73.9340590	1.7660560	165.2308830
O	73.7321380	1.9970050	166.4565070
O	74.9969450	2.0732670	164.6235160
C	74.8433850	7.4481990	165.0106580
H	75.0364950	8.4861510	165.3226400
H	75.8053540	6.9351900	164.8520860
C	74.0754120	6.6714940	166.0870140
O	73.4524280	7.3392420	166.9548180
O	74.1424160	5.4199900	166.0152870
C	76.9204190	7.4924060	168.9204310
H	76.2976630	7.5221480	169.8258260
H	77.9820940	7.5323190	169.2209980
C	76.6411350	6.1917550	168.1816580
O	75.8116440	5.3943100	168.6310880
N	77.3344120	5.9300970	167.0565830
H	77.1303940	5.0347770	166.5863170
H	77.8910980	6.6426360	166.5860740

C	76.0733720	1.9314100	172.2829160
H	75.2663940	2.6490300	172.5260380
H	75.7035300	1.3163230	171.4457600
C	77.3067520	2.7577750	171.8215670
O	77.4010510	2.9378130	170.5705070
O	78.0950090	3.2364230	172.6652040
C	72.8811240	5.2459970	171.5245380
H	72.0437460	5.7590840	171.0237710
C	72.9624290	3.7830830	171.0672700
O	73.4264060	3.5490220	169.9482570
N	72.5368830	2.7908490	171.8837100
H	72.1324790	2.9431420	172.8094800
Ca	74.2482060	3.8394360	167.7273800
C	76.8264910	2.2199750	167.3305800
C	78.3007620	2.3543330	167.6792150
C	78.8587240	1.1422600	168.4250290
O	76.4175600	3.2356660	166.4411230
O	76.0173030	2.2899020	168.5083760
H	76.6222200	1.2423740	166.8532850
H	78.8559850	2.5353150	166.7467540
H	78.3966270	3.2532620	168.3037350
H	79.8955080	1.3386320	168.7457090
H	78.8594760	0.2380510	167.7883730
H	78.2616710	0.9376020	169.3290170
H	75.9192940	2.8116070	165.6429250
H	76.5384680	2.5777960	169.3627540
C	81.1471720	4.4447950	164.5262940
O	80.1363560	3.5094790	164.8925950
C	80.1900310	2.3300780	164.0900850
C	81.6109830	2.3407060	163.4656370
C	81.8759900	3.8438200	163.2979110
O	81.6820960	1.6521770	162.2524190
O	81.2488860	4.2738250	162.0984850

C	79.9388420	1.0987630	164.8716590
H	81.3705470	0.7351620	162.3759720
H	81.7323660	5.0447460	161.7519400
H	80.6684800	5.3938820	164.2018150
H	79.4689010	2.4047380	163.2504710
H	82.3330840	1.9457300	164.2096620
H	82.9616500	4.0536950	163.2759220
H	80.3843840	0.9924370	165.8667280
H	79.5925990	0.2129140	164.3323960

Transition state and Intermediate1 for the OH group migration in the simple model calculations.

Units in Å

none-I1

C	77.19523119	1.81062839	166.49664449
C	77.77890837	2.03551260	167.84087492
C	78.69561560	0.88539837	168.26093319
O	76.79515702	2.94077745	165.83788994
O	76.69357369	2.18688471	168.78520992
H	76.64945260	0.89173529	166.29061414
H	78.35218186	2.97271548	167.79955881
H	79.53661976	0.77106426	167.57209878
H	78.13692211	-0.05401569	168.29020797
H	79.10236909	1.06016139	169.26218199
H	76.30794714	2.69726505	165.04374689
H	77.07552157	2.42717271	169.63893896

none-TS2

C	-0.63941645	-0.34079192	0.35798415
C	0.46853189	-0.51653903	-0.39271876
C	1.83588645	-0.72414542	0.17305056
O	-1.87236938	-0.27719863	-0.20827362
O	0.45694492	1.74343714	-0.17392110
H	-0.58693025	-0.23344030	1.43673680
H	0.33424435	-0.62138110	-1.46595604
H	2.18625351	-1.74834191	0.00023957
H	1.85879306	-0.53376988	1.24829243
H	2.54475088	-0.04089094	-0.29835301
H	-2.51697176	0.01514513	0.44378473
H	-0.18964362	1.83928831	-0.89261194

