Supplementary information for

"Mechanistic insight into the selective catalytic reduction of NO_x with propene on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface"

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Supporting Information list:

Convergence test for size of supercell of CeO_2 is performed (Table S1), the surface formation energy (E_{surf}) of 2 × 2 supercell is the same as 3 × 2, 2 × 3, and 3 × 3 supercell. E_{surf} is calculated by the following formula: $E_{surf} = (E_{slab} – n\ E_{bulk}) / 2A_{slab}$, where E_{slab} is the energy of surface, E_{bulk} is the energy of optimized bulk, A_{slab} is the area of surface and n is the number of atoms in the optimized bulk cell. To save computing resources, 2 × 2 supercell is selected to build $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

Table S1 Surface formation energies of CeO_2 (110) surface for different size of supercell.

Size of supercell	2 × 2	3 × 2	2 × 3	3 × 3
Surface energy (kcal mol^{-1} $Å^{-2}$)	0.0029	0.0029	0.0029	0.0029

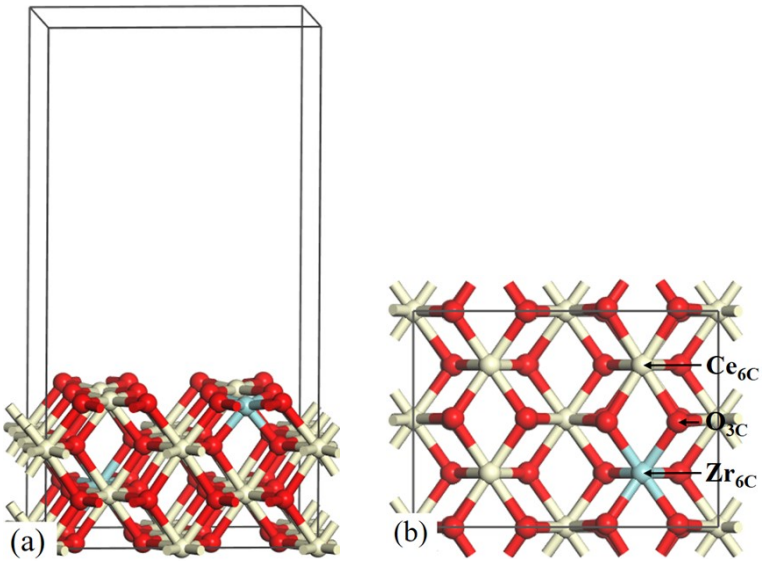

Fig. S1 Schematic structure models for the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface: (a) side view and (b) top view. Key: Ce, ivory; Zr, cyan; O, red.

Table S2 The bond distances for O_2, NO, N_2, and CO_2 molecules.

Molecule	O_2	NO	N_2	CO_2
Calculated value (Å)	1.225	1.164	1.107	1.177
Experimental value (Å)	1.207	1.151	1.098	1.160

Table S3 Adsorption energies (E_{ads}) for NO and NO_3 gas molecules on the possible adsorption sites of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

Gas Molecule	Adsorption Sites	E_{ads}(kcal/mol)	Figure
NO	Ce_T	-2.77	1(a)
	Zr_T	-3.68	1(b)
	O_{T1}	-21.18	1(c)
	O_{T2}	-40.59	1(d)
NO_3	$brid_1$	-40.84	1(e)
	$brid_2$	-40.84	1(f)
	biden	-39.20	1(g)
	monoden	-36.13	1(h)

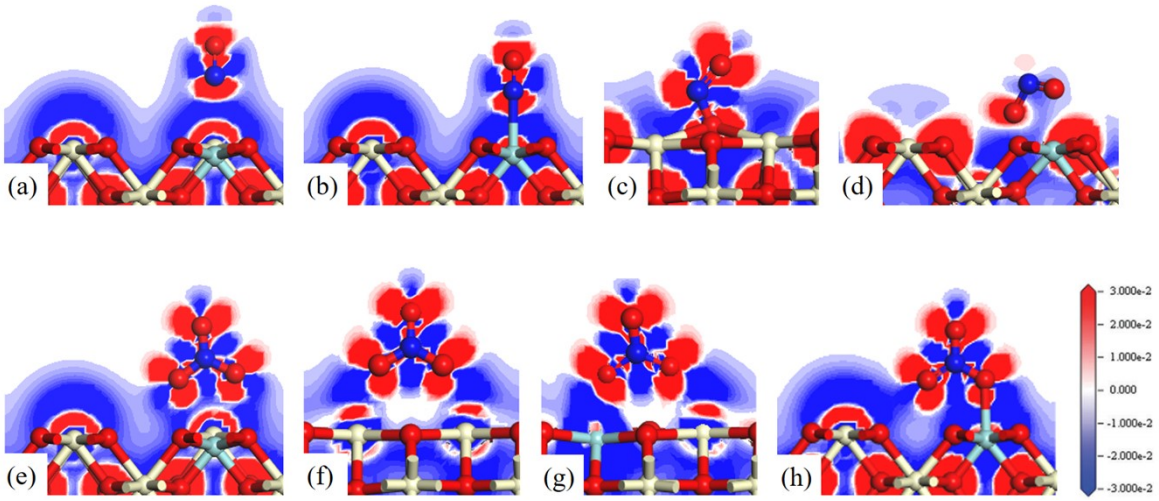

Fig. S2 The deformation electron density for adsorption geometries of (a) NO on Ce_T site, (b) NO on Zr_T site, (c) NO on O_{T1} site, (d) NO on O_{T2} site, (e) NO_3 on $brid_1$ site, (f) NO_3 on $brid_2$ site, (g) NO_3 on biden site, and (h) NO_3 on monoden site.

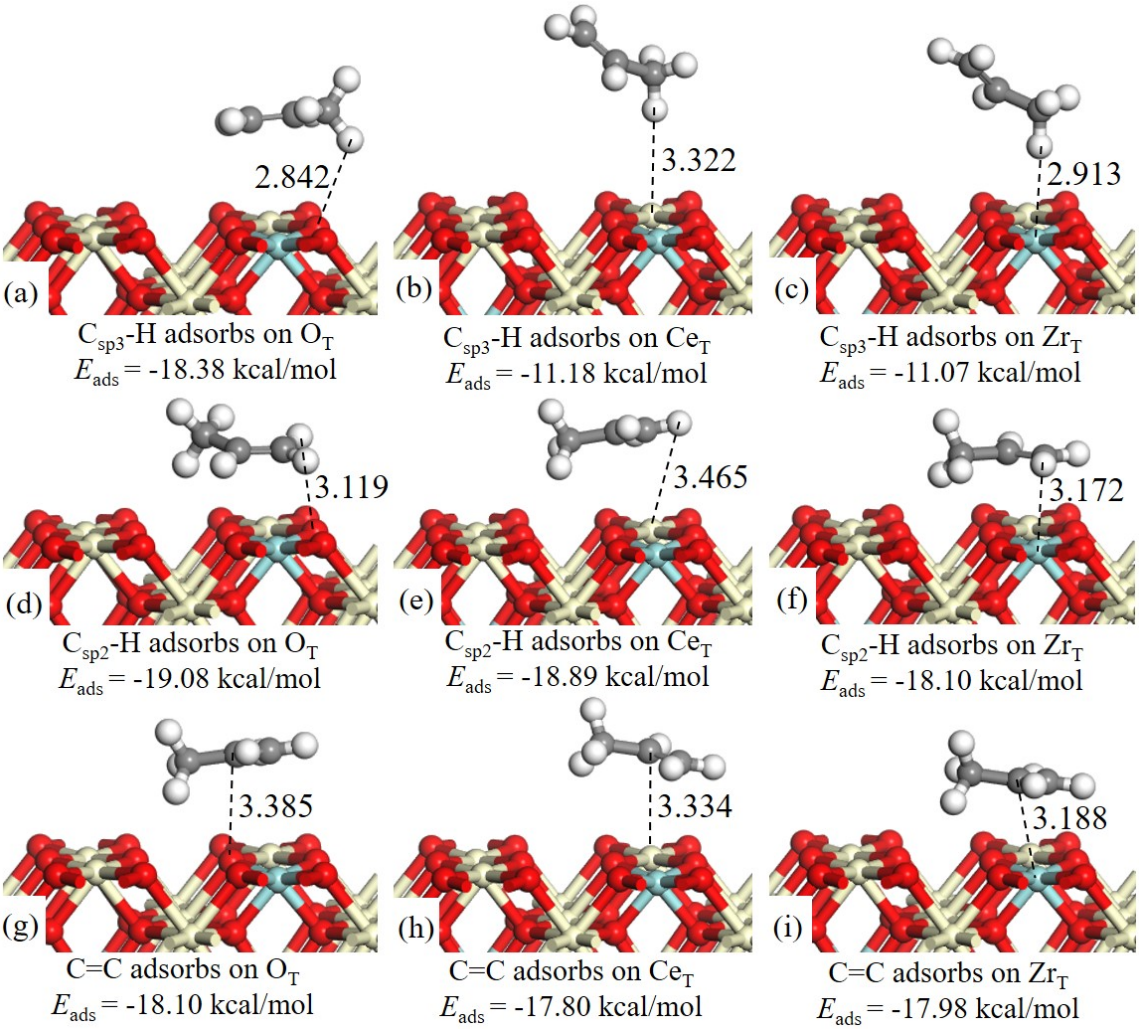

Fig. S3 Optimized adsorption configurations of (a) C_{sp3}-H of C_3H_6 on O_T site, (b) C_{sp3}-H of C_3H_6 on Ce_T site, (c) C_{sp3}-H of C_3H_6 on Zr_T site, (d) C_{sp2}-H of C_3H_6 on O_T site, (e) C_{sp2}-H of C_3H_6 on Ce_T site, (f) C_{sp2}-H of C_3H_6 on Zr_T site, (g) C=C of C_3H_6 on O_T site, (h) C=C of C_3H_6 on Ce_T site, and (i) C=C of C_3H_6 on Zr_T site. Key: C, gray; H, white.

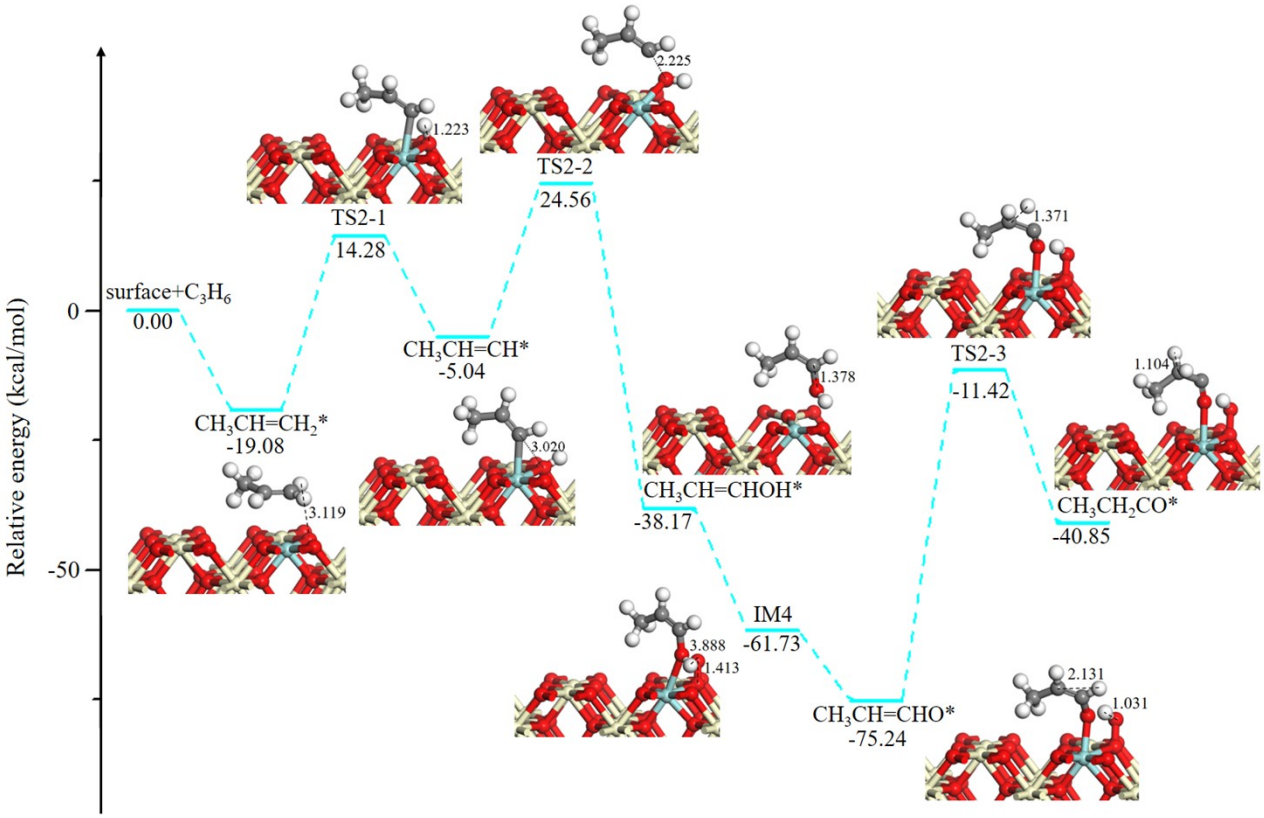

Fig. S4 Energy profile and corresponding optimized configurations of C_3H_6 oxidation from C_{sp2}-H site on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

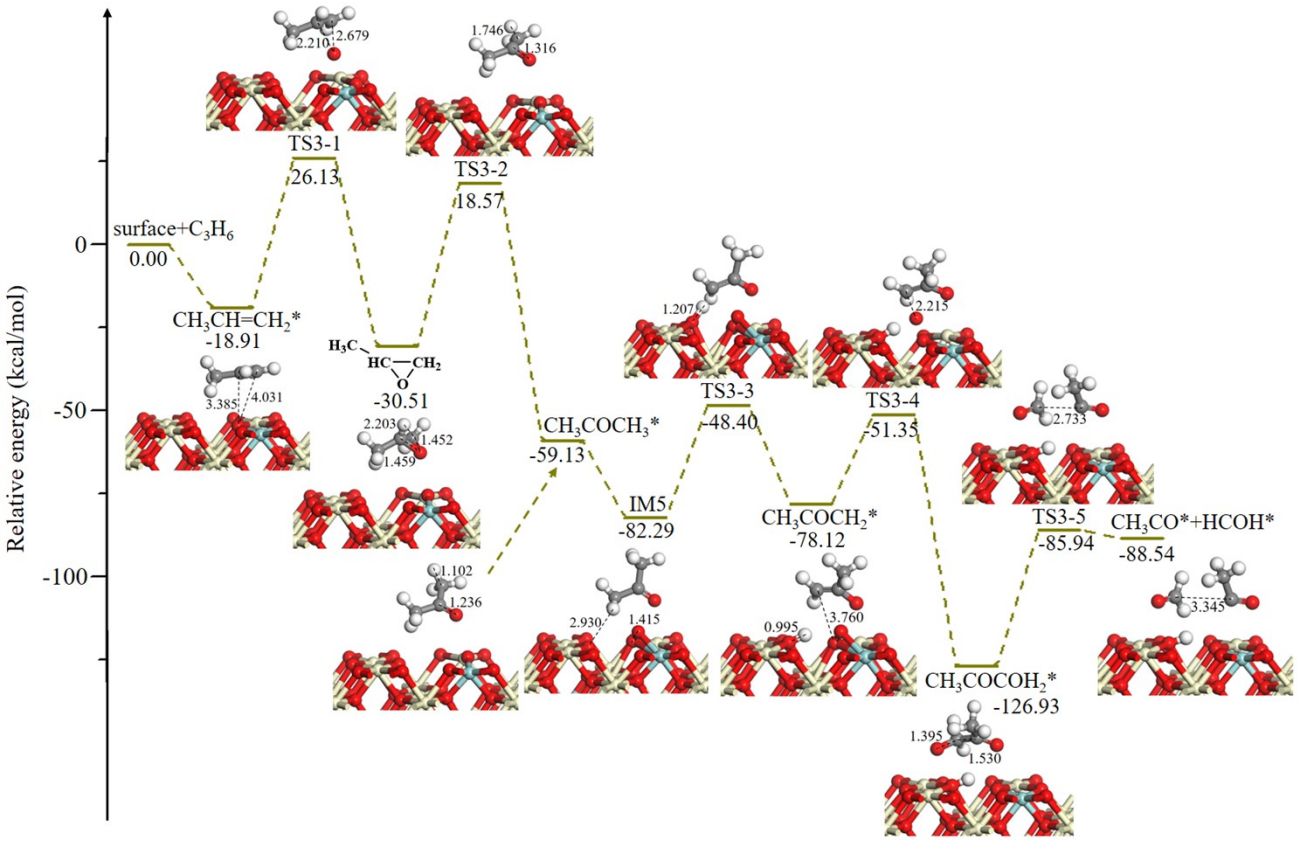

Fig. S5 Energy profile and corresponding optimized configurations of C_3H_6 oxidation from C=C site on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

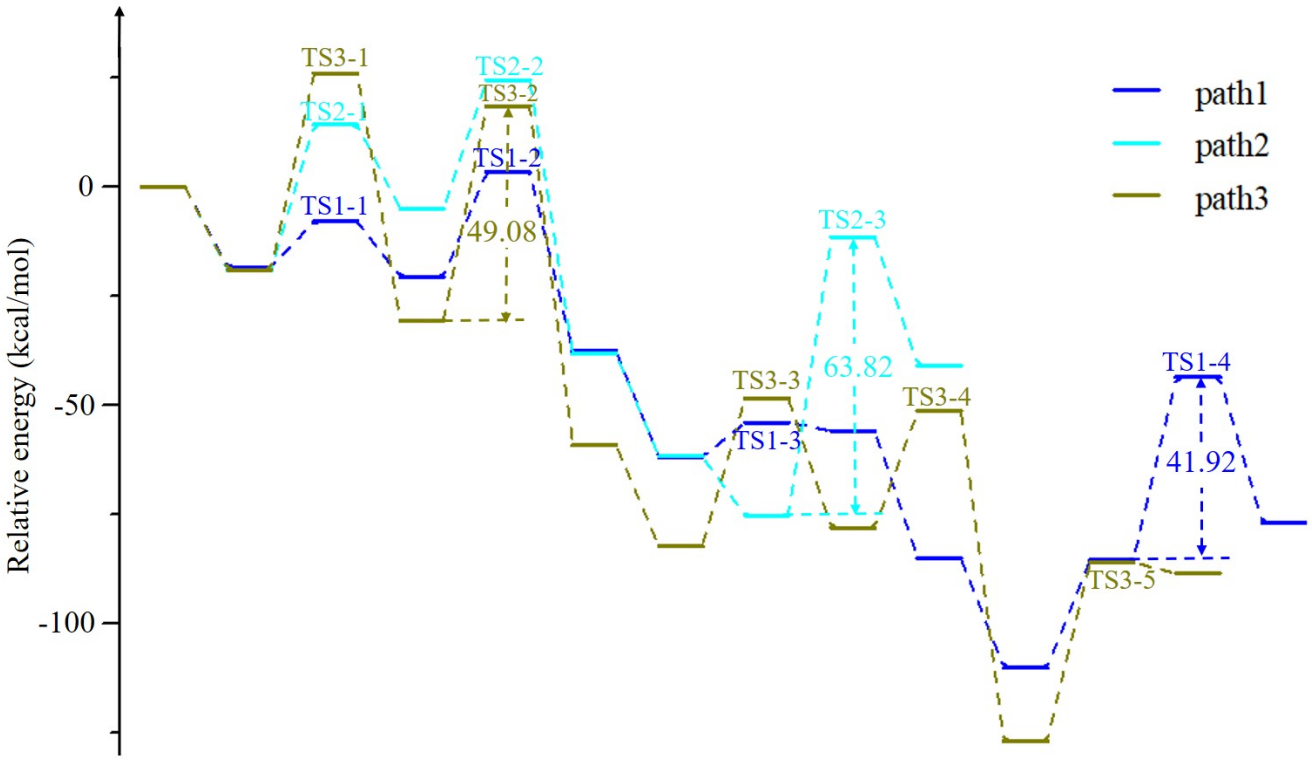

Fig. S6 Energy profiles of C_3H_6 oxidation on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

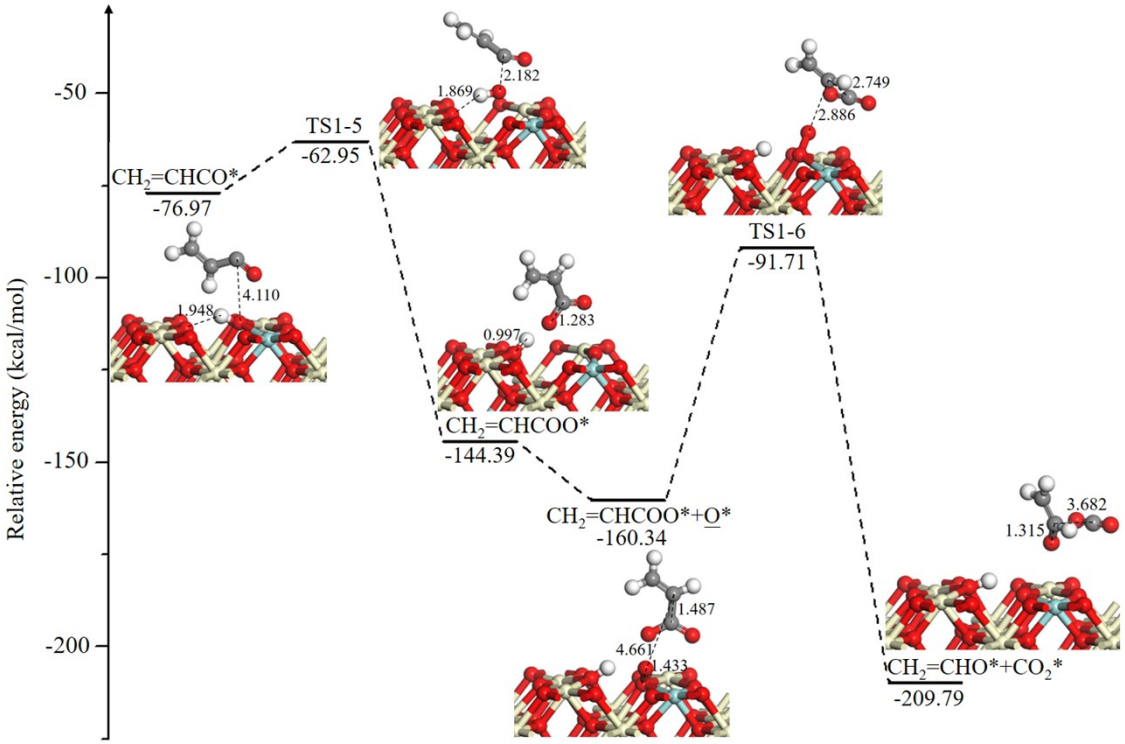

Fig. S7 Energy profile and corresponding optimized configurations of acryloyl oxidation on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

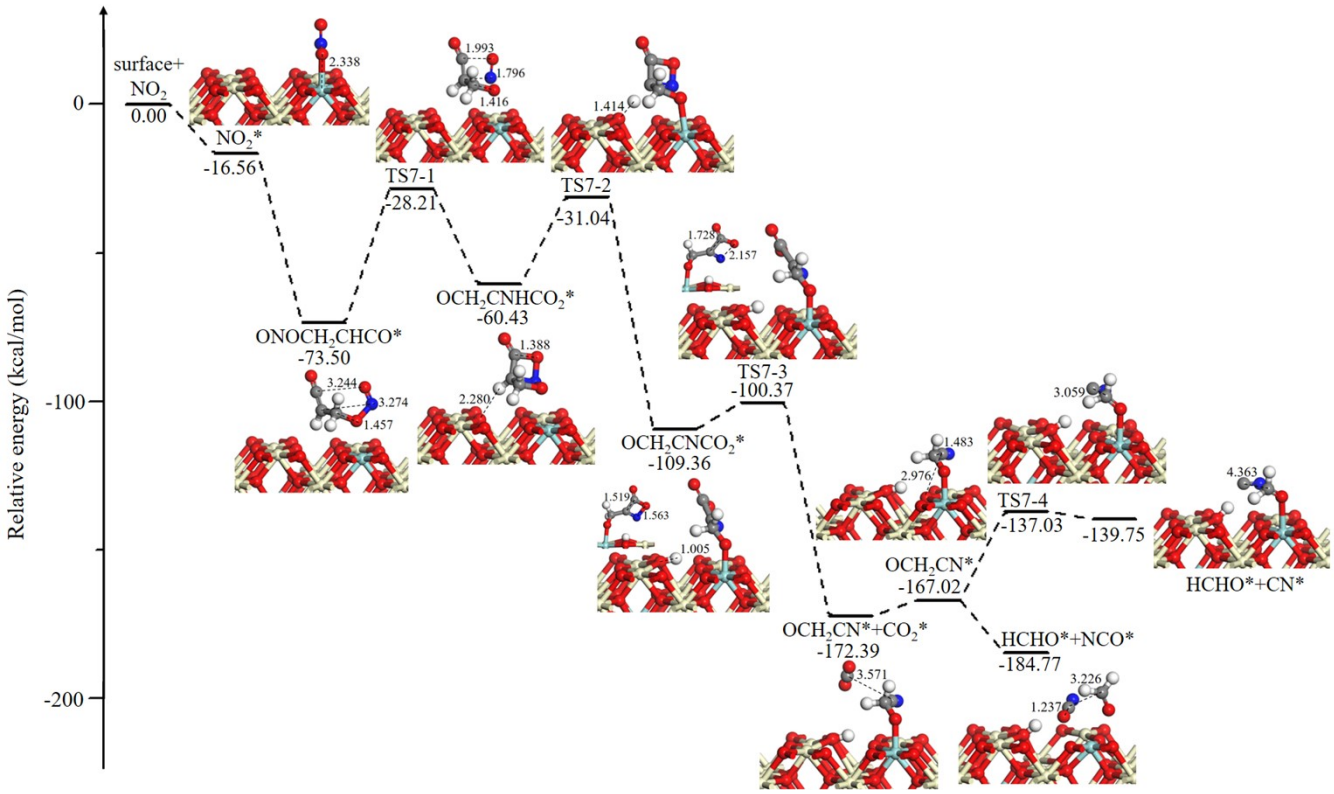

Fig. S8 Energy profile and corresponding optimized configurations of NO_2* and CH_2=CHCO* reaction on the $Ce_{0.875}Zr_{0.125}O_2$ (110) surface.

Table S4 Cartesian coordinates for all the optimized geometries of reactants, transition states and products.

$Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411734	-0.028586	5.770129
3	O	4.058250	1.913077	0.000000
4	O	4.063301	1.913079	3.895275
5	O	4.058250	0.000000	1.913077
6	O	3.999266	-0.028586	5.770129
7	O	1.352750	1.913077	0.000000
8	O	1.347699	1.913079	3.895275
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.004514	0.000025	3.948453
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.705500	1.913128	5.659458
13	O	6.763750	0.000000	1.913077
14	O	6.855993	0.102732	5.760344
15	O	9.469250	1.913077	0.000000
16	O	9.431712	1.913071	3.851941
17	O	9.469250	0.000000	1.913077
18	O	9.377007	0.102733	5.760344
19	O	6.763750	1.913077	0.000000
20	O	6.801287	1.913070	3.851940
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.415514	0.000025	3.948453
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.116500	1.913950	5.431412
25	O	1.352750	3.826155	1.913077
26	O	1.411777	3.854803	5.770184
27	O	4.058250	5.739232	0.000000
28	O	4.004600	5.739230	3.742568
29	O	4.058250	3.826155	1.913077
30	O	3.999223	3.854803	5.770184
31	O	1.352750	5.739232	0.000000
32	O	1.406400	5.739229	3.742568
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004651	3.826114	3.948509
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.705500	5.739211	5.595430
37	O	6.763750	3.826155	1.913077
38	O	6.855208	3.723386	5.761023
39	O	9.469250	5.739232	0.000000
40	O	9.472064	5.739172	3.928675
41	O	9.469250	3.826155	1.913077
42	O	9.377791	3.723386	5.761024
43	O	6.763750	5.739232	0.000000
44	O	6.760936	5.739172	3.928675
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.415651	3.826114	3.948509
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.116500	5.739836	5.682187

NO adsorbes on Ce_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.412024	-0.028368	5.770688
3	O	4.058250	1.913077	0.000000
4	O	4.062600	1.912994	3.894477

5	O	4.058250	0.000000	1.913077
6	O	3.998976	-0.028369	5.770687
7	O	1.352750	1.913077	0.000000
8	O	1.348399	1.912993	3.894477
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.006239	-0.000833	3.948713
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.705500	1.913152	5.658926
13	O	6.763750	0.000000	1.913077
14	O	6.853887	0.113051	5.758246
15	O	9.469250	1.913077	0.000000
16	O	9.431504	1.913155	3.846008
17	O	9.469250	0.000000	1.913077
18	O	9.379113	0.113051	5.758246
19	O	6.763750	1.913077	0.000000
20	O	6.801496	1.913155	3.846008
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.417239	-0.000835	3.948713
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.116500	1.915352	5.429538
25	O	1.352750	3.826155	1.913077
26	O	1.412142	3.854436	5.770673
27	O	4.058250	5.739232	0.000000
28	O	4.002595	5.739260	3.741742
29	O	4.058250	3.826155	1.913077
30	O	3.998857	3.854436	5.770673
31	O	1.352750	5.739232	0.000000
32	O	1.408406	5.739260	3.741743
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.006649	3.826968	3.948925
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.705500	5.739076	5.595070
37	O	6.763750	3.826155	1.913077
38	O	6.853958	3.713868	5.758232
39	O	9.469250	5.739232	0.000000
40	O	9.477247	5.739273	3.925493
41	O	9.469250	3.826155	1.913077
42	O	9.379042	3.713868	5.758232
43	O	6.763750	5.739232	0.000000
44	O	6.755754	5.739273	3.925493
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417649	3.826967	3.948925
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.116500	5.739861	5.700264
49	N	8.116500	5.939259	8.498269
50	O	8.116501	6.064221	9.654957

NO adsorbes on Zr_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411988	-0.027333	5.770701
3	O	4.058250	1.913077	0.000000
4	O	4.060342	1.913078	3.892623
5	O	4.058250	0.000000	1.913077
6	O	3.999012	-0.027333	5.770700
7	O	1.352750	1.913077	0.000000
8	O	1.350658	1.913077	3.892623
9	Ce	0.000000	0.000000	0.000000

10	Ce	-0.003264	0.001993	3.944511
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.705500	1.913079	5.658713
13	O	6.763750	0.000000	1.913077
14	O	6.853026	0.085058	5.752377
15	O	9.469250	1.913077	0.000000
16	O	9.435563	1.913078	3.857199
17	O	9.469250	0.000000	1.913077
18	O	9.379974	0.085058	5.752377
19	O	6.763750	1.913077	0.000000
20	O	6.797437	1.913078	3.857199
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.414264	0.001993	3.944511
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.116500	1.913079	5.454199
25	O	1.352750	3.826155	1.913077
26	O	1.411988	3.853489	5.770700
27	O	4.058250	5.739232	0.000000
28	O	4.002885	5.739228	3.741110
29	O	4.058250	3.826155	1.913077
30	O	3.999012	3.853489	5.770700
31	O	1.352750	5.739232	0.000000
32	O	1.408114	5.739228	3.741110
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.003264	3.824162	3.944509
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.705500	5.739228	5.593997
37	O	6.763750	3.826155	1.913077
38	O	6.853026	3.741098	5.752376
39	O	9.469250	5.739232	0.000000
40	O	9.473253	5.739229	3.916545
41	O	9.469250	3.826155	1.913077
42	O	9.379974	3.741098	5.752376
43	O	6.763750	5.739232	0.000000
44	O	6.759747	5.739228	3.916545
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.414264	3.824162	3.944509
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.116500	5.739229	5.671794
49	N	8.116500	1.913081	7.915342
50	O	8.116500	1.913083	9.077696

NO adsorbes on O_{T1} site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.315523	-0.052236	5.846883
3	O	4.058250	1.913077	0.000000
4	O	4.038849	2.007743	4.002981
5	O	4.058250	0.000000	1.913077
6	O	3.914046	-0.034301	5.767856
7	O	1.352750	1.913077	0.000000
8	O	1.316733	1.862310	3.904000
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.057172	-0.010081	3.898967
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.599656	1.778832	5.711653
13	O	6.763750	0.000000	1.913077
14	O	6.791558	0.123369	5.728648

15	O	9.469250	1.913077	0.000000
16	O	9.415338	1.912766	3.839789
17	O	9.469250	0.000000	1.913077
18	O	9.321288	0.111309	5.741316
19	O	6.763750	1.913077	0.000000
20	O	6.792928	1.915104	3.822513
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.407230	0.015879	3.944420
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.108915	1.920397	5.417389
25	O	1.352750	3.826155	1.913077
26	O	1.540177	3.841285	5.718799
27	O	4.058250	5.739232	0.000000
28	O	3.988979	5.670401	3.821588
29	O	4.058250	3.826155	1.913077
30	O	4.129101	3.814265	6.313527
31	O	1.352750	5.739232	0.000000
32	O	1.384515	5.768688	3.747112
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004168	3.814862	3.939232
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.622666	5.813815	5.630502
37	O	6.763750	3.826155	1.913077
38	O	6.834219	3.745218	5.701258
39	O	9.469250	5.739232	0.000000
40	O	9.459335	5.723086	3.926684
41	O	9.469250	3.826155	1.913077
42	O	9.380320	3.687142	5.768820
43	O	6.763750	5.739232	0.000000
44	O	6.750842	5.757026	3.896333
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.476831	3.836436	3.846551
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.096143	5.751647	5.680867
49	N	4.059594	4.321753	7.540970
50	O	4.106601	3.512846	8.447032

NO adsorbes on O_{T2} site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.484749	-0.030872	5.742089
3	O	4.058250	1.913077	0.000000
4	O	4.077636	1.899096	3.852213
5	O	4.058250	0.000000	1.913077
6	O	4.071700	-0.035336	5.740357
7	O	1.352750	1.913077	0.000000
8	O	1.380833	1.926222	3.884770
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.076586	-0.001835	3.872288
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.738563	1.910227	5.656353
13	O	6.763750	0.000000	1.913077
14	O	6.949841	0.032795	5.752607
15	O	9.469250	1.913077	0.000000
16	O	9.502279	1.865978	3.876984
17	O	9.469250	0.000000	1.913077
18	O	9.510334	0.060843	5.808158
19	O	6.763750	1.913077	0.000000

20	O	6.829583	2.029562	4.033268
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.433385	0.000980	3.945339
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.250580	1.726962	5.567797
25	O	1.352750	3.826155	1.913077
26	O	1.398697	3.860430	5.768019
27	O	4.058250	5.739232	0.000000
28	O	4.016288	5.753307	3.698228
29	O	4.058250	3.826155	1.913077
30	O	4.085460	3.873495	5.695848
31	O	1.352750	5.739232	0.000000
32	O	1.435189	5.722280	3.730830
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.019444	3.819446	3.927788
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.735533	5.736541	5.590836
37	O	6.763750	3.826155	1.913077
38	O	6.762782	3.013011	7.016599
39	O	9.469250	5.739232	0.000000
40	O	9.517464	5.781457	3.910987
41	O	9.469250	3.826155	1.913077
42	O	9.039754	3.779114	5.675531
43	O	6.763750	5.739232	0.000000
44	O	6.769224	5.621420	4.052286
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.340276	3.827047	3.797060
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.247944	5.880675	5.725232
49	N	7.319874	2.662465	8.116253
50	O	8.276924	1.844591	7.930981

NO_3 adsorbes on $brid_1$ site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.394743	-0.020797	5.752756
3	O	4.058250	1.913077	0.000000
4	O	4.061937	1.912026	3.872412
5	O	4.058250	0.000000	1.913077
6	O	4.008249	-0.025420	5.752588
7	O	1.352750	1.913077	0.000000
8	O	1.349396	1.911871	3.871920
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.000557	0.002586	3.937645
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.706134	1.921102	5.717855
13	O	6.763750	0.000000	1.913077
14	O	6.873925	0.104994	5.778978
15	O	9.469250	1.913077	0.000000
16	O	9.424391	1.912390	3.854190
17	O	9.469250	0.000000	1.913077
18	O	9.353721	0.106270	5.783393
19	O	6.763750	1.913077	0.000000
20	O	6.808711	1.912439	3.854096
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.410683	0.002451	3.938162
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.116804	1.920134	5.447336

25	O	1.352750	3.826155	1.913077
26	O	1.402072	3.859937	5.668289
27	O	4.058250	5.739232	0.000000
28	O	4.006384	5.755045	3.724067
29	O	4.058250	3.826155	1.913077
30	O	4.018034	3.853690	5.673247
31	O	1.352750	5.739232	0.000000
32	O	1.404285	5.754281	3.721647
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.002053	3.824337	3.923873
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.706006	5.731717	5.663627
37	O	6.763750	3.826155	1.913077
38	O	6.880741	3.722239	5.780102
39	O	9.469250	5.739232	0.000000
40	O	9.471049	5.742156	3.930573
41	O	9.469250	3.826155	1.913077
42	O	9.357421	3.723648	5.778117
43	O	6.763750	5.739232	0.000000
44	O	6.762067	5.741762	3.930390
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.409192	3.824166	3.924028
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.116593	5.739336	5.700199
49	N	2.815250	3.849836	8.754988
50	O	2.963369	3.849563	9.979904
51	O	2.729043	2.736251	8.127968
52	O	2.741129	4.956584	8.124038

NO_3 adsorbes on $brid_2$ site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411172	-0.028160	5.763129
3	O	4.058250	1.913077	0.000000
4	O	4.058767	1.910593	3.882802
5	O	4.058250	0.000000	1.913077
6	O	4.002260	-0.028919	5.765734
7	O	1.352750	1.913077	0.000000
8	O	1.352847	1.911562	3.881987
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.011907	-0.003114	3.940876
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.706820	1.919415	5.659437
13	O	6.763750	0.000000	1.913077
14	O	6.863766	0.076691	5.763778
15	O	9.469250	1.913077	0.000000
16	O	9.429356	1.905326	3.861702
17	O	9.469250	0.000000	1.913077
18	O	9.367259	0.074669	5.751538
19	O	6.763750	1.913077	0.000000
20	O	6.804440	1.899062	3.865463
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.425923	-0.003044	3.945595
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.118376	1.976295	5.517960
25	O	1.352750	3.826155	1.913077
26	O	1.418311	3.852155	5.763908
27	O	4.058250	5.739232	0.000000

28	O	3.997262	5.741842	3.733797
29	O	4.058250	3.826155	1.913077
30	O	3.994217	3.852959	5.764011
31	O	1.352750	5.739232	0.000000
32	O	1.417579	5.741332	3.732705
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.006221	3.827835	3.923235
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.706750	5.729972	5.601759
37	O	6.763750	3.826155	1.913077
38	O	6.842883	3.754620	5.652060
39	O	9.469250	5.739232	0.000000
40	O	9.471076	5.746287	3.903022
41	O	9.469250	3.826155	1.913077
42	O	9.392373	3.746363	5.657727
43	O	6.763750	5.739232	0.000000
44	O	6.766084	5.750266	3.904513
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.418533	3.827631	3.924907
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.121664	5.735488	5.742580
49	N	8.275595	3.395294	8.555008
50	O	8.480579	3.232850	9.759375
51	O	8.149297	2.347267	7.809358
52	O	8.180690	4.567955	8.074451

NO_3 adsorbes on biden site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.417309	-0.031149	5.767835
3	O	4.058250	1.913077	0.000000
4	O	4.061970	1.909943	3.880609
5	O	4.058250	0.000000	1.913077
6	O	3.999098	-0.019529	5.749478
7	O	1.352750	1.913077	0.000000
8	O	1.345477	1.912026	3.894825
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.013313	-0.009970	3.950605
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.713758	1.910481	5.667064
13	O	6.763750	0.000000	1.913077
14	O	6.866373	0.145158	5.732948
15	O	9.469250	1.913077	0.000000
16	O	9.429175	1.912563	3.821916
17	O	9.469250	0.000000	1.913077
18	O	9.376444	0.143470	5.745383
19	O	6.763750	1.913077	0.000000
20	O	6.798450	1.909850	3.817741
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.422795	-0.003228	3.936377
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.119472	1.913299	5.422058
25	O	1.352750	3.826155	1.913077
26	O	1.417525	3.854313	5.765471
27	O	4.058250	5.739232	0.000000
28	O	3.995005	5.740303	3.736406
29	O	4.058250	3.826155	1.913077
30	O	4.000306	3.845397	5.748202

31	O	1.352750	5.739232	0.000000
32	O	1.411734	5.737085	3.742229
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.016430	3.832090	3.951736
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.704739	5.738408	5.612994
37	O	6.763750	3.826155	1.913077
38	O	6.867047	3.680343	5.726383
39	O	9.469250	5.739232	0.000000
40	O	9.477243	5.738133	3.943288
41	O	9.469250	3.826155	1.913077
42	O	9.373682	3.685607	5.747509
43	O	6.763750	5.739232	0.000000
44	O	6.752193	5.737937	3.931489
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.416081	3.833080	3.936145
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.085117	5.740755	5.805284
49	N	7.750988	5.747736	8.805310
50	O	7.631904	5.754699	10.026186
51	O	8.905188	5.755605	8.236085
52	O	6.737316	5.732215	8.021374

NO_3 adsorbes on monoden site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.420559	-0.016615	5.770694
3	O	4.058250	1.913077	0.000000
4	O	4.058070	1.913367	3.885269
5	O	4.058250	0.000000	1.913077
6	O	4.000785	-0.044824	5.740390
7	O	1.352750	1.913077	0.000000
8	O	1.355231	1.912989	3.889372
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.004507	0.002414	3.947508
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.719368	1.913810	5.674996
13	O	6.763750	0.000000	1.913077
14	O	6.869015	0.015720	5.695341
15	O	9.469250	1.913077	0.000000
16	O	9.430877	1.913273	3.869508
17	O	9.469250	0.000000	1.913077
18	O	9.378380	0.077259	5.728491
19	O	6.763750	1.913077	0.000000
20	O	6.795235	1.913270	3.883241
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.417807	-0.002913	3.924549
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.102226	1.914107	5.524754
25	O	1.352750	3.826155	1.913077
26	O	1.421403	3.842427	5.770533
27	O	4.058250	5.739232	0.000000
28	O	3.997451	5.738833	3.722175
29	O	4.058250	3.826155	1.913077
30	O	4.001706	3.871549	5.740233
31	O	1.352750	5.739232	0.000000
32	O	1.412285	5.739138	3.740578
33	Ce	0.000000	3.826155	0.000000