K-I1

K	-2.12912034	-0.42803077	-0.17492044
C	0.84174988	1.17545627	-0.21673069
C	1.35374989	-0.09507260	0.35622617
C	2.66908143	-0.51115688	-0.28958367
O	-0.40695592	1.58391837	0.21870841
O	0.32726627	-1.11948275	0.16701227
H	1.52477551	1.95254608	-0.53689270
H	1.48828730	0.01854722	1.44459474
H	3.43916159	0.24742161	-0.12977904
H	2.54425856	-0.66190521	-1.36340909
H	3.03942208	-1.44030933	0.15108663
H	-0.51023756	2.53448952	0.08841946
H	0.68949471	-1.95653130	0.48290336

K-TS2

K	75.18374887	4.52971417	167.99548959
C	76.98562560	1.82986803	166.70030433
C	78.02920730	2.08946409	167.53340092
C	78.77807343	1.04172490	168.28349251
O	76.39879981	2.82483599	165.98694288
O	75.98011661	2.33630361	168.70482655
H	76.61926637	0.82387494	166.52409575
H	78.38541760	3.11373526	167.59332921
H	79.80624502	0.97486246	167.91153045
H	78.32366945	0.05331216	168.19206190
H	78.85114983	1.29698759	169.34446324
H	75.85126916	2.45561665	165.28319119
H	76.14210895	1.56930016	169.26997149

Na-I1

Na	74.98868795	3.49038995	167.86881064
C	77.07349216	1.80204743	166.48521412
C	77.80623683	2.10956511	167.74073525

C	78.55813187	0.89680890	168.26997356
O	76.17882374	2.77512361	166.05841950
O	76.81818286	2.58771940	168.71268250
H	77.51689453	1.18002502	165.71808821
H	78.50638426	2.94412327	167.57291940
H	79.29893109	0.55454220	167.54342582
H	77.87255956	0.07511796	168.48338088
H	79.10111270	1.14840054	169.18459354
H	75.96123699	2.65197083	165.12654103
H	77.25402545	2.68616480	169.56751556

Na-TS2

Na	75.30357059	4.17690831	167.81001843
C	76.97072084	1.85680944	166.71829798
C	78.01938892	2.09361777	167.55137788
C	78.77066310	1.02351510	168.26408872
O	76.35670357	2.88448510	166.06154845
O	75.96624303	2.39369562	168.72066479
H	76.60055717	0.85962474	166.50561402
H	78.37747749	3.11512878	167.64053718
H	79.79222197	0.96242842	167.87266244
H	78.30831726	0.04077179	168.15866983
H	78.86673961	1.25634655	169.32840250
H	75.86407161	2.55423478	165.29931502
H	76.13802284	1.72203360	169.39190277

Ca-I1

Ca	74.96055809	3.51534260	167.88316252
C	77.08019188	1.77161848	166.47613032
C	77.84703431	2.09293800	167.70065415
C	78.57402591	0.90087274	168.28840327
O	76.14068958	2.75420928	166.08358597
O	76.82040733	2.64230705	168.68728807

H	77.42847278	1.10489854	165.69931418
H	78.52870743	2.93727791	167.53545604
H	79.31720781	0.53891018	167.57273956
H	77.89206593	0.08176143	168.52080258
H	79.12555638	1.18455638	169.18788054
H	76.01210866	2.76329530	165.12118743
H	77.20767391	2.61401111	169.57569537

Ca-TS2

Ca	74.96829052	4.11317526	167.79686840
C	76.94789217	1.84335257	166.80893215
C	78.09978867	2.04572963	167.55077728
C	78.83738724	0.96814797	168.21947390
O	76.33825291	2.89610432	166.15903481
O	75.82088202	2.50837600	168.72316744
H	76.54531097	0.85742335	166.59552715
H	78.50028572	3.05637494	167.59791997
H	79.83108896	0.88639128	167.74656194
H	78.35151737	-0.00604299	168.17963391
H	79.06764789	1.23903363	169.25797480
H	76.10705521	2.65773894	165.24483525
H	75.91929835	1.87379512	169.44239299