34	Ce	-0.003915	3.823837	3.946881
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.718915	5.739266	5.600881
37	O	6.763750	3.826155	1.913077
38	O	6.868523	3.809540	5.697819
39	O	9.469250	5.739232	0.000000
40	O	9.472924	5.739552	3.895363
41	O	9.469250	3.826155	1.913077
42	O	9.379854	3.747122	5.728140
43	O	6.763750	5.739232	0.000000
44	O	6.760257	5.738989	3.864616
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417281	3.829106	3.924229
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.108486	5.739639	5.672149
49	N	6.904163	1.911610	8.451653
50	O	6.927580	1.911300	9.690478
51	O	8.044642	1.913643	7.815039
52	O	5.846239	1.908925	7.791420

NO_2-O_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.488189	-0.050062	5.743321
3	O	4.058250	1.913077	0.000000
4	O	4.081996	1.902314	3.848166
5	O	4.058250	0.000000	1.913077
6	O	4.070217	-0.022472	5.738931
7	O	1.352750	1.913077	0.000000
8	O	1.377077	1.922638	3.886094
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.078422	-0.023648	3.883444
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.740071	1.905095	5.649812
13	O	6.763750	0.000000	1.913077
14	O	6.957571	0.083734	5.742373
15	O	9.469250	1.913077	0.000000
16	O	9.499728	1.850823	3.847305
17	O	9.469250	0.000000	1.913077
18	O	9.525607	0.127170	5.852753
19	O	6.763750	1.913077	0.000000
20	O	6.836512	2.058707	4.036509
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.438830	0.002543	3.949547
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.299657	1.734925	5.501598
25	O	1.352750	3.826155	1.913077
26	O	1.396228	3.864751	5.763045
27	O	4.058250	5.739232	0.000000
28	O	4.016919	5.753450	3.706879
29	O	4.058250	3.826155	1.913077
30	O	4.090302	3.848929	5.699086
31	O	1.352750	5.739232	0.000000
32	O	1.441582	5.718371	3.729453
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.005138	3.833760	3.916536
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.747692	5.731678	5.603688

37	O	6.763750	3.826155	1.913077
38	O	7.665696	2.387534	7.862800
39	O	9.469250	5.739232	0.000000
40	O	9.526718	5.774650	3.938997
41	O	9.469250	3.826155	1.913077
42	O	9.009724	3.711168	5.717176
43	O	6.763750	5.739232	0.000000
44	O	6.761875	5.637229	4.045562
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.342114	3.842949	3.795968
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.195219	5.874380	5.790983
49	N	8.209586	3.303314	8.469722
50	O	9.063544	3.297283	9.313990
51	O	6.609261	4.757503	7.261152
52	O	7.592030	4.790782	8.196658

TS

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.455841972	-0.043611506	5.745606455
4.058250000	1.913077397	0.000000000
4.075640780	1.907929533	3.858411342
4.058250000	0.000000000	1.913077397
4.038757425	-0.021923288	5.740090596
1.352750000	1.913077397	0.000000000
1.362561083	1.919415970	3.879962701
0.000000000	0.000000000	0.000000000
0.036775902	-0.014213655	3.903510017
2.705500000	1.913077397	1.913077397
2.714169611	1.901938098	5.650398746
6.763750000	0.000000000	1.913077397
6.928463393	0.101098272	5.740099923
9.469250000	1.913077397	0.000000000
9.470921641	1.874547038	3.853942073
9.469250000	0.000000000	1.913077397
9.476256979	0.140827351	5.812119495
6.763750000	1.913077397	0.000000000
6.825260889	2.036368846	3.997236527
5.411000000	0.000000000	0.000000000
5.443681226	-0.000811911	3.965827371
8.116500000	1.913077397	1.913077397
8.265330004	1.759663183	5.523569906
1.352750000	3.826154793	1.913077397
1.388335910	3.859857184	5.755569560
4.058250000	5.739232190	0.000000000
4.010463302	5.747559271	3.713977513
4.058250000	3.826154793	1.913077397
4.039425562	3.843841166	5.698388211
1.352750000	5.739232190	0.000000000
1.425911952	5.725122559	3.726653929
0.000000000	3.826154793	0.000000000
-0.014266350	3.831405176	3.918250639
2.705500000	5.739232190	1.913077397
2.722351930	5.739854262	5.599553577
6.763750000	3.826154793	1.913077397
7.855578357	2.370526363	7.869690002
9.469250000	5.739232190	0.000000000

9.515536505	5.764325112	3.916572751
9.469250000	3.826154793	1.913077397
9.149251476	3.717524541	5.694206637
6.763750000	5.739232190	0.000000000
6.757600302	5.663546885	3.992020503
5.411000000	3.826154793	0.000000000
5.347353488	3.854663409	3.830768905
8.116500000	5.739232190	1.913077397
8.157900656	5.833029800	5.802708284
8.202770810	3.357807648	8.533557097
8.879274282	3.258497414	9.547491203
6.612639244	4.465149197	6.802885773
7.801115483	4.589036423	8.168890877

Cartesian coordinates of NO_3*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407805	-0.028301	5.765962
3	O	4.058250	1.913077	0.000000
4	O	4.057699	1.910134	3.883060
5	O	4.058250	0.000000	1.913077
6	O	4.006603	-0.028594	5.763184
7	O	1.352750	1.913077	0.000000
8	O	1.353096	1.910612	3.882879
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.026086	0.002049	3.946071
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.704785	1.919390	5.660009
13	O	6.763750	0.000000	1.913077
14	O	6.880888	0.103241	5.761801
15	O	9.469250	1.913077	0.000000
16	O	9.426672	1.903084	3.865981
17	O	9.469250	0.000000	1.913077
18	O	9.358035	0.081388	5.761482
19	O	6.763750	1.913077	0.000000
20	O	6.801405	1.906814	3.856681
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.439694	0.004658	3.942862
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.108103	1.966530	5.519303
25	O	1.352750	3.826155	1.913077
26	O	1.420346	3.847976	5.761400
27	O	4.058250	5.739232	0.000000
28	O	3.994676	5.740991	3.729283
29	O	4.058250	3.826155	1.913077
30	O	3.996165	3.853186	5.757799
31	O	1.352750	5.739232	0.000000
32	O	1.409706	5.739939	3.733941
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.002034	3.829352	3.918015
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.707661	5.732965	5.596889
37	O	6.763750	3.826155	1.913077
38	O	8.123558	2.347012	7.796411
39	O	9.469250	5.739232	0.000000
40	O	9.471478	5.752335	3.897284
41	O	9.469250	3.826155	1.913077
42	O	9.397361	3.765916	5.656897

43	O	6.763750	5.739232	0.000000
44	O	6.757955	5.758136	3.904593
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.412240	3.833079	3.916918
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.121848	5.671725	5.737944
49	N	8.117718	3.389866	8.560618
50	O	8.126477	3.222286	9.780649
51	O	6.842459	3.754841	5.649624
52	O	8.102672	4.566826	8.076200

C_{sp3}-H of C_3H_6 adsorbes on O_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.401448	-0.024247	5.784023
3	O	4.058250	1.913077	0.000000
4	O	4.052739	1.915392	3.897477
5	O	4.058250	0.000000	1.913077
6	O	3.990031	-0.030824	5.775394
7	O	1.352750	1.913077	0.000000
8	O	1.345108	1.913606	3.896428
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.008951	0.005272	3.953308
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.698413	1.916647	5.657887
13	O	6.763750	0.000000	1.913077
14	O	6.840187	0.110615	5.748157
15	O	9.469250	1.913077	0.000000
16	O	9.432423	1.909410	3.847029
17	O	9.469250	0.000000	1.913077
18	O	9.363650	0.114408	5.759953
19	O	6.763750	1.913077	0.000000
20	O	6.796425	1.911483	3.842044
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.405066	0.002543	3.950767
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.110007	1.906151	5.423165
25	O	1.352750	3.826155	1.913077
26	O	1.394072	3.865266	5.781430
27	O	4.058250	5.739232	0.000000
28	O	3.994245	5.737117	3.747098
29	O	4.058250	3.826155	1.913077
30	O	3.988885	3.851689	5.778705
31	O	1.352750	5.739232	0.000000
32	O	1.399007	5.743069	3.746109
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.012469	3.831198	3.946102
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.696322	5.742129	5.598422
37	O	6.763750	3.826155	1.913077
38	O	6.841873	3.715003	5.757948
39	O	9.469250	5.739232	0.000000
40	O	9.467511	5.741483	3.920898
41	O	9.469250	3.826155	1.913077
42	O	9.366317	3.722492	5.750018
43	O	6.763750	5.739232	0.000000
44	O	6.746442	5.737025	3.920899
45	Ce	5.411000	3.826155	0.000000

46	Ce	5.415208	3.823160	3.950461
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.103627	5.727851	5.681765
49	C	8.833469	5.781669	8.926830
50	C	9.678317	4.569820	9.160983
51	C	7.496292	5.784839	8.777065
52	H	10.288452	4.697583	10.072881
53	H	10.373240	4.402562	8.319048
54	H	9.064556	3.664408	9.276833
55	H	6.942318	6.712188	8.600977
56	H	6.913244	4.857783	8.822555
57	H	9.369156	6.738449	8.856750

C_{sp3}-H of C_3H_6 adsorbes on Ce_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.412538	-0.033275	5.770461
3	O	4.058250	1.913077	0.000000
4	O	4.066024	1.910906	3.890016
5	O	4.058250	0.000000	1.913077
6	O	3.999871	-0.013715	5.771161
7	O	1.352750	1.913077	0.000000
8	O	1.348626	1.908852	3.894057
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000126	-0.000157	3.947739
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.706008	1.908659	5.656812
13	O	6.763750	0.000000	1.913077
14	O	6.857114	0.084833	5.759069
15	O	9.469250	1.913077	0.000000
16	O	9.439109	1.912175	3.848085
17	O	9.469250	0.000000	1.913077
18	O	9.378678	0.116282	5.762812
19	O	6.763750	1.913077	0.000000
20	O	6.809248	1.912655	3.859657
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.418974	0.004367	3.950576
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.134556	1.912634	5.435336
25	O	1.352750	3.826155	1.913077
26	O	1.410501	3.862053	5.771828
27	O	4.058250	5.739232	0.000000
28	O	4.007132	5.739426	3.749269
29	O	4.058250	3.826155	1.913077
30	O	3.999250	3.842541	5.770223
31	O	1.352750	5.739232	0.000000
32	O	1.412170	5.738189	3.742504
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.003283	3.823737	3.952632
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.708973	5.736624	5.596684
37	O	6.763750	3.826155	1.913077
38	O	6.856359	3.745127	5.757438
39	O	9.469250	5.739232	0.000000
40	O	9.476599	5.739021	3.927356
41	O	9.469250	3.826155	1.913077
42	O	9.377730	3.708688	5.761859
43	O	6.763750	5.739232	0.000000

44	O	6.758837	5.744338	3.915342
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.420338	3.823284	3.952511
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.106263	5.743787	5.677866
49	C	6.947610	4.864894	10.577406
50	C	8.152376	5.612324	10.098927
51	C	5.994379	5.358383	11.378273
52	H	8.198113	5.616726	8.996534
53	H	9.084661	5.126232	10.439320
54	H	8.157126	6.656182	10.447161
55	H	5.139721	4.751117	11.691497
56	H	6.031063	6.389549	11.745230
57	H	6.860753	3.827235	10.229068

C_{sp3}-H of C_3H_6 adsorbes on Zr_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411807	-0.031030	5.771205
3	O	4.058250	1.913077	0.000000
4	O	4.065576	1.913285	3.892881
5	O	4.058250	0.000000	1.913077
6	O	3.998529	-0.024838	5.768164
7	O	1.352750	1.913077	0.000000
8	O	1.350722	1.913379	3.897647
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000488	-0.000334	3.948775
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.711214	1.908890	5.661452
13	O	6.763750	0.000000	1.913077
14	O	6.856244	0.084865	5.753824
15	O	9.469250	1.913077	0.000000
16	O	9.437125	1.912938	3.841990
17	O	9.469250	0.000000	1.913077
18	O	9.376992	0.120320	5.757820
19	O	6.763750	1.913077	0.000000
20	O	6.804352	1.913965	3.853411
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.415467	-0.000193	3.947333
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.132095	1.912983	5.425528
25	O	1.352750	3.826155	1.913077
26	O	1.411874	3.856769	5.770841
27	O	4.058250	5.739232	0.000000
28	O	4.005027	5.738718	3.745413
29	O	4.058250	3.826155	1.913077
30	O	3.999095	3.850764	5.771293
31	O	1.352750	5.739232	0.000000
32	O	1.408993	5.739798	3.742340
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.001688	3.826122	3.951583
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.706384	5.737171	5.596436
37	O	6.763750	3.826155	1.913077
38	O	6.854469	3.740674	5.759178
39	O	9.469250	5.739232	0.000000
40	O	9.472253	5.738903	3.933274
41	O	9.469250	3.826155	1.913077

42	O	9.377748	3.702910	5.760480
43	O	6.763750	5.739232	0.000000
44	O	6.763571	5.738396	3.918349
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.416261	3.826436	3.949430
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.105257	5.743170	5.678226
49	C	7.001799	2.424561	9.991373
50	C	8.283285	1.886621	9.438335
51	C	6.209566	1.782710	10.860545
52	H	9.144116	2.517607	9.723031
53	H	8.267217	1.876767	8.335483
54	H	8.479170	0.858921	9.781886
55	H	5.285779	2.231961	11.236707
56	H	6.452568	0.775372	11.217307
57	H	6.714528	3.428718	9.655089

C_{sp2}-H of C_3H_6 adsorbes on O_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411560	-0.029385	5.777379
3	O	4.058250	1.913077	0.000000
4	O	4.061187	1.913544	3.894791
5	O	4.058250	0.000000	1.913077
6	O	3.998345	-0.024294	5.785164
7	O	1.352750	1.913077	0.000000
8	O	1.349891	1.911790	3.893256
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.003980	0.003902	3.947770
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.704512	1.910415	5.657484
13	O	6.763750	0.000000	1.913077
14	O	6.849590	0.057730	5.745816
15	O	9.469250	1.913077	0.000000
16	O	9.433334	1.917308	3.859507
17	O	9.469250	0.000000	1.913077
18	O	9.376624	0.094304	5.749164
19	O	6.763750	1.913077	0.000000
20	O	6.805678	1.912071	3.870160
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.415874	-0.000650	3.945023
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.126638	1.932687	5.460218
25	O	1.352750	3.826155	1.913077
26	O	1.412100	3.855121	5.772796
27	O	4.058250	5.739232	0.000000
28	O	4.003857	5.737256	3.749152
29	O	4.058250	3.826155	1.913077
30	O	4.003233	3.846765	5.793433
31	O	1.352750	5.739232	0.000000
32	O	1.409749	5.740200	3.744927
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.006401	3.824925	3.944186
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.704065	5.738077	5.597818
37	O	6.763750	3.826155	1.913077
38	O	6.848045	3.760931	5.730345
39	O	9.469250	5.739232	0.000000

40	O	9.475174	5.739200	3.911356
41	O	9.469250	3.826155	1.913077
42	O	9.377012	3.730791	5.751829
43	O	6.763750	5.739232	0.000000
44	O	6.759336	5.742114	3.897239
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417604	3.825010	3.941934
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.109291	5.745540	5.655482
49	C	6.997139	1.873177	8.409782
50	C	6.085607	2.998270	8.773428
51	C	8.343871	1.916471	8.413651
52	H	5.339739	2.662101	9.515778
53	H	5.541388	3.348832	7.878087
54	H	6.635175	3.851492	9.202173
55	H	8.951739	1.043559	8.151718
56	H	8.888429	2.824244	8.695857
57	H	6.507390	0.945463	8.084553

C_{sp2}-H of C_3H_6 adsorbes on Ce_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.406204	-0.032192	5.775129
3	O	4.058250	1.913077	0.000000
4	O	4.059914	1.912866	3.897198
5	O	4.058250	0.000000	1.913077
6	O	3.994717	-0.024466	5.783333
7	O	1.352750	1.913077	0.000000
8	O	1.345853	1.911648	3.896449
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.008420	-0.002138	3.948344
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.701100	1.913213	5.660683
13	O	6.763750	0.000000	1.913077
14	O	6.843497	0.131723	5.754583
15	O	9.469250	1.913077	0.000000
16	O	9.433112	1.912800	3.849258
17	O	9.469250	0.000000	1.913077
18	O	9.371817	0.099834	5.753444
19	O	6.763750	1.913077	0.000000
20	O	6.798900	1.918315	3.837867
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419060	0.003364	3.956076
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.109484	1.910227	5.422067
25	O	1.352750	3.826155	1.913077
26	O	1.409506	3.853242	5.770887
27	O	4.058250	5.739232	0.000000
28	O	4.001383	5.738609	3.747452
29	O	4.058250	3.826155	1.913077
30	O	3.996787	3.851301	5.783447
31	O	1.352750	5.739232	0.000000
32	O	1.406305	5.736010	3.743675
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004335	3.824445	3.943071
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.698198	5.740368	5.593995
37	O	6.763750	3.826155	1.913077

38	O	6.848491	3.707344	5.759660
39	O	9.469250	5.739232	0.000000
40	O	9.476811	5.735622	3.918615
41	O	9.469250	3.826155	1.913077
42	O	9.372007	3.727027	5.756675
43	O	6.763750	5.739232	0.000000
44	O	6.757569	5.736730	3.934195
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.413291	3.825335	3.947191
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.121496	5.722253	5.690811
49	C	7.010283	5.257296	8.854220
50	C	5.549631	5.436413	8.586571
51	C	7.940494	6.227220	8.800590
52	H	4.974313	5.265624	9.516217
53	H	5.203196	4.696891	7.843617
54	H	5.325502	6.447819	8.211122
55	H	8.991366	6.027426	9.031304
56	H	7.670379	7.256928	8.545015
57	H	7.328650	4.241077	9.119358

C_{sp2}-H of C_3H_6 adsorbes on Zr_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.411718	-0.027633	5.773790
3	O	4.058250	1.913077	0.000000
4	O	4.061914	1.912396	3.892092
5	O	4.058250	0.000000	1.913077
6	O	4.000388	-0.025533	5.780155
7	O	1.352750	1.913077	0.000000
8	O	1.353019	1.913371	3.892032
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.006247	0.004450	3.944817
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.704423	1.911984	5.655190
13	O	6.763750	0.000000	1.913077
14	O	6.851149	0.047958	5.756776
15	O	9.469250	1.913077	0.000000
16	O	9.439412	1.920695	3.849564
17	O	9.469250	0.000000	1.913077
18	O	9.380656	0.111147	5.735424
19	O	6.763750	1.913077	0.000000
20	O	6.810036	1.909185	3.877385
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419804	0.001654	3.949263
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.144942	1.928677	5.463716
25	O	1.352750	3.826155	1.913077
26	O	1.408856	3.857170	5.774281
27	O	4.058250	5.739232	0.000000
28	O	4.003253	5.737857	3.746563
29	O	4.058250	3.826155	1.913077
30	O	3.999568	3.846156	5.785067
31	O	1.352750	5.739232	0.000000
32	O	1.409292	5.738591	3.743993
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.003396	3.825542	3.944117
35	Zr	2.705500	5.739232	1.913077

36	Ce	2.706081	5.737656	5.593865
37	O	6.763750	3.826155	1.913077
38	O	6.842255	3.778387	5.734208
39	O	9.469250	5.739232	0.000000
40	O	9.475196	5.736905	3.914392
41	O	9.469250	3.826155	1.913077
42	O	9.372915	3.717961	5.756455
43	O	6.763750	5.739232	0.000000
44	O	6.759891	5.745646	3.893384
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.415427	3.823899	3.941260
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.103649	5.747294	5.650560
49	C	7.246660	2.418715	8.448489
50	C	5.821883	1.970380	8.432623
51	C	8.331217	1.622872	8.377612
52	H	5.245290	2.614775	7.748021
53	H	5.381660	2.071458	9.443082
54	H	5.725489	0.926830	8.095498
55	H	9.344502	2.030055	8.420332
56	H	8.232817	0.536490	8.312419
57	H	7.401972	3.500972	8.528465

C=C of C_3H_6 adsorbes on O_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.410163	-0.029180	5.776530
3	O	4.058250	1.913077	0.000000
4	O	4.060803	1.917015	3.898494
5	O	4.058250	0.000000	1.913077
6	O	3.997322	-0.024879	5.779044
7	O	1.352750	1.913077	0.000000
8	O	1.347361	1.911421	3.895659
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.007969	-0.001037	3.949546
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.702883	1.913234	5.659713
13	O	6.763750	0.000000	1.913077
14	O	6.847975	0.128439	5.754550
15	O	9.469250	1.913077	0.000000
16	O	9.431638	1.911199	3.846076
17	O	9.469250	0.000000	1.913077
18	O	9.375142	0.097626	5.754968
19	O	6.763750	1.913077	0.000000
20	O	6.797714	1.914512	3.835045
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.416526	0.001066	3.952245
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.106460	1.912086	5.418779
25	O	1.352750	3.826155	1.913077
26	O	1.412422	3.852346	5.772882
27	O	4.058250	5.739232	0.000000
28	O	4.003374	5.738371	3.747224
29	O	4.058250	3.826155	1.913077
30	O	4.001997	3.858777	5.786593
31	O	1.352750	5.739232	0.000000
32	O	1.407739	5.739856	3.743536
33	Ce	0.000000	3.826155	0.000000

34	Ce	-0.005260	3.825103	3.945015
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.700307	5.740523	5.594600
37	O	6.763750	3.826155	1.913077
38	O	6.853082	3.697375	5.757035
39	O	9.469250	5.739232	0.000000
40	O	9.476228	5.738491	3.919204
41	O	9.469250	3.826155	1.913077
42	O	9.378552	3.728051	5.749695
43	O	6.763750	5.739232	0.000000
44	O	6.758858	5.736140	3.934063
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.415304	3.825415	3.945578
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.127830	5.729046	5.691955
49	C	7.090721	5.109612	8.824039
50	C	5.649106	5.424087	8.585326
51	C	8.103465	5.995820	8.823065
52	H	5.052191	5.159622	9.478598
53	H	5.264808	4.812240	7.748283
54	H	5.492551	6.488954	8.352136
55	H	9.134652	5.684495	9.016967
56	H	7.926651	7.065298	8.663879
57	H	7.323727	4.052395	9.002501

C=C of C_3H_6 adsorbes on Ce_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.414886	-0.024050	5.778470
3	O	4.058250	1.913077	0.000000
4	O	4.064744	1.914054	3.898271
5	O	4.058250	0.000000	1.913077
6	O	4.003688	-0.024399	5.783810
7	O	1.352750	1.913077	0.000000
8	O	1.351626	1.914982	3.896041
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.004720	0.004009	3.948701
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.706900	1.917174	5.661430
13	O	6.763750	0.000000	1.913077
14	O	6.857285	0.110009	5.766227
15	O	9.469250	1.913077	0.000000
16	O	9.435760	1.916331	3.839796
17	O	9.469250	0.000000	1.913077
18	O	9.383700	0.123331	5.752292
19	O	6.763750	1.913077	0.000000
20	O	6.801911	1.915865	3.848805
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.420249	0.001675	3.953939
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.122958	1.910481	5.422947
25	O	1.352750	3.826155	1.913077
26	O	1.413563	3.861509	5.778121
27	O	4.058250	5.739232	0.000000
28	O	4.004666	5.741698	3.743194
29	O	4.058250	3.826155	1.913077
30	O	4.003335	3.857834	5.775193
31	O	1.352750	5.739232	0.000000

32	O	1.411444	5.741692	3.742789
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.002650	3.827385	3.945920
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.706961	5.742375	5.593916
37	O	6.763750	3.826155	1.913077
38	O	6.860064	3.723500	5.768299
39	O	9.469250	5.739232	0.000000
40	O	9.481088	5.738782	3.931264
41	O	9.469250	3.826155	1.913077
42	O	9.381485	3.713707	5.755311
43	O	6.763750	5.739232	0.000000
44	O	6.758500	5.741596	3.929168
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417614	3.828120	3.950445
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.121430	5.730760	5.693025
49	C	8.066998	6.240220	8.987570
50	C	6.602368	6.037642	9.228296
51	C	8.960763	5.266515	8.744362
52	H	6.002213	6.650107	8.533394
53	H	6.334388	6.357119	10.251938
54	H	6.311176	4.981870	9.108524
55	H	10.019313	5.487026	8.579352
56	H	8.666938	4.212655	8.710842
57	H	8.419048	7.279476	9.010262

C=C of C_3H_6 adsorbes on Zr_T site of $Ce_{0.875}Zr_{0.125}O_2$ (110) surface

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407862	-0.023099	5.779747
3	O	4.058250	1.913077	0.000000
4	O	4.049855	1.913313	3.895115
5	O	4.058250	0.000000	1.913077
6	O	4.000248	-0.023614	5.796071
7	O	1.352750	1.913077	0.000000
8	O	1.349466	1.913385	3.891391
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.007596	0.002513	3.949428
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.698977	1.914398	5.657622
13	O	6.763750	0.000000	1.913077
14	O	6.844410	0.100702	5.736853
15	O	9.469250	1.913077	0.000000
16	O	9.424905	1.909446	3.873300
17	O	9.469250	0.000000	1.913077
18	O	9.372618	0.061632	5.747801
19	O	6.763750	1.913077	0.000000
20	O	6.792254	1.914036	3.853752
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.413318	0.003865	3.945367
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.094992	1.899040	5.459497
25	O	1.352750	3.826155	1.913077
26	O	1.407546	3.852154	5.778166
27	O	4.058250	5.739232	0.000000
28	O	4.002102	5.744932	3.747518
29	O	4.058250	3.826155	1.913077

30	O	3.998042	3.860258	5.778183
31	O	1.352750	5.739232	0.000000
32	O	1.407554	5.739721	3.748415
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004834	3.823475	3.943226
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.703821	5.740752	5.600747
37	O	6.763750	3.826155	1.913077
38	O	6.848949	3.729293	5.741841
39	O	9.469250	5.739232	0.000000
40	O	9.477202	5.737323	3.896274
41	O	9.469250	3.826155	1.913077
42	O	9.380478	3.766501	5.738435
43	O	6.763750	5.739232	0.000000
44	O	6.757004	5.735632	3.909123
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.411759	3.824742	3.943468
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.130336	5.721797	5.647929
49	C	7.480847	1.283901	8.526399
50	C	6.007971	1.432410	8.722919
51	C	8.364577	2.286976	8.372015
52	H	5.705876	0.993668	9.692398
53	H	5.473251	0.883224	7.928430
54	H	5.698906	2.488580	8.699372
55	H	9.436174	2.101193	8.255156
56	H	8.039434	3.330184	8.389613
57	H	7.860550	0.256215	8.513358

TS1-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.382005070	-0.025729418	5.746544124
4.058250000	1.913077397	0.000000000
4.045334660	1.911455257	3.893981266
4.058250000	0.000000000	1.913077397
3.975632276	-0.032935483	5.771135007
1.352750000	1.913077397	0.000000000
1.328269035	1.925712181	3.895083091
0.000000000	0.000000000	0.000000000
-0.019066962	-0.004898912	3.938269102
2.705500000	1.913077397	1.913077397
2.699037101	1.904286768	5.666150801
6.763750000	0.000000000	1.913077397
6.833149077	0.180985876	5.779839499
9.469250000	1.913077397	0.000000000
9.408126752	2.001671689	3.920566897
9.469250000	0.000000000	1.913077397
9.358735930	0.079997110	5.723864973
6.763750000	1.913077397	0.000000000
6.772428911	1.892778577	3.830215608
5.411000000	0.000000000	0.000000000
5.392383012	0.000874651	3.914217029
8.116500000	1.913077397	1.913077397
8.046072021	1.867790534	5.470845105
1.352750000	3.826154793	1.913077397
1.392226963	3.870831616	5.801773057
4.058250000	5.739232190	0.000000000

3.977624917	5.739658783	3.739353384
4.058250000	3.826154793	1.913077397
3.991906892	3.854523305	5.763382367
1.352750000	5.739232190	0.000000000
1.385827544	5.727613862	3.745542637
0.000000000	3.826154793	0.000000000
0.037184384	3.824692705	3.920610951
2.705500000	5.739232190	1.913077397
2.701377099	5.744604479	5.607873449
6.763750000	3.826154793	1.913077397
6.962827180	3.704914808	5.681560487
9.469250000	5.739232190	0.000000000
9.470284224	5.660529367	3.989497577
9.469250000	3.826154793	1.913077397
9.474398980	3.606656115	6.220171988
6.763750000	5.739232190	0.000000000
6.731218216	5.773718054	3.943623790
5.411000000	3.826154793	0.000000000
5.424384580	3.831587779	3.935650069
8.116500000	5.739232190	1.913077397
8.074886820	5.843721988	5.768559377
8.358484589	6.150156035	8.728508849
9.407156705	5.234561158	8.804868951
7.034118761	5.874565235	8.457777362
10.354477630	5.570011551	9.218540001
10.039568317	4.145891096	6.811852232
9.171491135	4.177448906	8.964799496
6.274363689	6.665245362	8.482090496
6.668819602	4.836061339	8.409269463
8.632999459	7.210169273	8.831092962

CH_2=CHCH_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.383234	-0.030153	5.754257
3	O	4.058250	1.913077	0.000000
4	O	4.049584	1.915656	3.895181
5	O	4.058250	0.000000	1.913077
6	O	3.969060	-0.039997	5.777395
7	O	1.352750	1.913077	0.000000
8	O	1.335947	1.919211	3.875845
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.023875	-0.006393	3.938346
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.697877	1.904437	5.653590
13	O	6.763750	0.000000	1.913077
14	O	6.813686	0.191087	5.786246
15	O	9.469250	1.913077	0.000000
16	O	9.411722	1.970052	3.869032
17	O	9.469250	0.000000	1.913077
18	O	9.354671	0.110057	5.731939
19	O	6.763750	1.913077	0.000000
20	O	6.769575	1.891309	3.814310
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.387412	0.000331	3.914411
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.051593	1.860700	5.437696
25	O	1.352750	3.826155	1.913077

26	O	1.329680	3.838854	5.799959
27	O	4.058250	5.739232	0.000000
28	O	3.983213	5.736871	3.738923
29	O	4.058250	3.826155	1.913077
30	O	3.976906	3.863079	5.768741
31	O	1.352750	5.739232	0.000000
32	O	1.396199	5.728952	3.728090
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.025602	3.829782	3.842034
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.688631	5.737651	5.600383
37	O	6.763750	3.826155	1.913077
38	O	6.959495	3.705277	5.678583
39	O	9.469250	5.739232	0.000000
40	O	9.475259	5.671087	3.989239
41	O	9.469250	3.826155	1.913077
42	O	9.454258	3.534189	6.135236
43	O	6.763750	5.739232	0.000000
44	O	6.739533	5.781357	3.947877
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.432204	3.839349	3.941276
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.076688	5.853890	5.786290
49	C	8.028414	6.435137	8.657980
50	C	9.209340	5.704919	8.608634
51	C	6.754022	5.946428	8.380140
52	H	10.173945	6.198683	8.737280
53	H	10.376232	3.476707	6.487461
54	H	9.200825	4.615999	8.516911
55	H	5.893916	6.617199	8.348101
56	H	6.562741	4.872766	8.278064
57	H	8.126322	7.521035	8.781292

TS1-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.381738288	-0.024708263	5.758583655
4.058250000	1.913077397	0.000000000
4.050798572	1.910218093	3.884510201
4.058250000	0.000000000	1.913077397
3.969475732	-0.055203389	5.771304147
1.352750000	1.913077397	0.000000000
1.339473496	1.928336097	3.871954371
0.000000000	0.000000000	0.000000000
-0.006685926	0.007535403	3.933713707
2.705500000	1.913077397	1.913077397
2.698271951	1.889137564	5.655373792
6.763750000	0.000000000	1.913077397
6.794688873	0.151990054	5.840018884
9.469250000	1.913077397	0.000000000
9.413881031	2.019430641	3.964211577
9.469250000	0.000000000	1.913077397
9.356928180	0.123964465	5.812105093
6.763750000	1.913077397	0.000000000
6.753244999	1.893555794	3.860038476
5.411000000	0.000000000	0.000000000
5.370180952	-0.025017922	3.905462645
8.116500000	1.913077397	1.913077397

7.979276838	1.775709512	5.473110752
1.352750000	3.826154793	1.913077397
1.408618288	3.802450591	5.808399209
4.058250000	5.739232190	0.000000000
3.982346079	5.727017898	3.731773725
4.058250000	3.826154793	1.913077397
4.009193083	3.860130076	5.756878772
1.352750000	5.739232190	0.000000000
1.404331629	5.732402335	3.727113529
0.000000000	3.826154793	0.000000000
0.043782416	3.864620840	3.813417939
2.705500000	5.739232190	1.913077397
2.690384668	5.747257711	5.605563068
6.763750000	3.826154793	1.913077397
7.267440029	3.656313613	5.891349786
9.469250000	5.739232190	0.000000000
9.467820229	5.701927394	3.984600566
9.469250000	3.826154793	1.913077397
9.839924884	4.243595654	6.591503142
6.763750000	5.739232190	0.000000000
6.729865206	5.737516445	3.993739200
5.411000000	3.826154793	0.000000000
5.403944170	3.836207886	3.909435466
8.116500000	5.739232190	1.913077397
8.161203918	5.841361854	5.812001045
8.524529200	5.714164222	8.945549527
9.484259839	4.702526381	8.700441437
7.164699332	5.453301034	8.952131174
10.496341898	4.854230496	9.050901236
10.816862429	4.011062648	6.538374118
9.151070942	3.675074497	8.551824597
6.449655322	6.206326951	9.283302289
6.780861703	4.470383475	8.676812798
8.862650593	6.692245121	9.270716129

CH_2=CHCH_2OH*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.373162	-0.014030	5.762852
3	O	4.058250	1.913077	0.000000
4	O	4.036874	1.898484	3.878643
5	O	4.058250	0.000000	1.913077
6	O	3.960985	-0.062587	5.769880
7	O	1.352750	1.913077	0.000000
8	O	1.341753	1.938880	3.873439
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.012294	0.019850	3.957201
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.699565	1.879227	5.658797
13	O	6.763750	0.000000	1.913077
14	O	6.756984	0.097291	5.876835
15	O	9.469250	1.913077	0.000000
16	O	9.414755	2.029181	3.995901
17	O	9.469250	0.000000	1.913077
18	O	9.342022	0.136694	5.841219
19	O	6.763750	1.913077	0.000000
20	O	6.719304	1.896731	3.879268
21	Ce	5.411000	0.000000	0.000000

22	Ce	5.342990	-0.041990	3.887541
23	Ce	8.116500	1.913077	1.913077
24	Zr	7.970407	1.727283	5.474041
25	O	1.352750	3.826155	1.913077
26	O	1.222641	3.870562	5.867893
27	O	4.058250	5.739232	0.000000
28	O	3.970946	5.726100	3.727879
29	O	4.058250	3.826155	1.913077
30	O	3.999287	3.850503	5.754761
31	O	1.352750	5.739232	0.000000
32	O	1.406346	5.737243	3.728041
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.051057	3.849086	3.760313
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.677917	5.745084	5.616753
37	O	6.763750	3.826155	1.913077
38	O	7.572906	3.621028	6.060381
39	O	9.469250	5.739232	0.000000
40	O	9.485379	5.674928	4.068764
41	O	9.469250	3.826155	1.913077
42	O	10.080673	4.750186	7.145706
43	O	6.763750	5.739232	0.000000
44	O	6.724548	5.715687	4.018355
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.373807	3.831436	3.871343
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.121815	5.916495	5.836233
49	C	8.880595	5.132425	9.142671
50	C	9.710554	4.137610	8.379837
51	C	7.557259	5.026718	9.334909
52	H	10.618883	3.874099	8.956786
53	H	10.944141	4.305483	6.696422
54	H	9.126531	3.215805	8.206332
55	H	6.994845	5.801183	9.865470
56	H	6.997241	4.163026	8.959450
57	H	9.418515	6.022257	9.496272

IM1

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.371854	-0.029504	5.743876
3	O	4.058250	1.913077	0.000000
4	O	4.035242	1.922540	3.882004
5	O	4.058250	0.000000	1.913077
6	O	3.959114	-0.032959	5.747938
7	O	1.352750	1.913077	0.000000
8	O	1.330677	1.905525	3.862120
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.028024	-0.006330	3.948223
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.702737	1.912029	5.644241
13	O	6.763750	0.000000	1.913077
14	O	6.770889	0.144696	5.821799
15	O	9.469250	1.913077	0.000000
16	O	9.402622	1.968637	3.941673
17	O	9.469250	0.000000	1.913077
18	O	9.316991	0.035321	5.729414
19	O	6.763750	1.913077	0.000000

20	O	6.741287	1.861810	3.808914
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.378807	-0.014299	3.867320
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.011976	1.780821	5.492509
25	O	1.352750	3.826155	1.913077
26	O	1.424759	3.838639	5.693399
27	O	4.058250	5.739232	0.000000
28	O	3.965924	5.733845	3.727939
29	O	4.058250	3.826155	1.913077
30	O	4.008864	3.870891	5.791882
31	O	1.352750	5.739232	0.000000
32	O	1.384923	5.744117	3.720293
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.028030	3.829427	3.864669
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.674271	5.745171	5.590062
37	O	6.763750	3.826155	1.913077
38	O	6.936708	3.713270	5.635447
39	O	9.469250	5.739232	0.000000
40	O	9.459012	5.696492	3.944136
41	O	9.469250	3.826155	1.913077
42	O	8.129503	4.949418	8.188030
43	O	6.763750	5.739232	0.000000
44	O	6.707784	5.787103	3.910231
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.407178	3.830513	3.947532
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.041059	5.847382	5.750223
49	C	6.639066	5.842513	9.840903
50	C	6.929412	4.679296	8.945993
51	C	5.492986	6.532393	9.834804
52	H	7.102782	3.772380	9.555397
53	H	8.531557	4.052609	7.893992
54	H	6.082508	4.473427	8.265526
55	H	5.318367	7.369394	10.517249
56	H	4.687749	6.290075	9.134028
57	H	7.447306	6.121151	10.528307
58	O	9.543675	3.993042	6.007306
59	O	9.229300	2.936034	6.932637

TS1-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.373436166	-0.032682833	5.737526362
4.058250000	1.913077397	0.000000000
4.038235112	1.921190460	3.884566086
4.058250000	0.000000000	1.913077397
3.955767640	-0.035923088	5.737973571
1.352750000	1.913077397	0.000000000
1.329198334	1.905134741	3.859747419
0.000000000	0.000000000	0.000000000
-0.040663289	-0.012956884	3.943990955
2.705500000	1.913077397	1.913077397
2.689085704	1.910117171	5.648494944
6.763750000	0.000000000	1.913077397
6.766718824	0.156496060	5.825773542
9.469250000	1.913077397	0.000000000

9.394842732	1.962943808	3.938840013
9.469250000	0.000000000	1.913077397
9.308784877	0.045937642	5.733449144
6.763750000	1.913077397	0.000000000
6.750521461	1.851812980	3.819145710
5.411000000	0.000000000	0.000000000
5.362844389	-0.010866852	3.888175703
8.116500000	1.913077397	1.913077397
8.012376782	1.792302700	5.499913077
1.352750000	3.826154793	1.913077397
1.435799760	3.833264826	5.691437750
4.058250000	5.739232190	0.000000000
3.970192651	5.731873354	3.726527794
4.058250000	3.826154793	1.913077397
4.016909265	3.868253024	5.783835597
1.352750000	5.739232190	0.000000000
1.387753903	5.740355887	3.716313783
0.000000000	3.826154793	0.000000000
0.033820242	3.836359124	3.862230611
2.705500000	5.739232190	1.913077397
2.688365192	5.738196910	5.587950971
6.763750000	3.826154793	1.913077397
6.953344768	3.679672264	5.647237312
9.469250000	5.739232190	0.000000000
9.457509907	5.692861134	3.941363318
9.469250000	3.826154793	1.913077397
8.102911422	4.941427860	8.175384066
6.763750000	5.739232190	0.000000000
6.711358880	5.782877263	3.930646511
5.411000000	3.826154793	0.000000000
5.437054704	3.826291099	3.947805447
8.116500000	5.739232190	1.913077397
8.037993355	5.835928362	5.816163385
6.534184545	5.891547867	9.852075984
6.909458988	4.730092784	8.949235764
5.343460486	6.515740227	9.864499825
7.066720486	3.822691231	9.568064545
8.718122272	3.894803126	7.770650241
6.069099679	4.479924294	8.278099992
5.103749658	7.338228163	10.526140468
4.526617793	6.230810001	9.195140891
7.325472110	6.225599926	10.539669471
9.556821843	3.986526523	5.975626392
9.326621683	3.116545117	7.102289648

CH_2=CHCH_2O*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.368240	-0.056730	5.773630
3	O	4.058250	1.913077	0.000000
4	O	4.042654	1.916293	3.872590
5	O	4.058250	0.000000	1.913077
6	O	3.946230	-0.043758	5.732819
7	O	1.352750	1.913077	0.000000
8	O	1.323415	1.896017	3.857907
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.053036	-0.020701	3.959649
11	Ce	2.705500	1.913077	1.913077

12	Ce	2.700271	1.887128	5.640388
13	O	6.763750	0.000000	1.913077
14	O	6.704741	0.224221	5.774043
15	O	9.469250	1.913077	0.000000
16	O	9.397561	2.005283	3.938436
17	O	9.469250	0.000000	1.913077
18	O	9.302134	0.102628	5.752853
19	O	6.763750	1.913077	0.000000
20	O	6.743909	1.870924	3.779477
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.369342	-0.019001	3.882731
23	Ce	8.116500	1.913077	1.913077
24	Zr	7.958770	1.797135	5.457993
25	O	1.352750	3.826155	1.913077
26	O	1.387581	3.669401	5.850043
27	O	4.058250	5.739232	0.000000
28	O	3.958010	5.732175	3.737751
29	O	4.058250	3.826155	1.913077
30	O	4.007339	3.874496	5.740169
31	O	1.352750	5.739232	0.000000
32	O	1.392053	5.706889	3.760410
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.020634	3.834303	3.851180
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.694769	5.738463	5.640318
37	O	6.763750	3.826155	1.913077
38	O	6.990642	3.630225	5.698672
39	O	9.469250	5.739232	0.000000
40	O	9.474389	5.717171	3.909773
41	O	9.469250	3.826155	1.913077
42	O	7.203851	5.729007	7.877945
43	O	6.763750	5.739232	0.000000
44	O	6.697364	5.772522	3.952400
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.414728	3.830501	3.962006
47	Ce	8.116500	5.739232	1.913077
48	Ce	7.984313	5.893861	5.859372
49	C	4.891404	6.047851	8.555406
50	C	6.120385	5.170423	8.561602
51	C	3.627102	5.613425	8.715608
52	H	6.409013	5.018381	9.628551
53	H	10.613513	2.851052	6.802936
54	H	5.865904	4.170279	8.154292
55	H	2.791765	6.315965	8.818287
56	H	3.402814	4.550255	8.856959
57	H	5.093978	7.116539	8.419500
58	O	9.660639	4.228783	5.976995
59	O	9.628404	3.034398	6.822069