Mg-I1

Mg	75.25222701	3.39530332	167.79324995
C	77.09154973	1.77222574	166.46452309
C	77.85113385	2.09711122	167.69581598
C	78.57355320	0.91547391	168.30020724
O	76.07718674	2.72308892	166.12879350
O	76.78466126	2.64677656	168.67305249
H	77.48082588	1.19263691	165.63847339
H	78.51747305	2.95672438	167.55175215
H	79.33288978	0.56399904	167.59443479

H	77.89776324	0.08767323	168.51809715
H	79.11025821	1.20842098	169.20548843
H	75.85708228	2.72959399	165.18223223
H	77.10809577	2.61297079	169.58617961

Mg-TS2

Mg	75.08215600	3.82196255	167.64509208
C	76.94067809	1.82385654	166.82466572
C	78.09372219	2.02757003	167.56642802
C	78.85361881	0.94205655	168.18182409
O	76.28345734	2.91017903	166.22713934
O	75.81297497	2.56114668	168.73540469
H	76.53405139	0.84860891	166.57579974
H	78.47012572	3.04484776	167.65664204
H	79.84937201	0.91031012	167.70095461
H	78.39301197	-0.04190061	168.10992399
H	79.09524330	1.18466955	169.22646723
H	76.14053073	2.77032552	165.27346211
H	75.78575548	2.13596737	169.59929634

The QM region of the QM/MM optimized structure without the metal ion (Figure 7)
Units in Å

TS2	E = -1965.016306 (a.u.)		
C	69.613448	4.625988	168.763155
H	68.916338	4.140616	168.070231
H	70.399652	3.894155	169.013557
C	70.313102	5.788431	168.087275
O	70.653101	6.819861	168.684138
N	70.588252	5.581994	166.783130
H	71.445526	5.986966	166.352559
H	70.274776	4.728727	166.326232
C	72.771808	-2.716986	168.722834
H	73.163777	-3.395630	167.933585
H	72.640537	-3.358021	169.613692
C	73.787196	-1.651915	169.033018
N	74.942974	-2.000198	169.713944
C	75.672849	-0.893761	169.716952
H	76.671215	-0.784699	170.138234
N	75.065943	0.142614	169.096018
H	75.458787	1.135782	169.011864
C	73.859298	-0.324338	168.647025
H	73.204147	0.302821	168.048163
C	72.907544	0.977055	164.020009
H	72.887147	1.437924	163.019135
H	73.053546	-0.107051	163.873508
C	74.106220	1.457364	164.864924
O	74.272615	0.947229	165.973563
O	74.872040	2.323505	164.309521
C	74.750402	7.429582	164.755183
H	75.185513	8.386836	165.091036
H	75.589726	6.716462	164.643483
C	73.792725	6.876854	165.834592

O	73.991145	7.260730	167.016319
O	72.894745	6.094071	165.452010
C	76.325301	7.733147	169.590935
H	75.276101	7.868683	169.907867
H	76.968290	8.038611	170.430063
C	76.576401	6.233653	169.432510
O	77.194056	5.662398	170.331959
N	76.033273	5.610374	168.369449
H	76.009934	4.577484	168.396364
H	75.341708	6.114721	167.801956
C	76.447190	1.805345	172.302865
H	75.633607	2.547305	172.382750
H	76.343156	1.351520	171.306979
C	77.808498	2.546228	172.424349
O	78.487793	2.692369	171.389544
O	78.118902	2.959022	173.577095
C	72.587169	5.043804	171.575703
H	71.853012	5.646105	171.016758
C	72.478263	3.582022	171.113706
O	72.164320	3.334260	169.967152
N	72.736782	2.593664	172.051868
H	73.291800	2.820666	172.880709
C	77.046118	2.142176	166.682694
C	78.054230	2.319390	167.611844
C	78.661757	1.213515	168.418671
O	76.664243	3.073429	165.864322
O	76.152796	2.652104	168.971719
H	76.511618	1.180898	166.619870
H	78.926491	1.106278	165.363403
H	78.520854	3.309361	167.645258
H	79.691151	0.987495	168.065760
H	78.066721	0.285719	168.335307
H	78.724293	1.511590	169.482338