CH_2=CHCHO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407045	-0.054434	5.754571
3	O	4.058250	1.913077	0.000000
4	O	4.073606	1.904575	3.871653
5	O	4.058250	0.000000	1.913077
6	O	4.013830	-0.069300	5.784805
7	O	1.352750	1.913077	0.000000

8	O	1.357331	1.919866	3.865109
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.009370	-0.010007	3.886510
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.708644	1.873078	5.642128
13	O	6.763750	0.000000	1.913077
14	O	6.822656	0.211375	5.850122
15	O	9.469250	1.913077	0.000000
16	O	9.443057	1.931841	3.921491
17	O	9.469250	0.000000	1.913077
18	O	9.371603	0.138450	5.842198
19	O	6.763750	1.913077	0.000000
20	O	6.819696	1.950811	3.900079
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.376365	-0.014543	3.878028
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.117582	1.809383	5.521647
25	O	1.352750	3.826155	1.913077
26	O	1.293083	3.746403	5.900844
27	O	4.058250	5.739232	0.000000
28	O	3.982292	5.729605	3.729840
29	O	4.058250	3.826155	1.913077
30	O	4.037035	3.843469	5.794074
31	O	1.352750	5.739232	0.000000
32	O	1.405058	5.706970	3.745513
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.021426	3.836301	3.825699
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.688150	5.737288	5.624071
37	O	6.763750	3.826155	1.913077
38	O	6.819211	3.521733	6.186613
39	O	9.469250	5.739232	0.000000
40	O	9.457219	5.750914	3.974729
41	O	9.469250	3.826155	1.913077
42	O	7.608861	5.915898	8.378377
43	O	6.763750	5.739232	0.000000
44	O	6.727942	5.715622	4.052545
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.394398	3.827992	3.863797
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.083324	6.008448	5.837690
49	C	5.469356	6.908527	8.773506
50	C	6.662508	6.180557	9.145858
51	C	4.462689	7.087415	9.661367
52	H	6.726966	5.835242	10.202807
53	H	10.840776	3.241456	6.708882
54	H	5.908679	3.434374	6.556939
55	H	3.550662	7.629324	9.397899
56	H	4.520915	6.693254	10.681884
57	H	5.415410	7.300458	7.750120
58	O	9.321871	3.869731	5.791739
59	O	9.823420	3.098394	6.935991

IM2

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.402500	-0.039714	5.767231
3	O	4.058250	1.913077	0.000000

4	O	4.041905	1.894057	3.877224
5	O	4.058250	0.000000	1.913077
6	O	3.994217	-0.053892	5.777733
7	O	1.352750	1.913077	0.000000
8	O	1.327803	1.905405	3.907519
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.019433	-0.018673	3.936532
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.701044	1.888993	5.642106
13	O	6.763750	0.000000	1.913077
14	O	6.809333	0.120139	5.767933
15	O	9.469250	1.913077	0.000000
16	O	9.396103	1.935595	3.892573
17	O	9.469250	0.000000	1.913077
18	O	9.361295	0.034680	5.717366
19	O	6.763750	1.913077	0.000000
20	O	6.748609	1.867305	3.815242
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.411547	-0.043844	3.876690
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.032478	1.792138	5.465725
25	O	1.352750	3.826155	1.913077
26	O	1.434125	3.851495	5.752704
27	O	4.058250	5.739232	0.000000
28	O	3.991696	5.726233	3.732892
29	O	4.058250	3.826155	1.913077
30	O	4.017178	3.842936	5.782214
31	O	1.352750	5.739232	0.000000
32	O	1.405906	5.741033	3.728763
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.000139	3.846624	3.907509
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.705726	5.727014	5.595217
37	O	6.763750	3.826155	1.913077
38	O	6.891766	3.672852	5.700121
39	O	9.469250	5.739232	0.000000
40	O	9.474151	5.730406	3.895027
41	O	9.469250	3.826155	1.913077
42	O	7.507142	5.445160	8.327249
43	O	6.763750	5.739232	0.000000
44	O	6.753521	5.737734	3.917685
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.408854	3.811161	3.952622
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.151241	5.728700	5.707474
49	C	5.620744	6.882056	8.628751
50	C	6.615354	5.907074	9.048770
51	C	4.652645	7.249911	9.491695
52	H	6.540534	5.548125	10.102497
53	H	9.187047	3.122230	7.195251
54	H	7.852451	2.983032	7.997406
55	H	3.873727	7.960410	9.205403
56	H	4.610006	6.851940	10.511281
57	H	5.682429	7.273475	7.604062
58	O	9.472830	3.901516	5.813878
59	O	8.603677	2.420762	7.696630

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.412755	-0.027974	5.779285
3	O	4.058250	1.913077	0.000000
4	O	4.044628	1.888874	3.891681
5	O	4.058250	0.000000	1.913077
6	O	4.005814	-0.069332	5.782664
7	O	1.352750	1.913077	0.000000
8	O	1.331277	1.905442	3.894165
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.020997	-0.014996	3.946967
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.691840	1.892527	5.644737
13	O	6.763750	0.000000	1.913077
14	O	6.867704	0.145496	5.740143
15	O	9.469250	1.913077	0.000000
16	O	9.421149	1.923553	3.847033
17	O	9.469250	0.000000	1.913077
18	O	9.390000	0.059104	5.745022
19	O	6.763750	1.913077	0.000000
20	O	6.770348	1.899557	3.810095
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.411269	-0.053029	3.898446
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.074873	1.908674	5.408273
25	O	1.352750	3.826155	1.913077
26	O	1.411366	3.843760	5.762881
27	O	4.058250	5.739232	0.000000
28	O	3.995255	5.720197	3.731825
29	O	4.058250	3.826155	1.913077
30	O	3.999444	3.844500	5.770330
31	O	1.352750	5.739232	0.000000
32	O	1.407298	5.740065	3.734540
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.001028	3.841102	3.912938
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.696992	5.723168	5.594850
37	O	6.763750	3.826155	1.913077
38	O	6.851754	3.649154	5.748873
39	O	9.469250	5.739232	0.000000
40	O	9.472081	5.735675	3.905052
41	O	9.469250	3.826155	1.913077
42	O	7.673651	5.656359	8.360183
43	O	6.763750	5.739232	0.000000
44	O	6.750734	5.727373	3.947039
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.410104	3.808745	3.951132
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.161743	5.719363	5.732744
49	C	5.569171	6.765285	8.622675
50	C	6.710323	5.974213	9.062547
51	C	4.538068	6.961412	9.468180
52	H	6.691825	5.641063	10.128908
53	H	3.659142	7.541166	9.173332
54	H	4.545708	6.557415	10.486491
55	H	5.579697	7.174858	7.602777
56	O	9.389890	3.768859	5.736949

TS1-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.400309279	-0.028900297	5.762609180
4.058250000	1.913077397	0.000000000
4.072587361	1.910120770	3.896663398
4.058250000	0.000000000	1.913077397
3.996041420	-0.018262875	5.791213663
1.352750000	1.913077397	0.000000000
1.350449493	1.914645764	3.887021787
0.000000000	0.000000000	0.000000000
0.009341123	-0.008827846	3.919270797
2.705500000	1.913077397	1.913077397
2.692038119	1.917953826	5.662706177
6.763750000	0.000000000	1.913077397
6.847940854	0.096923016	5.785464188
9.469250000	1.913077397	0.000000000
9.447909742	1.891489092	3.855370991
9.469250000	0.000000000	1.913077397
9.381971229	0.129045948	5.774891270
6.763750000	1.913077397	0.000000000
6.819194306	1.988866379	3.943440190
5.411000000	0.000000000	0.000000000
5.427006222	0.005371359	3.973895432
8.116500000	1.913077397	1.913077397
8.168525020	1.854334751	5.491852365
1.352750000	3.826154793	1.913077397
1.379523626	3.852389571	5.776753162
4.058250000	5.739232190	0.000000000
4.013945451	5.751085248	3.752029912
4.058250000	3.826154793	1.913077397
3.970088306	3.867170406	5.733653239
1.352750000	5.739232190	0.000000000
1.418361002	5.734496915	3.744920078
0.000000000	3.826154793	0.000000000
-0.015306001	3.820303433	3.941218836
2.705500000	5.739232190	1.913077397
2.690851082	5.742872190	5.618446745
6.763750000	3.826154793	1.913077397
6.714361671	3.886267468	6.250743592
9.469250000	5.739232190	0.000000000
9.492022786	5.742474683	3.944911909
9.469250000	3.826154793	1.913077397
7.716821216	6.007681201	8.719118737
6.763750000	5.739232190	0.000000000
6.769428391	5.699304666	3.977521747
5.411000000	3.826154793	0.000000000
5.371638892	3.847487340	3.958334017
8.116500000	5.739232190	1.913077397
8.143633140	5.772052947	5.758421709
5.487086484	6.747469991	8.573051043
6.583412710	5.755659436	8.343811687
4.610971361	7.026528945	9.550381305
6.513456480	4.590925165	7.367282715
3.816307853	7.781761934	9.369507317
4.613119699	6.577466794	10.532281996
5.392293901	7.327779675	7.627475576
9.290718096	3.696343527	5.731459201

CH_2=CHCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.433660	-0.030662	5.770672
3	O	4.058250	1.913077	0.000000
4	O	4.070769	1.908763	3.878225
5	O	4.058250	0.000000	1.913077
6	O	4.030048	-0.041896	5.777876
7	O	1.352750	1.913077	0.000000
8	O	1.356625	1.920442	3.892114
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.011528	0.012057	3.914163
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.705734	1.909825	5.651645
13	O	6.763750	0.000000	1.913077
14	O	6.872261	0.080401	5.756885
15	O	9.469250	1.913077	0.000000
16	O	9.451376	1.893669	3.842999
17	O	9.469250	0.000000	1.913077
18	O	9.405052	0.144609	5.808738
19	O	6.763750	1.913077	0.000000
20	O	6.816676	1.945793	3.888132
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.403989	-0.036750	3.924816
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.164046	1.834597	5.456022
25	O	1.352750	3.826155	1.913077
26	O	1.426011	3.874330	5.769117
27	O	4.058250	5.739232	0.000000
28	O	4.003429	5.722288	3.729580
29	O	4.058250	3.826155	1.913077
30	O	4.081669	3.838291	5.803299
31	O	1.352750	5.739232	0.000000
32	O	1.419163	5.744314	3.739166
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.003011	3.851186	3.929939
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.711025	5.738885	5.603951
37	O	6.763750	3.826155	1.913077
38	O	6.783100	3.526808	6.155647
39	O	9.469250	5.739232	0.000000
40	O	9.487453	5.777575	3.935038
41	O	9.469250	3.826155	1.913077
42	O	7.705170	5.976146	8.382653
43	O	6.763750	5.739232	0.000000
44	O	6.756539	5.656309	3.997083
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.390926	3.818656	3.846727
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.181524	5.808051	5.756287
49	C	5.575870	7.029978	8.690526
50	C	6.831984	6.402042	9.109089
51	C	4.576900	7.191909	9.576605
52	H	5.858884	3.470636	6.504180
53	H	3.619567	7.631051	9.282175
54	H	4.690543	6.873562	10.617696
55	H	5.501501	7.356306	7.637056

56	O	9.266101	3.731839	5.686364

TS2-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.407068767	-0.022473995	5.749148112
4.058250000	1.913077397	0.000000000
4.053144831	1.907987992	3.890161723
4.058250000	0.000000000	1.913077397
3.997972302	-0.024801988	5.774464332
1.352750000	1.913077397	0.000000000
1.336841038	1.914229229	3.888315724
0.000000000	0.000000000	0.000000000
-0.016695294	0.007126884	3.955385243
2.705500000	1.913077397	1.913077397
2.714793930	1.910518559	5.655444015
6.763750000	0.000000000	1.913077397
6.824869425	0.094042347	5.776855472
9.469250000	1.913077397	0.000000000
9.412607321	1.985127106	3.961728421
9.469250000	0.000000000	1.913077397
9.374444375	0.036925045	5.730254172
6.763750000	1.913077397	0.000000000
6.765778482	1.890304910	3.865295422
5.411000000	0.000000000	0.000000000
5.409848594	0.001792836	3.914765815
8.116500000	1.913077397	1.913077397
8.043275429	1.833279378	5.540265017
1.352750000	3.826154793	1.913077397
1.433565002	3.846645157	5.751452757
4.058250000	5.739232190	0.000000000
3.996792901	5.745397426	3.738517632
4.058250000	3.826154793	1.913077397
4.034074191	3.858154089	5.767647457
1.352750000	5.739232190	0.000000000
1.397859962	5.738834910	3.745371470
0.000000000	3.826154793	0.000000000
0.015320230	3.819793247	3.947777852
2.705500000	5.739232190	1.913077397
2.713446650	5.743110203	5.592268065
6.763750000	3.826154793	1.913077397
6.951424924	3.764075730	5.663332734
9.469250000	5.739232190	0.000000000
9.472089682	5.678285952	3.964044471
9.469250000	3.826154793	1.913077397
9.422945087	3.759003858	6.087015958
6.763750000	5.739232190	0.000000000
6.756506453	5.772279034	3.913521519
5.411000000	3.826154793	0.000000000
5.439058287	3.829172107	3.943138215
8.116500000	5.739232190	1.913077397
8.119262387	5.768280137	5.717461522
7.287863905	2.021649041	8.747965446
6.035320579	2.833240612	8.769335825
8.424421917	2.089368692	7.968602956
5.826755787	3.214365752	9.792695307
5.170127981	2.191166897	8.498699113
6.072379607	3.697329927	8.097867459

9.147595457	1.338604148	8.295781026
9.152039790	3.133586472	7.102336244
7.237632916	1.209857104	9.488731104

$CH_3CH=CH^*$

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.387187	-0.021425	5.744378
3	O	4.058250	1.913077	0.000000
4	O	4.041151	1.900845	3.883046
5	O	4.058250	0.000000	1.913077
6	O	3.970853	-0.036606	5.768971
7	O	1.352750	1.913077	0.000000
8	O	1.342777	1.924748	3.871493
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.024930	0.013031	3.928991
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.706905	1.900341	5.655198
13	O	6.763750	0.000000	1.913077
14	O	6.809044	0.053704	5.749248
15	O	9.469250	1.913077	0.000000
16	O	9.430157	1.961175	3.920116
17	O	9.469250	0.000000	1.913077
18	O	9.352974	0.025533	5.719255
19	O	6.763750	1.913077	0.000000
20	O	6.754641	1.895528	3.878010
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.397300	-0.002547	3.911073
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.055617	1.812485	5.587674
25	O	1.352750	3.826155	1.913077
26	O	1.369120	3.842529	5.804500
27	O	4.058250	5.739232	0.000000
28	O	3.983148	5.738108	3.735739
29	O	4.058250	3.826155	1.913077
30	O	3.994538	3.849150	5.751054
31	O	1.352750	5.739232	0.000000
32	O	1.393642	5.728272	3.731941
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.019756	3.817425	3.855912
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.695943	5.739102	5.591522
37	O	6.763750	3.826155	1.913077
38	O	6.969248	3.807897	5.646436
39	O	9.469250	5.739232	0.000000
40	O	9.459495	5.687219	3.926101
41	O	9.469250	3.826155	1.913077
42	O	9.514837	3.719508	5.994559
43	O	6.763750	5.739232	0.000000
44	O	6.747550	5.768145	3.881563
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.429569	3.820351	3.925577
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.066234	5.817899	5.684509
49	C	7.292896	2.153148	8.928199
50	C	5.875564	2.624063	8.751563
51	C	8.160619	1.854255	7.945309
52	H	5.672776	3.517375	9.371516

53	H	5.159663	1.845548	9.081499
54	H	5.664994	2.882501	7.704106
55	H	9.169618	1.529624	8.264563
56	H	10.344618	3.671275	6.524573
57	H	7.599769	2.040415	9.987560

TS2-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.381529212	-0.020660245	5.752842806
4.058250000	1.913077397	0.000000000
4.039865820	1.916631535	3.876439016
4.058250000	0.000000000	1.913077397
3.974121467	-0.036199059	5.761017759
1.352750000	1.913077397	0.000000000
1.339381361	1.918831740	3.863801170
0.000000000	0.000000000	0.000000000
-0.002736872	-0.003636365	3.922471813
2.705500000	1.913077397	1.913077397
2.700793896	1.902012331	5.651758773
6.763750000	0.000000000	1.913077397
6.808964850	0.088375046	5.815452281
9.469250000	1.913077397	0.000000000
9.408871549	1.986309858	3.994081188
9.469250000	0.000000000	1.913077397
9.369863120	0.031936936	5.773345642
6.763750000	1.913077397	0.000000000
6.753122623	1.915817346	3.911931969
5.411000000	0.000000000	0.000000000
5.371003186	0.006680327	3.894950594
8.116500000	1.913077397	1.913077397
8.096663440	1.766061099	5.615856220
1.352750000	3.826154793	1.913077397
1.320326608	3.852171045	5.760755486
4.058250000	5.739232190	0.000000000
3.983361822	5.734216947	3.726625808
4.058250000	3.826154793	1.913077397
4.027314860	3.859999419	5.752838752
1.352750000	5.739232190	0.000000000
1.398299932	5.731562449	3.718218574
0.000000000	3.826154793	0.000000000
0.077235208	3.824782203	3.802894667
2.705500000	5.739232190	1.913077397
2.687065812	5.736973487	5.599370791
6.763750000	3.826154793	1.913077397
7.308711403	3.769545380	5.833964057
9.469250000	5.739232190	0.000000000
9.476654730	5.652264935	3.998620056
9.469250000	3.826154793	1.913077397
9.513235550	2.820444707	6.969028234
6.763750000	5.739232190	0.000000000
6.728028674	5.751505349	3.938395958
5.411000000	3.826154793	0.000000000
5.407276608	3.826861846	3.891367853
8.116500000	5.739232190	1.913077397
8.058272741	5.877086533	5.738213347
7.518484656	1.973815414	9.327335426
6.153878935	2.470961669	8.960481064

8.562395166	1.623484130	8.585572173
5.675847075	3.021779905	9.785894959
5.530084632	1.579207612	8.745122723
6.186142848	3.089136521	8.060168595
9.455895796	1.149285383	8.941476442
10.408036742	2.369667474	6.935550297
7.686166481	1.781346239	10.425398582

$CH_3CH=CHOH$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.391648	-0.029854	5.768704
3	O	4.058250	1.913077	0.000000
4	O	4.035393	1.919051	3.865979
5	O	4.058250	0.000000	1.913077
6	O	3.985660	-0.034604	5.759778
7	O	1.352750	1.913077	0.000000
8	O	1.353413	1.913010	3.862023
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.027915	-0.011833	3.918537
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.694436	1.903781	5.660239
13	O	6.763750	0.000000	1.913077
14	O	6.810219	0.104135	5.855912
15	O	9.469250	1.913077	0.000000
16	O	9.439493	1.975680	4.039347
17	O	9.469250	0.000000	1.913077
18	O	9.423575	0.035291	5.885916
19	O	6.763750	1.913077	0.000000
20	O	6.754988	1.953761	3.963125
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.362422	0.004217	3.898339
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.061584	1.740895	5.555243
25	O	1.352750	3.826155	1.913077
26	O	1.309822	3.874305	5.753675
27	O	4.058250	5.739232	0.000000
28	O	3.979654	5.738726	3.714770
29	O	4.058250	3.826155	1.913077
30	O	4.065240	3.872554	5.757054
31	O	1.352750	5.739232	0.000000
32	O	1.414131	5.743015	3.711204
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.082000	3.835970	3.800984
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.697255	5.736477	5.608440
37	O	6.763750	3.826155	1.913077
38	O	7.817125	3.707462	6.098532
39	O	9.469250	5.739232	0.000000
40	O	9.482279	5.666510	4.045296
41	O	9.469250	3.826155	1.913077
42	O	9.151571	1.561218	7.777546
43	O	6.763750	5.739232	0.000000
44	O	6.715185	5.713746	4.003023
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.343938	3.837494	3.823266
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.062098	5.887424	5.756138

49	C	7.804842	1.675067	9.757224
50	C	6.566236	2.216560	9.101715
51	C	8.942440	1.351642	9.123069
52	H	5.754368	2.343209	9.835747
53	H	6.201837	1.535559	8.312098
54	H	6.743353	3.190180	8.614665
55	H	9.808606	0.939636	9.653949
56	H	9.578224	0.757993	7.274342
57	H	7.799297	1.514044	10.840054

IM4

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.396785	0.002582	5.758358
3	O	4.058250	1.913077	0.000000
4	O	4.033691	1.911814	3.888770
5	O	4.058250	0.000000	1.913077
6	O	3.979362	-0.042366	5.764140
7	O	1.352750	1.913077	0.000000
8	O	1.326374	1.914061	3.863549
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.020826	0.009043	3.944760
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.690403	1.914072	5.651726
13	O	6.763750	0.000000	1.913077
14	O	6.812735	0.128061	5.766790
15	O	9.469250	1.913077	0.000000
16	O	9.377866	1.970106	3.960834
17	O	9.469250	0.000000	1.913077
18	O	9.401916	0.006098	5.779056
19	O	6.763750	1.913077	0.000000
20	O	6.742168	1.882247	3.824680
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.388087	-0.012677	3.914211
23	Ce	8.116500	1.913077	1.913077
24	Zr	7.963006	1.846366	5.508010
25	O	1.352750	3.826155	1.913077
26	O	1.417858	3.862060	5.704444
27	O	4.058250	5.739232	0.000000
28	O	3.984244	5.729992	3.734226
29	O	4.058250	3.826155	1.913077
30	O	4.006318	3.858228	5.770108
31	O	1.352750	5.739232	0.000000
32	O	1.404182	5.756829	3.728071
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.047017	3.848179	3.870144
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.700537	5.744411	5.599309
37	O	6.763750	3.826155	1.913077
38	O	6.901639	3.658246	5.720836
39	O	9.469250	5.739232	0.000000
40	O	9.478024	5.708725	3.917564
41	O	9.469250	3.826155	1.913077
42	O	8.814582	1.374667	7.741351
43	O	6.763750	5.739232	0.000000
44	O	6.729916	5.742566	3.917384
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.412778	3.818276	3.932764

47	Ce	8.116500	5.739232	1.913077
48	Ce	8.107587	5.762132	5.722147
49	C	7.731967	1.717041	9.858443
50	C	6.584694	2.544542	9.370894
51	C	8.713146	1.205648	9.098456
52	H	5.803853	2.631246	10.143280
53	H	6.122917	2.119055	8.467246
54	H	6.908115	3.563015	9.107483
55	H	9.538569	0.634299	9.530927
56	H	9.320204	0.625498	7.242140
57	H	7.816591	1.517510	10.931055
58	O	9.486421	3.680406	5.937907
59	O	9.435491	4.508825	7.080899

$CH_3CH=CHO$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.369697	-0.007281	5.743486
3	O	4.058250	1.913077	0.000000
4	O	4.022480	1.912429	3.886384
5	O	4.058250	0.000000	1.913077
6	O	3.954881	-0.041832	5.757901
7	O	1.352750	1.913077	0.000000
8	O	1.325387	1.917741	3.856309
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.029330	0.012813	3.943845
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.684487	1.914294	5.649350
13	O	6.763750	0.000000	1.913077
14	O	6.772598	0.054198	5.785716
15	O	9.469250	1.913077	0.000000
16	O	9.394218	1.989965	3.963576
17	O	9.469250	0.000000	1.913077
18	O	9.313435	0.018192	5.707372
19	O	6.763750	1.913077	0.000000
20	O	6.733621	1.861735	3.862628
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.383978	-0.011734	3.903868
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.001649	1.748040	5.564610
25	O	1.352750	3.826155	1.913077
26	O	1.400593	3.857712	5.704641
27	O	4.058250	5.739232	0.000000
28	O	3.983695	5.732386	3.734706
29	O	4.058250	3.826155	1.913077
30	O	3.993293	3.856245	5.774157
31	O	1.352750	5.739232	0.000000
32	O	1.400715	5.755266	3.725387
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.044561	3.843339	3.863584
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.695656	5.741222	5.595192
37	O	6.763750	3.826155	1.913077
38	O	6.914532	3.791404	5.641408
39	O	9.469250	5.739232	0.000000
40	O	9.470035	5.684055	3.927742
41	O	9.469250	3.826155	1.913077
42	O	8.162787	2.070524	7.711191

43	O	6.763750	5.739232	0.000000
44	O	6.738146	5.771884	3.880401
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417758	3.822716	3.929844
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.055763	5.771351	5.696933
49	C	6.686609	0.987606	9.251676
50	C	5.401691	1.508766	8.689953
51	C	7.919721	1.285752	8.768648
52	H	4.710219	1.810836	9.498130
53	H	4.895161	0.738269	8.076760
54	H	5.582564	2.379281	8.039908
55	H	8.814498	0.876105	9.266402
56	H	8.964419	3.469784	7.747973
57	H	6.645605	0.316624	10.117592
58	O	9.468056	3.700151	5.950212
59	O	9.474119	4.246462	7.299791

TS2-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.366966981	-0.014279938	5.744254167
4.058250000	1.913077397	0.000000000
4.036351097	1.914478632	3.886390846
4.058250000	0.000000000	1.913077397
3.964652439	-0.041425222	5.768549932
1.352750000	1.913077397	0.000000000
1.324781598	1.914150336	3.861269971
0.000000000	0.000000000	0.000000000
-0.029047207	0.007930175	3.938388326
2.705500000	1.913077397	1.913077397
2.677154964	1.914433419	5.644251921
6.763750000	0.000000000	1.913077397
6.769257906	0.070025847	5.817227059
9.469250000	1.913077397	0.000000000
9.379025766	1.987828460	3.967430902
9.469250000	0.000000000	1.913077397
9.300308654	0.036772126	5.725240056
6.763750000	1.913077397	0.000000000
6.757613827	1.853085543	3.877275693
5.411000000	0.000000000	0.000000000
5.358922559	-0.013705027	3.888600098
8.116500000	1.913077397	1.913077397
7.986254053	1.763182283	5.522225260
1.352750000	3.826154793	1.913077397
1.405118937	3.869591677	5.706137595
4.058250000	5.739232190	0.000000000
3.983170847	5.727839571	3.734088988
4.058250000	3.826154793	1.913077397
4.003600033	3.852927216	5.784188933
1.352750000	5.739232190	0.000000000
1.393933782	5.749321045	3.718652024
0.000000000	3.826154793	0.000000000
0.059146417	3.838107133	3.851313353
2.705500000	5.739232190	1.913077397
2.685494425	5.738365241	5.591238926
6.763750000	3.826154793	1.913077397
6.928585011	3.754806998	5.674523944

9.469250000	5.739232190	0.000000000
9.468605617	5.683717928	3.948821155
9.469250000	3.826154793	1.913077397
8.111457577	2.157688615	7.955572639
6.763750000	5.739232190	0.000000000
6.733205506	5.770428869	3.898619572
5.411000000	3.826154793	0.000000000
5.420190669	3.820498287	3.933028099
8.116500000	5.739232190	1.913077397
8.067183322	5.778836594	5.687462543
6.682929559	0.980491133	9.413116338
5.366737612	1.363011349	8.771954819
7.957904669	1.295834314	8.907436221
4.504478269	1.268958720	9.472403897
5.208033696	0.657157774	7.926663119
5.390832537	2.377103328	8.323768641
7.635292798	1.629442914	10.155894151
9.049940570	3.531569459	7.796423537
6.713354689	0.080586046	10.027611450
9.482038845	3.641936693	5.966737887
9.541837235	4.259767793	7.293123579

CH_3CH_2CO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.366500	-0.015831	5.746987
3	O	4.058250	1.913077	0.000000
4	O	4.036779	1.915266	3.886605
5	O	4.058250	0.000000	1.913077
6	O	3.960961	-0.039100	5.756742
7	O	1.352750	1.913077	0.000000
8	O	1.326405	1.912911	3.862503
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.027980	0.012073	3.944322
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.685714	1.914127	5.649603
13	O	6.763750	0.000000	1.913077
14	O	6.768717	0.076306	5.822758
15	O	9.469250	1.913077	0.000000
16	O	9.381604	1.991481	3.965635
17	O	9.469250	0.000000	1.913077
18	O	9.303620	0.044646	5.745902
19	O	6.763750	1.913077	0.000000
20	O	6.749706	1.854334	3.869260
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.360959	-0.015208	3.894602
23	Ce	8.116500	1.913077	1.913077
24	Zr	7.978318	1.775493	5.522268
25	O	1.352750	3.826155	1.913077
26	O	1.409385	3.871778	5.705025
27	O	4.058250	5.739232	0.000000
28	O	3.983850	5.726966	3.734218
29	O	4.058250	3.826155	1.913077
30	O	4.010260	3.854028	5.783372
31	O	1.352750	5.739232	0.000000
32	O	1.395383	5.752218	3.717808
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.057935	3.838164	3.853892

35	Zr	2.705500	5.739232	1.913077
36	Ce	2.690141	5.740194	5.593091
37	O	6.763750	3.826155	1.913077
38	O	6.941763	3.737483	5.695405
39	O	9.469250	5.739232	0.000000
40	O	9.469604	5.684005	3.961483
41	O	9.469250	3.826155	1.913077
42	O	8.015849	2.052520	7.962673
43	O	6.763750	5.739232	0.000000
44	O	6.733984	5.768375	3.910585
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.418997	3.820129	3.939397
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.066620	5.795180	5.694970
49	C	6.563760	1.153687	9.667870
50	C	5.336557	1.193567	8.750267
51	C	7.822545	1.822197	9.152355
52	H	4.484556	0.707218	9.254060
53	H	5.523542	0.681975	7.796064
54	H	5.060618	2.237852	8.527743
55	H	6.359790	1.592599	10.660486
56	H	9.120649	3.600475	7.852373
57	H	6.884350	0.113062	9.883748
58	O	9.504173	3.596808	5.992372
59	O	9.581094	4.281042	7.291701

TS3-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.412881411	-0.038495800	5.760501705
4.058250000	1.913077397	0.000000000
4.048152781	1.919248535	3.873145660
4.058250000	0.000000000	1.913077397
3.987162435	-0.030956824	5.755719053
1.352750000	1.913077397	0.000000000
1.358940010	1.917982174	3.880043274
0.000000000	0.000000000	0.000000000
0.021999790	-0.027836294	3.887893296
2.705500000	1.913077397	1.913077397
2.701796447	1.908927377	5.662007485
6.763750000	0.000000000	1.913077397
6.818552030	0.141051487	5.817044009
9.469250000	1.913077397	0.000000000
9.480263240	1.889431223	3.836948632
9.469250000	0.000000000	1.913077397
9.468080174	0.125743632	5.821701662
6.763750000	1.913077397	0.000000000
6.789713593	2.024737106	3.976155064
5.411000000	0.000000000	0.000000000
5.435266460	0.003064442	3.957636187
8.116500000	1.913077397	1.913077397
8.212455047	1.712120243	5.476971374
1.352750000	3.826154793	1.913077397
1.370186373	3.868642951	5.750098085
4.058250000	5.739232190	0.000000000
3.982100197	5.738207615	3.719982492
4.058250000	3.826154793	1.913077397
4.087955203	3.858937905	5.754226227

1.352750000	5.739232190	0.000000000
1.431965547	5.734103020	3.726228229
0.000000000	3.826154793	0.000000000
-0.020202125	3.841125558	3.888871015
2.705500000	5.739232190	1.913077397
2.700825409	5.737635981	5.614619905
6.763750000	3.826154793	1.913077397
7.660082108	4.682552339	7.489562403
9.469250000	5.739232190	0.000000000
9.529064391	5.726493186	3.953941035
9.469250000	3.826154793	1.913077397
8.878795263	3.576949255	5.813590468
6.763750000	5.739232190	0.000000000
6.712217645	5.646738930	4.025105535
5.411000000	3.826154793	0.000000000
5.323447095	3.848095443	3.780330403
8.116500000	5.739232190	1.913077397
8.127540006	5.845434177	5.918522310
6.742925723	5.669845098	9.241614384
5.344789380	5.719374930	8.686205303
7.605984757	6.710655050	9.239066927
4.615805622	5.743620139	9.514923317
5.146023482	4.817223016	8.089669205
5.207975859	6.599411808	8.052303943
8.615426744	6.619008288	9.681498840
7.410943210	7.609475432	8.649907653
6.973570753	4.802262850	9.873009804

CH_3CHOCH_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.406610	-0.038755	5.757290
3	O	4.058250	1.913077	0.000000
4	O	4.046787	1.911349	3.871261
5	O	4.058250	0.000000	1.913077
6	O	4.000431	-0.041622	5.775586
7	O	1.352750	1.913077	0.000000
8	O	1.363262	1.912780	3.865219
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.027547	-0.007518	3.915974
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.701187	1.899971	5.656645
13	O	6.763750	0.000000	1.913077
14	O	6.815356	0.117034	5.883776
15	O	9.469250	1.913077	0.000000
16	O	9.461451	1.973388	3.960927
17	O	9.469250	0.000000	1.913077
18	O	9.404776	0.103743	5.867587
19	O	6.763750	1.913077	0.000000
20	O	6.769137	1.966220	3.959428
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.379535	-0.007231	3.924979
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.112777	1.723417	5.502410
25	O	1.352750	3.826155	1.913077
26	O	1.320410	3.870454	5.755359
27	O	4.058250	5.739232	0.000000
28	O	3.984289	5.737222	3.715347

29	O	4.058250	3.826155	1.913077
30	O	4.081285	3.864186	5.767480
31	O	1.352750	5.739232	0.000000
32	O	1.421109	5.738674	3.709129
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.074206	3.840517	3.805734
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.696292	5.734294	5.602113
37	O	6.763750	3.826155	1.913077
38	O	7.784983	6.085662	8.501373
39	O	9.469250	5.739232	0.000000
40	O	9.505858	5.679575	4.059116
41	O	9.469250	3.826155	1.913077
42	O	8.093679	3.616611	6.229970
43	O	6.763750	5.739232	0.000000
44	O	6.726552	5.683792	4.069263
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.335461	3.839998	3.812152
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.119696	5.912726	5.830889
49	C	6.600402	6.023866	9.350178
50	C	5.277243	5.837115	8.664372
51	C	7.374461	7.270799	9.232680
52	H	4.462521	6.025348	9.387862
53	H	5.173227	4.805893	8.288936
54	H	5.166110	6.536340	7.820035
55	H	8.073960	7.569139	10.020764
56	H	6.981701	8.070963	8.596307
57	H	6.777476	5.403733	10.238538

TS3-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.407391116	-0.041205323	5.749209834
4.058250000	1.913077397	0.000000000
4.047018819	1.912121175	3.873418410
4.058250000	0.000000000	1.913077397
3.992839723	-0.034364862	5.764908591
1.352750000	1.913077397	0.000000000
1.358483749	1.913025102	3.867395644
0.000000000	0.000000000	0.000000000
0.010238657	-0.020954550	3.921092337
2.705500000	1.913077397	1.913077397
2.696416220	1.900776100	5.650849080
6.763750000	0.000000000	1.913077397
6.810780138	0.115862375	5.867969056
9.469250000	1.913077397	0.000000000
9.458058807	1.969957218	3.952018912
9.469250000	0.000000000	1.913077397
9.407558868	0.101669739	5.853121771
6.763750000	1.913077397	0.000000000
6.770170850	1.971952531	3.956710186
5.411000000	0.000000000	0.000000000
5.391310875	-0.015114715	3.929021513
8.116500000	1.913077397	1.913077397
8.119971532	1.718964819	5.496121323
1.352750000	3.826154793	1.913077397
1.321668808	3.868963171	5.748163140

4.058250000	5.739232190	0.000000000
3.983915182	5.739137147	3.718448384
4.058250000	3.826154793	1.913077397
4.071605367	3.865067682	5.756855146
1.352750000	5.739232190	0.000000000
1.422064387	5.736376022	3.710803425
0.000000000	3.826154793	0.000000000
0.057905958	3.850785549	3.811657014
2.705500000	5.739232190	1.913077397
2.695558486	5.734247992	5.603124817
6.763750000	3.826154793	1.913077397
7.634917714	5.818280664	8.527248642
9.469250000	5.739232190	0.000000000
9.503166383	5.675718546	4.068366415
9.469250000	3.826154793	1.913077397
8.122618167	3.621601293	6.188299867
6.763750000	5.739232190	0.000000000
6.721094608	5.677957162	4.089307738
5.411000000	3.826154793	0.000000000
5.343670758	3.849376256	3.816719148
8.116500000	5.739232190	1.913077397
8.100937545	5.908995944	5.971802485
6.678429452	6.489164131	9.133004683
5.270362939	6.183532310	8.657889169
7.086234912	7.793045155	9.571825820
4.485327095	6.378273794	9.395487660
5.201942334	5.140971096	8.327406948
5.128908236	6.814882028	7.773571807
8.083202127	7.807762407	10.035795420
6.600476063	8.723790270	9.306959752
6.570485706	6.367588846	10.438596340

CH_3COCH_3*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.403045	-0.042746	5.750412
3	O	4.058250	1.913077	0.000000
4	O	4.045434	1.909112	3.876765
5	O	4.058250	0.000000	1.913077
6	O	4.000242	-0.036971	5.796662
7	O	1.352750	1.913077	0.000000
8	O	1.359497	1.914484	3.867436
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.026679	-0.012159	3.916047
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.692137	1.904127	5.655865
13	O	6.763750	0.000000	1.913077
14	O	6.815221	0.115978	5.874709
15	O	9.469250	1.913077	0.000000
16	O	9.459163	1.965506	3.954977
17	O	9.469250	0.000000	1.913077
18	O	9.408074	0.097949	5.860235
19	O	6.763750	1.913077	0.000000
20	O	6.771153	1.973527	3.962343
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.384914	-0.005360	3.926525
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.120773	1.718603	5.503367

25	O	1.352750	3.826155	1.913077
26	O	1.316383	3.868489	5.756171
27	O	4.058250	5.739232	0.000000
28	O	3.985389	5.743347	3.718606
29	O	4.058250	3.826155	1.913077
30	O	4.080706	3.872159	5.773055
31	O	1.352750	5.739232	0.000000
32	O	1.420051	5.735815	3.709762
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.068153	3.840402	3.807838
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.691043	5.731029	5.601070
37	O	6.763750	3.826155	1.913077
38	O	7.607789	6.189855	8.429943
39	O	9.469250	5.739232	0.000000
40	O	9.501093	5.677666	4.054388
41	O	9.469250	3.826155	1.913077
42	O	8.131419	3.616431	6.220318
43	O	6.763750	5.739232	0.000000
44	O	6.727303	5.680076	4.077934
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.335195	3.842857	3.814518
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.124322	5.903787	5.842072
49	C	6.649654	6.763228	8.959987
50	C	5.241534	6.451915	8.558754
51	C	6.879333	7.842061	9.983521
52	H	4.515843	6.681661	9.355164
53	H	5.158674	5.400671	8.242819
54	H	5.005047	7.082511	7.671746
55	H	7.953421	8.000495	10.145261
56	H	6.417412	8.780705	9.629951
57	H	6.386127	7.584128	10.935189

IM5

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.424963	-0.023820	5.759651
3	O	4.058250	1.913077	0.000000
4	O	4.060058	1.910477	3.900501
5	O	4.058250	0.000000	1.913077
6	O	4.011475	-0.049962	5.782023
7	O	1.352750	1.913077	0.000000
8	O	1.373350	1.917599	3.871597
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.007788	0.004411	3.886200
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.665099	1.926703	5.679022
13	O	6.763750	0.000000	1.913077
14	O	6.905584	0.005818	5.726525
15	O	9.469250	1.913077	0.000000
16	O	9.481648	1.877004	3.798713
17	O	9.469250	0.000000	1.913077
18	O	9.459829	0.131606	5.794039
19	O	6.763750	1.913077	0.000000
20	O	6.819420	1.972600	3.947341
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.412729	-0.024240	3.973881

23	Ce	8.116500	1.913077	1.913077
24	Zr	8.213751	1.768850	5.490452
25	O	1.352750	3.826155	1.913077
26	O	1.354244	3.861517	5.743948
27	O	4.058250	5.739232	0.000000
28	O	4.001623	5.740184	3.736975
29	O	4.058250	3.826155	1.913077
30	O	3.945691	3.854714	5.754312
31	O	1.352750	5.739232	0.000000
32	O	1.426978	5.740645	3.710344
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.021000	3.839948	3.834232
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.678555	5.743979	5.596297
37	O	6.763750	3.826155	1.913077
38	O	8.021540	5.924508	8.348948
39	O	9.469250	5.739232	0.000000
40	O	9.512485	5.777064	3.878477
41	O	9.469250	3.826155	1.913077
42	O	9.225542	3.730720	5.616625
43	O	6.763750	5.739232	0.000000
44	O	6.753357	5.675060	3.944909
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.369737	3.823777	3.885775
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.202094	5.781818	5.738147
49	C	7.024098	5.976529	9.077419
50	C	5.637725	6.002157	8.509861
51	C	7.187846	6.007955	10.572615
52	H	4.864644	6.095830	9.287645
53	H	5.485609	5.076139	7.927245
54	H	5.552309	6.832240	7.784135
55	H	8.249727	5.996570	10.852697
56	H	6.696389	6.905393	10.985000
57	H	6.674967	5.137601	11.014505
58	O	6.619344	4.034000	6.102409
59	O	6.892493	2.854621	6.834315

TS3-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.457652601	0.013688653	5.828726828
4.058250000	1.913077397	0.000000000
4.077694305	2.063839808	3.999124119
4.058250000	0.000000000	1.913077397
4.041057990	0.034335725	5.731430665
1.352750000	1.913077397	0.000000000
1.384461230	1.888098073	3.901431162
0.000000000	0.000000000	0.000000000
0.027719385	-0.016124096	3.900717495
2.705500000	1.913077397	1.913077397
2.679386428	1.856319295	5.720211474
6.763750000	0.000000000	1.913077397
6.903025800	0.055194929	5.680269281
9.469250000	1.913077397	0.000000000
9.490328947	1.844844205	3.816251663
9.469250000	0.000000000	1.913077397
9.474377856	0.128481064	5.847479161

6.763750000	1.913077397	0.000000000
6.841529750	2.023525485	3.944009990
5.411000000	0.000000000	0.000000000
5.439934435	0.022976311	3.953346233
8.116500000	1.913077397	1.913077397
8.224106039	1.754083376	5.516046671
1.352750000	3.826154793	1.913077397
1.543743673	3.784871810	5.771549651
4.058250000	5.739232190	0.000000000
4.017318351	5.710734972	3.748451129
4.058250000	3.826154793	1.913077397
4.260984528	4.460759424	6.375331498
1.352750000	5.739232190	0.000000000
1.432014423	5.735004331	3.747556336
0.000000000	3.826154793	0.000000000
-0.011122192	3.816181693	3.940492154
2.705500000	5.739232190	1.913077397
2.715475971	5.804930811	5.666613643
6.763750000	3.826154793	1.913077397
7.935350100	5.886135702	8.191008226
9.469250000	5.739232190	0.000000000
9.533979763	5.769390487	3.917676786
9.469250000	3.826154793	1.913077397
9.249475643	3.689810876	5.626034803
6.763750000	5.739232190	0.000000000
6.767785872	5.693854621	3.937909516
5.411000000	3.826154793	0.000000000
5.443849219	3.901296716	3.884671128
8.116500000	5.739232190	1.913077397
8.210009303	5.830606901	5.802219811
6.877056466	5.660653110	8.857518148
5.559741840	5.824377339	8.318533198
7.160595178	5.280463517	10.328805614
4.792884029	5.893205408	9.082406957
4.926635648	4.965629087	7.247084786
5.530559405	6.655944616	7.599808932
8.223636791	5.488055233	10.526589041
6.546265724	5.853737865	11.057512833
6.960980269	4.208859189	10.482372295
6.734217361	4.036015319	6.187154428
6.899499071	2.852930030	6.878429957