H	75.861099	2.754173	165.219465
H	76.822270	2.890439	169.650117
C	81.136733	4.443830	164.505826
O	80.133388	3.511676	164.877541
C	80.196560	2.326361	164.095146
C	81.595926	2.333754	163.463012
C	81.869191	3.833472	163.284275
O	81.674028	1.635066	162.247223
O	81.251788	4.252518	162.071892
C	79.941486	1.093041	164.940749
H	81.303997	0.739884	162.364157
H	81.703363	5.054937	161.758856
H	80.659788	5.394637	164.181248
H	79.452244	2.379853	163.272520
H	82.326761	1.941090	164.201580
H	82.955433	4.044788	163.261643
H	80.662569	1.048436	165.776686
H	80.056834	0.191384	164.308887

The optimized structures of OH group migration in the simple model calculation (Figure 8)

Units in Å

deprotonation I1 E = -457.530948154 (a.u.)

O	-0.158457281	-0.88201512	-0.165745527
C	-2.522782181	-0.08359782	-0.225862383
C	-1.023245475	0.173776363	-0.015395435
C	-3.258473603	1.266398436	0.168214953
O	-3.071533789	-1.132784195	0.347740692
H	-2.618861929	-0.074007513	-1.396565451
H	-4.32390184	1.132428819	-0.058677425
H	-3.160979697	1.409054977	1.253886043
H	-2.893690559	2.174393883	-0.349139516
H	-0.616231884	1.127532098	-0.389814459
H	0.758472697	-0.542264182	-0.279757534
C	3.349795569	0.053816429	0.303033433
O	2.489952434	0.019615151	-0.61366506
O	4.569502572	0.307211384	0.244141681
H	2.947715856	-0.185716283	1.340350641

deprotonation TS2 E = -457.468437600 (a.u.)

C	-0.964387972	-1.688677794	-1.55811056
C	-0.361959769	-1.021178813	-0.527283522
C	-1.947494053	-2.798054187	-1.306834823
O	0.542745118	-0.035558192	-0.792778569
O	0.573715045	-2.77337261	0.257988406
H	0.767792515	0.465192479	0.022049892
H	-1.738984455	-3.678725246	-1.935918229
H	-1.81912613	-3.137713907	-0.274861314
H	-3.019055758	-2.542600921	-1.485041188
H	-0.506567905	-1.601867931	-2.544295323
H	-0.796898775	-1.002811656	0.462445052

C	0.587614759	2.930196998	1.062545075
O	0.718181398	4.008927088	1.677728911
H	-0.073640948	2.969696259	0.137747559
O	1.078338896	1.799392926	1.30655832

OH I1 E = -534.021787556 (a.u.)

O	-0.5992022	0.024067946	0.891483533
C	1.737222639	-0.112341472	0.181527933
C	0.310455965	-0.566755523	0.056706396
C	1.916741392	1.397775896	-0.1362968
O	2.566441414	-0.879882174	-0.636226759
H	2.019447803	-0.216861614	1.258474535
H	2.986155693	1.615432428	-0.047677489
H	1.606279609	1.588168582	-1.171493112
H	1.324012508	2.03383255	0.53354089
H	-0.046017901	-0.860064178	-0.934171255
H	3.602029896	-0.532290334	-0.446463519
O	4.84451369	-0.022857922	-0.068936783
H	4.731478071	-0.059228164	0.892529488
H	-1.52758126	-0.239631655	0.646121951
C	-3.899364792	0.252125327	-0.199900812
O	-3.156487704	-0.646197079	0.283438704
O	-5.120610415	0.228090839	-0.430772246
H	-3.363373929	1.220044147	-0.454973373

OH TS2 E = -533.969416837 (a.u.)

C	-1.741734788	-1.229657321	0.296795569
C	-0.540285998	-0.608377997	0.053859089
C	-2.886537997	-1.259737106	-0.662832801
O	0.457188858	-0.654178572	0.951439012
O	-1.32327422	1.332152647	0.259014907
H	-2.287915928	1.352931643	-0.026575577
H	1.333535372	-0.45074659	0.52040728

H	-3.529204929	-0.343178894	-0.548061599
H	-2.532692105	-1.261665563	-1.703572983
H	-3.503532333	-2.162003839	-0.522696069
H	-1.925907142	-1.517441257	1.331781277
H	-0.254389775	-0.346714751	-0.960653699
O	-4.060545625	1.430558242	-0.208603631
H	-4.052691792	1.193505642	0.733150124
C	3.678251082	0.497802779	-0.073051377
O	4.874835437	0.557265723	-0.404314657
O	2.856991019	-0.451185254	-0.215673223
H	3.253081085	1.418229192	0.432699089

HCO2 I1 E = -647.465047468 (a.u.)