CH_3COCH_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.405353	-0.022452	5.807633
3	O	4.058250	1.913077	0.000000
4	O	4.067014	1.975765	3.925620
5	O	4.058250	0.000000	1.913077
6	O	3.982219	-0.012064	5.755312
7	O	1.352750	1.913077	0.000000
8	O	1.373518	1.899267	3.887772
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.007226	0.002389	3.871800
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.660542	1.867791	5.677840
13	O	6.763750	0.000000	1.913077
14	O	6.896160	0.037254	5.643033

15	O	9.469250	1.913077	0.000000
16	O	9.489085	1.879315	3.784067
17	O	9.469250	0.000000	1.913077
18	O	9.462057	0.148821	5.789780
19	O	6.763750	1.913077	0.000000
20	O	6.826951	1.992013	3.901856
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.447259	-0.013097	3.940548
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.223020	1.771194	5.483043
25	O	1.352750	3.826155	1.913077
26	O	1.482653	3.885715	5.692365
27	O	4.058250	5.739232	0.000000
28	O	4.004935	5.706631	3.776964
29	O	4.058250	3.826155	1.913077
30	O	4.049196	3.867559	6.100866
31	O	1.352750	5.739232	0.000000
32	O	1.433224	5.776698	3.725541
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.014059	3.863209	3.884298
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.670177	5.815351	5.620787
37	O	6.763750	3.826155	1.913077
38	O	7.976423	5.861857	8.088814
39	O	9.469250	5.739232	0.000000
40	O	9.519382	5.785624	3.887355
41	O	9.469250	3.826155	1.913077
42	O	9.289151	3.713131	5.613166
43	O	6.763750	5.739232	0.000000
44	O	6.744391	5.667831	3.917597
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.423021	3.834429	3.811133
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.210328	5.805739	5.817371
49	C	6.965411	5.680836	8.911108
50	C	5.795055	6.393282	8.800896
51	C	7.173770	4.626299	9.965766
52	H	4.978313	6.234449	9.510176
53	H	4.953447	3.922990	6.513326
54	H	5.683349	7.151738	8.021885
55	H	8.115754	4.815618	10.505810
56	H	6.344618	4.589664	10.687640
57	H	7.268002	3.644433	9.472213
58	O	6.630061	3.990935	6.031906
59	O	6.901235	2.818199	6.819728

TS3-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.374590654	-0.061488728	5.811987738
4.058250000	1.913077397	0.000000000
4.058996033	1.940939646	3.922283021
4.058250000	0.000000000	1.913077397
3.947778723	-0.060542608	5.736126250
1.352750000	1.913077397	0.000000000
1.352884108	1.874048546	3.897936088
0.000000000	0.000000000	0.000000000
-0.024936079	-0.025198208	3.895926897

2.705500000	1.913077397	1.913077397
2.653206892	1.806023045	5.677047793
6.763750000	0.000000000	1.913077397
6.828835046	0.103588896	5.697517488
9.469250000	1.913077397	0.000000000
9.437480951	1.886622165	3.837602662
9.469250000	0.000000000	1.913077397
9.355294586	0.196345622	5.828871037
6.763750000	1.913077397	0.000000000
6.803451724	1.942281603	3.841289137
5.411000000	0.000000000	0.000000000
5.425317138	-0.037791577	3.927693354
8.116500000	1.913077397	1.913077397
8.150683659	1.870187529	5.455446146
1.352750000	3.826154793	1.913077397
1.401387794	3.842742245	5.715290211
4.058250000	5.739232190	0.000000000
3.989230040	5.674115620	3.786308744
4.058250000	3.826154793	1.913077397
3.933106659	3.779713527	6.023552196
1.352750000	5.739232190	0.000000000
1.412194644	5.745306491	3.735616095
0.000000000	3.826154793	0.000000000
-0.057735972	3.833285819	3.955696274
2.705500000	5.739232190	1.913077397
2.619254141	5.762069332	5.630825554
6.763750000	3.826154793	1.913077397
8.018172983	6.004837453	8.395806237
9.469250000	5.739232190	0.000000000
9.513437091	5.794637854	3.985412002
9.469250000	3.826154793	1.913077397
9.202544267	3.723652860	5.699381224
6.763750000	5.739232190	0.000000000
6.775915721	5.692994032	3.960754212
5.411000000	3.826154793	0.000000000
5.436727154	3.815683703	3.900454539
8.116500000	5.739232190	1.913077397
8.083940565	5.875930819	5.918646651
6.843649510	5.703761707	8.896896892
5.676625426	6.359646802	8.474674734
6.731589025	4.572114282	9.897688916
4.711797510	6.150589917	8.947764481
4.801271024	3.902957410	6.522542253
5.781199753	7.277348612	7.881674318
7.440773709	4.663711941	10.742420416
5.718307207	4.495002502	10.312290323
6.946439259	3.630841543	9.382065195
6.162483069	4.725574572	7.059997653
6.504888266	3.402241937	5.909411637

CH_3COCOH_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.352788	-0.003921	5.806584
3	O	4.058250	1.913077	0.000000
4	O	4.034243	1.970801	3.868522
5	O	4.058250	0.000000	1.913077
6	O	3.952296	0.057947	5.682377

7	O	1.352750	1.913077	0.000000
8	O	1.316181	1.889156	3.876774
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.031204	-0.022412	3.944655
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.638764	1.843534	5.657658
13	O	6.763750	0.000000	1.913077
14	O	6.785127	0.154162	5.710962
15	O	9.469250	1.913077	0.000000
16	O	9.414132	1.913745	3.860679
17	O	9.469250	0.000000	1.913077
18	O	9.308856	0.072779	5.769336
19	O	6.763750	1.913077	0.000000
20	O	6.784369	1.930891	3.799109
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.393441	0.008348	3.913258
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.068015	1.920746	5.419727
25	O	1.352750	3.826155	1.913077
26	O	1.490148	3.814793	5.729916
27	O	4.058250	5.739232	0.000000
28	O	3.995268	5.694688	3.796768
29	O	4.058250	3.826155	1.913077
30	O	4.152434	3.743135	6.000590
31	O	1.352750	5.739232	0.000000
32	O	1.385485	5.755456	3.758597
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.002732	3.843840	3.953200
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.696541	5.796334	5.774408
37	O	6.763750	3.826155	1.913077
38	O	6.878129	5.541368	8.128799
39	O	9.469250	5.739232	0.000000
40	O	9.452587	5.740955	3.921462
41	O	9.469250	3.826155	1.913077
42	O	9.322805	3.751980	5.746276
43	O	6.763750	5.739232	0.000000
44	O	6.746224	5.725607	3.932015
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.419287	3.833049	3.843504
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.084790	5.758241	5.735605
49	C	5.732949	5.427576	8.582896
50	C	4.663935	6.498439	8.356176
51	C	5.344591	4.227001	9.398963
52	H	4.509865	6.985952	9.352121
53	H	5.079722	3.672283	6.368580
54	H	5.090518	7.254719	7.670555
55	H	5.488271	4.475420	10.467086
56	H	4.280615	3.997019	9.249141
57	H	5.984753	3.367876	9.157129
58	O	3.468141	5.958012	7.882625
59	O	6.753148	3.638429	5.776335

TS3-5

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.368951271	-0.021769490	5.813201839

4.058250000	1.913077397	0.000000000
4.043295298	1.970362815	3.899116410
4.058250000	0.000000000	1.913077397
3.954060949	0.025181788	5.709738738
1.352750000	1.913077397	0.000000000
1.323200710	1.890474475	3.888963439
0.000000000	0.000000000	0.000000000
-0.043128582	-0.009208882	3.933284915
2.705500000	1.913077397	1.913077397
2.648084811	1.851117116	5.660196761
6.763750000	0.000000000	1.913077397
6.789657219	0.150131173	5.738106420
9.469250000	1.913077397	0.000000000
9.422527661	1.916858696	3.829790764
9.469250000	0.000000000	1.913077397
9.332790524	0.128702885	5.740686858
6.763750000	1.913077397	0.000000000
6.791685467	1.925492604	3.808823640
5.411000000	0.000000000	0.000000000
5.414053825	0.004434018	3.926260191
8.116500000	1.913077397	1.913077397
8.094314196	1.915233182	5.415654129
1.352750000	3.826154793	1.913077397
1.507454471	3.841237687	5.726004235
4.058250000	5.739232190	0.000000000
3.993267390	5.692778704	3.797956517
4.058250000	3.826154793	1.913077397
4.144598225	3.786330776	6.055659028
1.352750000	5.739232190	0.000000000
1.396066454	5.760524893	3.757439026
0.000000000	3.826154793	0.000000000
-0.011105689	3.838938913	3.939728830
2.705500000	5.739232190	1.913077397
2.678774802	5.795543040	5.695339402
6.763750000	3.826154793	1.913077397
8.267058654	5.553308526	8.317647161
9.469250000	5.739232190	0.000000000
9.465137636	5.742358131	3.927456874
9.469250000	3.826154793	1.913077397
9.339860902	3.711671626	5.719469701
6.763750000	5.739232190	0.000000000
6.741842117	5.727182824	3.927224963
5.411000000	3.826154793	0.000000000
5.435969919	3.832992690	3.849551599
8.116500000	5.739232190	1.913077397
8.103247578	5.754337178	5.749529289
7.073091817	5.387642776	8.546186812
4.659172036	6.656273664	8.365665872
6.619663936	4.591061698	9.735277499
4.855954310	6.936599671	9.432435726
5.088886965	3.720475353	6.389622413
5.190687030	7.260933104	7.604599278
6.450935665	5.307094137	10.559062896
5.661224075	4.081058684	9.552438809
7.400879764	3.877650031	10.036811766
3.629672156	6.023769301	8.102154743
6.753346821	3.640676226	5.796710162

$CH_3CO^*+HCOH^*$

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.377510	-0.031249	5.819931
3	O	4.058250	1.913077	0.000000
4	O	4.047043	1.967757	3.914232
5	O	4.058250	0.000000	1.913077
6	O	3.957401	0.006146	5.727077
7	O	1.352750	1.913077	0.000000
8	O	1.327383	1.889098	3.895499
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.048525	-0.004810	3.933385
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.652895	1.851416	5.661996
13	O	6.763750	0.000000	1.913077
14	O	6.788580	0.144652	5.756984
15	O	9.469250	1.913077	0.000000
16	O	9.425782	1.915941	3.816890
17	O	9.469250	0.000000	1.913077
18	O	9.340783	0.155329	5.733912
19	O	6.763750	1.913077	0.000000
20	O	6.794331	1.921128	3.813190
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.426123	-0.000609	3.934467
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.104656	1.911805	5.419157
25	O	1.352750	3.826155	1.913077
26	O	1.514556	3.850631	5.725419
27	O	4.058250	5.739232	0.000000
28	O	3.993132	5.690884	3.796227
29	O	4.058250	3.826155	1.913077
30	O	4.138675	3.807148	6.082243
31	O	1.352750	5.739232	0.000000
32	O	1.400722	5.761444	3.755365
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.017889	3.834295	3.936532
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.669221	5.793576	5.659490
37	O	6.763750	3.826155	1.913077
38	O	8.943077	5.542896	8.211581
39	O	9.469250	5.739232	0.000000
40	O	9.469800	5.742030	3.934181
41	O	9.469250	3.826155	1.913077
42	O	9.344518	3.687329	5.710570
43	O	6.763750	5.739232	0.000000
44	O	6.740401	5.726011	3.925989
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.446495	3.832626	3.854719
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.114312	5.745099	5.780968
49	C	7.746150	5.358063	8.404408
50	C	4.698775	6.737089	8.403036
51	C	7.251314	4.825325	9.726575
52	H	5.073268	6.863691	9.444925
53	H	5.089100	3.745462	6.403801
54	H	5.239480	7.245720	7.580379
55	H	6.949080	5.689151	10.344533
56	H	6.363804	4.194524	9.578636

57	H	8.050159	4.276077	10.257164
58	O	3.693006	6.061320	8.205003
59	O	6.751012	3.640144	5.811481

TS1-5

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.430034555	-0.055960860	5.772704707
4.058250000	1.913077397	0.000000000
4.060287220	1.902095604	3.861835611
4.058250000	0.000000000	1.913077397
4.019708723	-0.041616000	5.755579814
1.352750000	1.913077397	0.000000000
1.353191570	1.914233779	3.893335120
0.000000000	0.000000000	0.000000000
0.041252365	-0.029822129	3.911233020
2.705500000	1.913077397	1.913077397
2.695177032	1.897933038	5.657047568
6.763750000	0.000000000	1.913077397
6.864988312	0.080071540	5.796544979
9.469250000	1.913077397	0.000000000
9.466543427	1.869281074	3.843049563
9.469250000	0.000000000	1.913077397
9.437047568	0.127160284	5.828620876
6.763750000	1.913077397	0.000000000
6.806808055	2.040733212	4.014942961
5.411000000	0.000000000	0.000000000
5.408869121	0.012031065	3.949851252
8.116500000	1.913077397	1.913077397
8.267509487	1.757285496	5.478302900
1.352750000	3.826154793	1.913077397
1.372848987	3.873942648	5.759082204
4.058250000	5.739232190	0.000000000
4.002887237	5.727221288	3.737451113
4.058250000	3.826154793	1.913077397
4.012271654	3.786651557	5.773533168
1.352750000	5.739232190	0.000000000
1.421355525	5.730575637	3.735435834
0.000000000	3.826154793	0.000000000
-0.018028897	3.839433539	3.923901002
2.705500000	5.739232190	1.913077397
2.697570364	5.735425020	5.609704841
6.763750000	3.826154793	1.913077397
6.537725788	4.274903438	6.934964383
9.469250000	5.739232190	0.000000000
9.475211971	5.745572007	3.980304544
9.469250000	3.826154793	1.913077397
8.006585144	5.869434208	8.484966714
6.763750000	5.739232190	0.000000000
6.728218041	5.656377071	4.014453293
5.411000000	3.826154793	0.000000000
5.319735306	3.839197312	3.794417472
8.116500000	5.739232190	1.913077397
8.090316146	5.814967118	5.771850331
5.844439712	6.178556288	9.424983318
6.878771685	5.499396263	8.708950525
4.790998612	5.629963066	10.067516617
5.560808817	4.127468920	6.763848510

4.054486136	6.274000581	10.541791090
4.628995481	4.554461037	10.069608171
6.020490909	7.261283988	9.489975654
9.027190300	3.675794634	5.774381224

CH_2=CHCOO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.379349	-0.040103	5.798323
3	O	4.058250	1.913077	0.000000
4	O	4.039301	1.952298	3.911573
5	O	4.058250	0.000000	1.913077
6	O	3.962383	-0.034572	5.750067
7	O	1.352750	1.913077	0.000000
8	O	1.352550	1.906462	3.880573
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.009579	0.001487	3.908445
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.660670	1.835699	5.677776
13	O	6.763750	0.000000	1.913077
14	O	6.822998	0.139210	5.788434
15	O	9.469250	1.913077	0.000000
16	O	9.468661	1.944193	3.894820
17	O	9.469250	0.000000	1.913077
18	O	9.428898	0.128241	5.836003
19	O	6.763750	1.913077	0.000000
20	O	6.788253	2.000973	3.940429
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.390807	-0.009392	3.929331
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.174768	1.720134	5.478922
25	O	1.352750	3.826155	1.913077
26	O	1.420378	3.867003	5.730625
27	O	4.058250	5.739232	0.000000
28	O	3.974168	5.700043	3.748795
29	O	4.058250	3.826155	1.913077
30	O	4.228318	3.840421	6.014689
31	O	1.352750	5.739232	0.000000
32	O	1.408006	5.755259	3.722941
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.017674	3.853187	3.833690
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.653319	5.784353	5.617024
37	O	6.763750	3.826155	1.913077
38	O	6.145751	5.105820	7.439719
39	O	9.469250	5.739232	0.000000
40	O	9.504199	5.715386	4.021896
41	O	9.469250	3.826155	1.913077
42	O	8.009458	5.836677	8.421816
43	O	6.763750	5.739232	0.000000
44	O	6.714630	5.662734	4.041428
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.389017	3.830420	3.744828
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.085326	5.909402	5.888130
49	C	6.352125	4.891298	9.830273
50	C	6.858064	5.298180	8.488774
51	C	5.190521	4.250798	10.014428

52	H	4.903865	4.120451	6.692200
53	H	4.849961	3.947322	11.007540
54	H	4.550292	4.004048	9.163119
55	H	7.012538	5.138729	10.666453
56	O	8.419738	3.641682	6.049811

CH_2=CHCOO*+<u>O</u>*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.409223	-0.038329	5.791467
3	O	4.058250	1.913077	0.000000
4	O	4.063956	1.949544	3.922596
5	O	4.058250	0.000000	1.913077
6	O	3.980899	-0.032957	5.764347
7	O	1.352750	1.913077	0.000000
8	O	1.363660	1.894386	3.891527
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.001786	0.001458	3.877125
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.668907	1.838438	5.671103
13	O	6.763750	0.000000	1.913077
14	O	6.907236	0.045708	5.662775
15	O	9.469250	1.913077	0.000000
16	O	9.473709	1.887994	3.778630
17	O	9.469250	0.000000	1.913077
18	O	9.456909	0.203750	5.780386
19	O	6.763750	1.913077	0.000000
20	O	6.814263	1.951587	3.878379
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.461442	-0.022966	3.939224
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.206182	1.811916	5.474460
25	O	1.352750	3.826155	1.913077
26	O	1.528009	3.859032	5.707084
27	O	4.058250	5.739232	0.000000
28	O	4.001493	5.688658	3.778274
29	O	4.058250	3.826155	1.913077
30	O	4.108954	3.815263	6.098194
31	O	1.352750	5.739232	0.000000
32	O	1.431025	5.768688	3.742029
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.031349	3.839031	3.957994
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.681306	5.796171	5.625101
37	O	6.763750	3.826155	1.913077
38	O	7.151020	5.759815	8.123518
39	O	9.469250	5.739232	0.000000
40	O	9.503666	5.783433	3.938026
41	O	9.469250	3.826155	1.913077
42	O	9.381551	5.793204	8.068846
43	O	6.763750	5.739232	0.000000
44	O	6.742475	5.695917	3.885139
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.427606	3.834310	3.813966
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.223009	5.867030	5.867663
49	C	8.352921	5.588589	10.199694
50	C	8.280754	5.721711	8.720454

51	C	7.266986	5.471619	10.973982
52	H	4.925780	3.726403	6.645854
53	H	7.344203	5.366228	12.059945
54	H	6.268688	5.475220	10.527574
55	H	9.364829	5.582747	10.615918
56	O	9.361460	3.664920	5.668233
57	O	6.753629	3.955945	5.798091
58	O	6.787762	2.880198	6.743928

TS1-6

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.386507934	-0.035351126	5.804929765
4.058250000	1.913077397	0.000000000
4.073249358	1.974467964	3.932649148
4.058250000	0.000000000	1.913077397
3.977300423	-0.036566349	5.771852767
1.352750000	1.913077397	0.000000000
1.346850751	1.877241714	3.895841640
0.000000000	0.000000000	0.000000000
-0.023339320	-0.008271650	3.906276604
2.705500000	1.913077397	1.913077397
2.666832379	1.834657978	5.680037229
6.763750000	0.000000000	1.913077397
6.839744751	0.099515094	5.717888702
9.469250000	1.913077397	0.000000000
9.443304935	1.885498328	3.800012933
9.469250000	0.000000000	1.913077397
9.406752169	0.176920983	5.770135255
6.763750000	1.913077397	0.000000000
6.816127326	2.025114090	3.940491186
5.411000000	0.000000000	0.000000000
5.452573623	0.014588403	3.969207171
8.116500000	1.913077397	1.913077397
8.243304056	1.843494496	5.458665270
1.352750000	3.826154793	1.913077397
1.536119659	3.855971781	5.707736655
4.058250000	5.739232190	0.000000000
4.012563943	5.686847401	3.783021452
4.058250000	3.826154793	1.913077397
4.155035778	3.835708452	6.101334487
1.352750000	5.739232190	0.000000000
1.422031162	5.766849071	3.744694759
0.000000000	3.826154793	0.000000000
0.002732282	3.826856919	3.919735666
2.705500000	5.739232190	1.913077397
2.664791627	5.788657521	5.633574647
6.763750000	3.826154793	1.913077397
8.737239332	7.786232524	8.867313170
9.469250000	5.739232190	0.000000000
9.488723685	5.756045035	3.930744123
9.469250000	3.826154793	1.913077397
10.592489387	6.361981042	8.595149543
6.763750000	5.739232190	0.000000000
6.745515546	5.663240495	3.947028319
5.411000000	3.826154793	0.000000000
5.382359050	3.852547700	3.773386994
8.116500000	5.739232190	1.913077397

8.158379820	5.831785338	5.719275698
8.405483658	4.844584635	9.960517817
9.635400381	7.013307203	8.802590170
7.424426982	5.102911187	10.789236885
5.046116091	3.789610977	6.543826175
7.377087130	4.563442929	11.742676952
6.626521098	5.849005211	10.617812326
9.170153335	4.073780922	9.954255619
9.404298555	3.657480888	5.651831835
6.882513735	3.635094546	6.251018995
7.367688958	4.525269278	7.286243756