O	1.7397266	-0.629444834	-0.388679185
C	-0.194327007	0.821217193	0.001079411
C	0.996769303	0.073332694	0.501213178
C	-0.394638156	2.136836379	0.774066051
O	-1.390267548	0.033737352	0.097345605
H	0.000234007	1.065496673	-1.056615247
H	-1.303903897	2.634234514	0.42586603
H	-0.513240196	1.921518993	1.842989488
H	0.463144795	2.809346912	0.652256759
H	1.005582068	-0.276097486	1.535757325
H	-2.134535557	0.598659767	-0.219570602
H	2.480538304	-1.113841779	0.090192802
C	-4.14939122	1.77082649	-1.695927432
O	-3.35382089	1.842075199	-0.72011274
O	-4.995262376	2.588387039	-2.094536343
H	-4.074013081	0.80366232	-2.290477805
C	3.661725574	-3.102744841	1.056538006
O	3.718216628	-1.850391927	0.883096818
O	4.514684081	-3.866897167	1.532212986
H	2.68915063	-3.579512703	0.723168833

HCO2 TS2 E = -647.420233963 (a.u.)

C	-0.947730478	0.03125536	-0.749998313
C	-0.122549291	0.611382475	0.184657233
C	-2.171812483	-0.76351304	-0.422329935
O	0.912223427	1.369412273	-0.169309033
O	0.534885615	-1.334670997	0.749632002
H	0.40713149	-1.883830569	-0.050630954
H	1.271503943	1.876478678	0.629416001
H	-2.123132644	-1.769033639	-0.858281479
H	-2.287616711	-0.869601265	0.659742785
H	-3.083983942	-0.284699899	-0.818629721
H	-0.612261827	0.056023466	-1.784267529
H	-0.431425824	0.678184774	1.224200964
O	0.183150573	-3.454620377	-1.567168959
C	-0.765968636	-4.10395254	-2.05135732
H	-0.446759772	-5.056186036	-2.611724791
O	-1.999038066	-3.906309634	-2.040389842
C	1.298012945	4.036804956	1.752178805
O	1.544736969	5.007427918	2.481831212
H	0.627491473	4.234440808	0.860140249
O	1.691459168	2.83705587	1.854296077

none I1 E = -458.257827687 (a.u.)

O	0.004790497	-0.842573277	0.542469411
C	2.225873169	0.072270078	0.259408028
C	0.787952474	0.056194008	-0.062189874
C	2.856939979	1.448549319	0.023936721
O	2.957988004	-0.920036524	-0.543488637
H	2.334961491	-0.215348275	1.316218916
H	3.934985432	1.434495538	0.226814749
H	2.72294168	1.742550562	-1.021273722
H	2.399843504	2.212339369	0.659584757

H	0.408613848	0.553308256	-0.953861208
H	3.842692877	-0.992724039	-0.157653891
H	-0.961732909	-0.76957956	0.153337027
C	-3.089689492	0.16273555	0.211975133
O	-2.29706459	-0.575958404	-0.460760654
O	-4.257088188	0.465277554	-0.035852797
H	-2.637768483	0.582789635	1.15911474

none TS2 E = -458.240764535 (a.u.)

C	2.400190921	-0.410276291	-0.136272574
C	1.030552819	-0.586700386	0.18336199
C	3.322553222	0.47076859	0.637421224
O	0.249795997	-1.359799124	-0.45105622
O	0.772982807	1.374280951	-0.588111326
H	0.610282505	0.975037589	-1.455715348
H	-1.221040959	-1.149834486	-0.050799002
H	3.577472406	1.378170021	0.07491599
H	2.852627336	0.803496923	1.567967774
H	4.266221983	-0.032254039	0.898029935
H	2.737969697	-0.83968571	-1.077452438
H	0.718623661	-0.19336488	1.164994396
C	-2.452265326	0.343614071	0.035706902
O	-3.546635827	0.837383237	0.204028172
O	-2.199654406	-0.949514857	0.1853717
H	-1.560255003	0.935197016	-0.245105165

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