CH_2=CHO*+CO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.370972	-0.035061	5.810910
3	O	4.058250	1.913077	0.000000
4	O	4.047296	1.960786	3.942830
5	O	4.058250	0.000000	1.913077
6	O	3.944522	-0.034181	5.778669
7	O	1.352750	1.913077	0.000000
8	O	1.333168	1.881453	3.905123
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.048851	-0.003301	3.932166
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.659100	1.836630	5.681791
13	O	6.763750	0.000000	1.913077
14	O	6.795866	0.136663	5.689840
15	O	9.469250	1.913077	0.000000
16	O	9.425174	1.919760	3.818733
17	O	9.469250	0.000000	1.913077
18	O	9.350721	0.159471	5.732439
19	O	6.763750	1.913077	0.000000
20	O	6.799211	1.931252	3.806154
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.439893	-0.001929	3.933852
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.112984	1.903803	5.423700
25	O	1.352750	3.826155	1.913077
26	O	1.512849	3.850552	5.712096
27	O	4.058250	5.739232	0.000000
28	O	3.995057	5.689778	3.786689
29	O	4.058250	3.826155	1.913077
30	O	4.116560	3.841902	6.134870
31	O	1.352750	5.739232	0.000000
32	O	1.408620	5.762329	3.747103
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.011217	3.834323	3.931161
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.668949	5.791896	5.623162
37	O	6.763750	3.826155	1.913077
38	O	9.595355	8.757217	8.733890
39	O	9.469250	5.739232	0.000000
40	O	9.482981	5.736391	3.935183
41	O	9.469250	3.826155	1.913077
42	O	11.097034	6.949808	8.742777
43	O	6.763750	5.739232	0.000000
44	O	6.738798	5.721041	3.903375

45	Ce	5.411000	3.826155	0.000000
46	Ce	5.452514	3.828345	3.854351
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.107210	5.721281	5.778760
49	C	8.277589	4.805803	9.051733
50	C	10.333411	7.842500	8.717102
51	C	7.677297	4.978589	10.263524
52	H	5.069394	3.778390	6.441496
53	H	7.810278	4.235332	11.053153
54	H	7.059654	5.857437	10.464756
55	H	8.890103	3.905963	8.872350
56	O	9.345444	3.684371	5.719917
57	O	6.743083	3.671889	5.774723
58	O	8.179474	5.651516	8.049021

$C_2H_3COONO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.413249	-0.028419	5.770940
3	O	4.058250	1.913077	0.000000
4	O	4.062340	1.913643	3.895064
5	O	4.058250	0.000000	1.913077
6	O	3.998423	-0.027835	5.771387
7	O	1.352750	1.913077	0.000000
8	O	1.347236	1.913241	3.891141
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.008705	0.000717	3.942859
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.698854	1.908718	5.651835
13	O	6.763750	0.000000	1.913077
14	O	6.860281	0.109746	5.756477
15	O	9.469250	1.913077	0.000000
16	O	9.428181	1.911519	3.854345
17	O	9.469250	0.000000	1.913077
18	O	9.380648	0.085924	5.748097
19	O	6.763750	1.913077	0.000000
20	O	6.800417	1.908778	3.845898
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.418569	-0.000892	3.949169
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.107002	1.918516	5.439566
25	O	1.352750	3.826155	1.913077
26	O	1.410331	3.854895	5.772668
27	O	4.058250	5.739232	0.000000
28	O	4.003742	5.735187	3.747044
29	O	4.058250	3.826155	1.913077
30	O	4.000077	3.847461	5.791795
31	O	1.352750	5.739232	0.000000
32	O	1.409476	5.741578	3.742074
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.008748	3.830655	3.942862
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.701504	5.740312	5.596228
37	O	6.763750	3.826155	1.913077
38	O	6.836412	3.694794	5.754200
39	O	9.469250	5.739232	0.000000
40	O	9.472224	5.749676	3.911062
41	O	9.469250	3.826155	1.913077

42	O	9.373684	3.751532	5.716241
43	O	6.763750	5.739232	0.000000
44	O	6.762557	5.738685	3.934876
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.419026	3.824431	3.950644
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.135034	5.753050	5.693141
49	N	8.250436	3.158235	9.062595
50	O	8.405532	3.115037	10.251052
51	O	8.341837	2.334974	8.196137
52	O	7.963001	4.638523	8.527415
53	C	5.807407	4.646917	9.705285
54	C	7.039399	5.350651	9.312579
55	C	5.194916	3.753227	8.910142
56	O	7.272136	6.524396	9.506750
57	H	5.351120	5.009573	10.631165
58	H	4.227143	3.337629	9.205533
59	H	5.590891	3.463872	7.930035

TS4-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.410459654	-0.027919579	5.761991859
4.058250000	1.913077397	0.000000000
4.058611984	1.918494750	3.891786322
4.058250000	0.000000000	1.913077397
3.993582069	-0.020603174	5.765408780
1.352750000	1.913077397	0.000000000
1.350920573	1.913750237	3.885532982
0.000000000	0.000000000	0.000000000
-0.014043668	-0.005572073	3.932782398
2.705500000	1.913077397	1.913077397
2.697593135	1.914585503	5.659515334
6.763750000	0.000000000	1.913077397
6.862142647	0.114855835	5.742964727
9.469250000	1.913077397	0.000000000
9.428602940	1.910759317	3.847393976
9.469250000	0.000000000	1.913077397
9.375137633	0.100871369	5.727777664
6.763750000	1.913077397	0.000000000
6.811114084	1.915557925	3.853851087
5.411000000	0.000000000	0.000000000
5.429985130	-0.001242517	3.947191195
8.116500000	1.913077397	1.913077397
8.130992866	1.918996164	5.471181365
1.352750000	3.826154793	1.913077397
1.415031123	3.856710049	5.760636519
4.058250000	5.739232190	0.000000000
3.998631205	5.736283028	3.744563055
4.058250000	3.826154793	1.913077397
4.002118560	3.846888528	5.790846334
1.352750000	5.739232190	0.000000000
1.416083753	5.740577716	3.735671477
0.000000000	3.826154793	0.000000000
-0.017137751	3.834215113	3.935894773
2.705500000	5.739232190	1.913077397
2.705174931	5.739216346	5.606175519
6.763750000	3.826154793	1.913077397

6.847918688	3.715474333	5.741330516
9.469250000	5.739232190	0.000000000
9.476038362	5.744499122	3.918326223
9.469250000	3.826154793	1.913077397
9.375649611	3.725863940	5.710461813
6.763750000	5.739232190	0.000000000
6.758347898	5.743718272	3.931332725
5.411000000	3.826154793	0.000000000
5.430066772	3.832533616	3.946670765
8.116500000	5.739232190	1.913077397
8.129065106	5.748116016	5.791141111
8.491423785	2.821591644	8.991500259
9.578142415	3.068357024	9.414497350
8.175356844	2.102522921	8.046800827
8.113931948	5.309705539	8.231071192
6.918456217	3.721915769	9.616415478
7.161187055	5.170582615	9.088220134
5.977939718	2.945632911	8.910500971
6.356310210	6.000762606	9.522771485
6.876826190	3.663830018	10.726179274
5.473224256	2.087673364	9.368149895
5.915268338	3.090801442	7.826595533

$CO_2C_2H_3NO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.412221	-0.027930	5.765712
3	O	4.058250	1.913077	0.000000
4	O	4.061355	1.917494	3.892133
5	O	4.058250	0.000000	1.913077
6	O	3.994711	-0.018912	5.774697
7	O	1.352750	1.913077	0.000000
8	O	1.350474	1.914713	3.887620
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.007866	-0.004064	3.941475
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.696362	1.915953	5.655595
13	O	6.763750	0.000000	1.913077
14	O	6.848190	0.114556	5.746087
15	O	9.469250	1.913077	0.000000
16	O	9.442474	1.905119	3.829894
17	O	9.469250	0.000000	1.913077
18	O	9.375896	0.101895	5.726566
19	O	6.763750	1.913077	0.000000
20	O	6.805449	1.905528	3.839288
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.420972	0.000884	3.952014
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.132311	1.900603	5.432251
25	O	1.352750	3.826155	1.913077
26	O	1.416179	3.857325	5.764709
27	O	4.058250	5.739232	0.000000
28	O	4.001182	5.734236	3.747614
29	O	4.058250	3.826155	1.913077
30	O	4.007359	3.844514	5.795773
31	O	1.352750	5.739232	0.000000
32	O	1.413798	5.738900	3.739387
33	Ce	0.000000	3.826155	0.000000

34	Ce	-0.011485	3.827924	3.941279
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.705545	5.739220	5.604763
37	O	6.763750	3.826155	1.913077
38	O	6.841148	3.710249	5.752227
39	O	9.469250	5.739232	0.000000
40	O	9.475141	5.744241	3.916107
41	O	9.469250	3.826155	1.913077
42	O	9.375557	3.704391	5.726548
43	O	6.763750	5.739232	0.000000
44	O	6.751949	5.748466	3.926611
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.419722	3.828690	3.946255
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.113454	5.755195	5.725863
49	N	8.674289	2.835752	8.869319
50	O	9.850967	3.024780	8.825916
51	O	7.938787	1.936611	7.992357
52	O	8.085339	5.526007	8.263431
53	C	7.483978	3.443527	9.425498
54	C	7.211650	5.005834	8.995947
55	C	6.675946	2.430216	8.613327
56	O	6.150494	5.384721	9.490069
57	H	7.474934	3.409013	10.522955
58	H	6.205384	1.604953	9.160799
59	H	6.044389	2.863308	7.827083

TS4-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.411591698	-0.027452770	5.765628196
4.058250000	1.913077397	0.000000000
4.062350312	1.919465203	3.892521583
4.058250000	0.000000000	1.913077397
3.995909122	-0.016929738	5.776007388
1.352750000	1.913077397	0.000000000
1.351374321	1.915526626	3.887769072
0.000000000	0.000000000	0.000000000
-0.005533895	-0.003438558	3.938167732
2.705500000	1.913077397	1.913077397
2.696691064	1.916349892	5.654272120
6.763750000	0.000000000	1.913077397
6.848170230	0.107915563	5.747140227
9.469250000	1.913077397	0.000000000
9.443951557	1.907876602	3.830118121
9.469250000	0.000000000	1.913077397
9.376765007	0.101522153	5.723467675
6.763750000	1.913077397	0.000000000
6.807387367	1.911280904	3.844615532
5.411000000	0.000000000	0.000000000
5.419735320	0.003349904	3.949756659
8.116500000	1.913077397	1.913077397
8.138894217	1.904368859	5.433377496
1.352750000	3.826154793	1.913077397
1.416348450	3.859415122	5.764297235
4.058250000	5.739232190	0.000000000
4.002058888	5.734842385	3.748738150
4.058250000	3.826154793	1.913077397

4.007982622	3.844879103	5.799187401
1.352750000	5.739232190	0.000000000
1.413928482	5.739774629	3.738819743
0.000000000	3.826154793	0.000000000
-0.010499245	3.829057480	3.940472145
2.705500000	5.739232190	1.913077397
2.704666676	5.741249873	5.600933229
6.763750000	3.826154793	1.913077397
6.843903702	3.723655470	5.754473115
9.469250000	5.739232190	0.000000000
9.474538068	5.741835952	3.916528479
9.469250000	3.826154793	1.913077397
9.374757130	3.708162220	5.724677193
6.763750000	5.739232190	0.000000000
6.754219494	5.745979453	3.925015838
5.411000000	3.826154793	0.000000000
5.421071260	3.828733834	3.947751811
8.116500000	5.739232190	1.913077397
8.117970823	5.756257952	5.705255994
8.652552544	2.830638391	8.895425504
9.826000366	3.013979045	8.882194231
7.940098948	1.912392757	7.981115016
8.103475953	5.568785494	8.334365036
7.481605798	3.347578359	9.458391251
7.188300957	5.194070001	9.040123743
6.671552249	2.394027894	8.599399502
6.174914154	5.549782792	9.588120599
7.454467162	3.344222904	10.552308205
6.176655036	1.562325289	9.115576177
6.053209933	2.842524458	7.802811434

$C_2H_3NO_2$*+CO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407935	-0.037426	5.769376
3	O	4.058250	1.913077	0.000000
4	O	4.067421	1.914018	3.894963
5	O	4.058250	0.000000	1.913077
6	O	3.996085	-0.016903	5.801183
7	O	1.352750	1.913077	0.000000
8	O	1.353291	1.911555	3.887848
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.005413	-0.000692	3.934013
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.694867	1.910566	5.652183
13	O	6.763750	0.000000	1.913077
14	O	6.832093	0.043656	5.749828
15	O	9.469250	1.913077	0.000000
16	O	9.453362	1.915562	3.833937
17	O	9.469250	0.000000	1.913077
18	O	9.375915	0.116824	5.722059
19	O	6.763750	1.913077	0.000000
20	O	6.819743	1.918651	3.884611
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.421601	0.002021	3.951969
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.169499	1.913146	5.461423
25	O	1.352750	3.826155	1.913077

26	O	1.411295	3.860470	5.762200
27	O	4.058250	5.739232	0.000000
28	O	4.006124	5.735923	3.757385
29	O	4.058250	3.826155	1.913077
30	O	4.003867	3.828558	5.813975
31	O	1.352750	5.739232	0.000000
32	O	1.414471	5.739133	3.737413
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004900	3.824198	3.934811
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.700240	5.737650	5.596556
37	O	6.763750	3.826155	1.913077
38	O	6.839405	3.794316	5.751275
39	O	9.469250	5.739232	0.000000
40	O	9.477630	5.734451	3.912719
41	O	9.469250	3.826155	1.913077
42	O	9.373338	3.700600	5.738759
43	O	6.763750	5.739232	0.000000
44	O	6.758881	5.741759	3.890174
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.420385	3.828411	3.945371
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.102313	5.740275	5.665730
49	N	8.050753	2.682585	9.109043
50	O	9.173027	2.923580	9.464500
51	O	7.660257	1.701659	7.881964
52	O	8.298179	6.006599	8.603017
53	C	6.781897	2.888009	9.357378
54	C	8.063571	6.755774	9.478454
55	C	6.275243	2.070158	8.226917
56	O	7.821104	7.460291	10.383837
57	H	6.397738	3.486260	10.182322
58	H	5.692075	1.168570	8.464315
59	H	5.820231	2.655299	7.408895

$C_2H_3NO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.403195	-0.035920	5.765240
3	O	4.058250	1.913077	0.000000
4	O	4.062340	1.917056	3.896635
5	O	4.058250	0.000000	1.913077
6	O	3.991237	-0.020435	5.788495
7	O	1.352750	1.913077	0.000000
8	O	1.351908	1.911258	3.889705
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000393	-0.001554	3.932290
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.693754	1.911503	5.656832
13	O	6.763750	0.000000	1.913077
14	O	6.834704	0.065414	5.751289
15	O	9.469250	1.913077	0.000000
16	O	9.446003	1.908222	3.847340
17	O	9.469250	0.000000	1.913077
18	O	9.372349	0.092946	5.734101
19	O	6.763750	1.913077	0.000000
20	O	6.811959	1.914366	3.878822
21	Ce	5.411000	0.000000	0.000000

22	Ce	5.413231	0.005913	3.947343
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.146889	1.899965	5.467205
25	O	1.352750	3.826155	1.913077
26	O	1.408496	3.858753	5.763567
27	O	4.058250	5.739232	0.000000
28	O	4.002620	5.735458	3.752858
29	O	4.058250	3.826155	1.913077
30	O	4.000637	3.837524	5.811109
31	O	1.352750	5.739232	0.000000
32	O	1.410064	5.738585	3.737782
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.012087	3.820995	3.945671
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.698362	5.737701	5.595591
37	O	6.763750	3.826155	1.913077
38	O	6.834005	3.783946	5.742758
39	O	9.469250	5.739232	0.000000
40	O	9.473721	5.736476	3.911614
41	O	9.469250	3.826155	1.913077
42	O	9.365384	3.719132	5.744957
43	O	6.763750	5.739232	0.000000
44	O	6.758465	5.748744	3.898065
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.420136	3.828779	3.947171
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.106188	5.760312	5.660974
49	N	8.471848	2.849486	8.951850
50	O	9.655120	2.928872	9.136896
51	O	7.767980	1.823190	7.931684
52	C	7.298499	3.308151	9.319921
53	C	6.514525	2.443635	8.402032
54	H	7.142926	4.079088	10.074311
55	H	5.877579	1.677898	8.874560
56	H	6.008809	2.962700	7.570609

TS4-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.400894513	-0.030808446	5.767614327
4.058250000	1.913077397	0.000000000
4.060817498	1.917147002	3.890854521
4.058250000	0.000000000	1.913077397
3.984391959	-0.020351345	5.788339473
1.352750000	1.913077397	0.000000000
1.354619566	1.910878967	3.881647599
0.000000000	0.000000000	0.000000000
-0.020943726	0.007940088	3.944305978
2.705500000	1.913077397	1.913077397
2.700477982	1.908605159	5.654563580
6.763750000	0.000000000	1.913077397
6.809887239	-0.057176606	5.667180924
9.469250000	1.913077397	0.000000000
9.448888389	1.906356435	3.851417916
9.469250000	0.000000000	1.913077397
9.352024921	0.086611826	5.744981727
6.763750000	1.913077397	0.000000000
6.801442055	1.918452057	3.904144920

5.411000000	0.000000000	0.000000000
5.412966640	-0.016265882	3.927865911
8.116500000	1.913077397	1.913077397
8.107103465	1.906707009	5.539489788
1.352750000	3.826154793	1.913077397
1.403085546	3.851781599	5.757632336
4.058250000	5.739232190	0.000000000
3.999657802	5.731884250	3.745958412
4.058250000	3.826154793	1.913077397
3.994294507	3.839394678	5.817002376
1.352750000	5.739232190	0.000000000
1.411985664	5.739305388	3.731134342
0.000000000	3.826154793	0.000000000
-0.024528648	3.816729586	3.940212488
2.705500000	5.739232190	1.913077397
2.691570267	5.737989368	5.591725720
6.763750000	3.826154793	1.913077397
6.806758472	3.810872639	5.760259044
9.469250000	5.739232190	0.000000000
9.479083222	5.744727157	3.895033852
9.469250000	3.826154793	1.913077397
9.338993881	3.731584342	5.720776513
6.763750000	5.739232190	0.000000000
6.765564424	5.710422625	3.853628314
5.411000000	3.826154793	0.000000000
5.423412929	3.826681546	3.950795981
8.116500000	5.739232190	1.913077397
8.104386155	5.741135409	5.683074604
8.668751440	3.272027857	9.185022171
8.532849131	4.509713043	8.838552622
7.562718020	1.743723476	7.630585194
7.255547660	3.208289026	9.352808999
6.584860662	2.396526800	8.369851135
6.728037794	3.850083464	10.067913920
5.817724949	1.686442217	8.799819164
5.957802524	3.117424486	7.771045202

CH_2CHONO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.405836	-0.035287	5.768770
3	O	4.058250	1.913077	0.000000
4	O	4.063400	1.915930	3.896928
5	O	4.058250	0.000000	1.913077
6	O	3.993501	-0.019955	5.793627
7	O	1.352750	1.913077	0.000000
8	O	1.351074	1.911352	3.889170
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.003791	-0.003457	3.935993
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.695291	1.911506	5.653887
13	O	6.763750	0.000000	1.913077
14	O	6.840067	0.071708	5.771445
15	O	9.469250	1.913077	0.000000
16	O	9.446597	1.904846	3.843207
17	O	9.469250	0.000000	1.913077
18	O	9.372511	0.102433	5.742599
19	O	6.763750	1.913077	0.000000

20	O	6.814923	1.903924	3.869343
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419411	0.004097	3.953006
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.151234	1.904803	5.457848
25	O	1.352750	3.826155	1.913077
26	O	1.408886	3.858678	5.765376
27	O	4.058250	5.739232	0.000000
28	O	4.003609	5.736991	3.753710
29	O	4.058250	3.826155	1.913077
30	O	4.002565	3.836703	5.820947
31	O	1.352750	5.739232	0.000000
32	O	1.411281	5.739460	3.737654
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.011201	3.823193	3.941534
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.700206	5.737614	5.594783
37	O	6.763750	3.826155	1.913077
38	O	6.830744	3.772491	5.707529
39	O	9.469250	5.739232	0.000000
40	O	9.471965	5.739658	3.919108
41	O	9.469250	3.826155	1.913077
42	O	9.371732	3.714103	5.728942
43	O	6.763750	5.739232	0.000000
44	O	6.760648	5.753079	3.906154
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.421558	3.827569	3.942450
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.105967	5.741964	5.679684
49	N	8.478320	2.995924	8.918335
50	O	8.002390	4.339786	8.572882
51	O	7.769859	2.070460	7.932216
52	C	7.154551	3.493907	9.316805
53	C	6.450675	2.520328	8.401422
54	H	6.897387	3.794689	10.336119
55	H	5.952128	1.685225	8.911743
56	H	5.850052	2.961676	7.590884

TS4-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.403315461	-0.041163359	5.760830373
4.058250000	1.913077397	0.000000000
4.064980052	1.916215295	3.891580099
4.058250000	0.000000000	1.913077397
3.988725614	-0.016051546	5.782278430
1.352750000	1.913077397	0.000000000
1.349330679	1.910125137	3.886994018
0.000000000	0.000000000	0.000000000
-0.004804742	-0.007643085	3.935510668
2.705500000	1.913077397	1.913077397
2.691219847	1.909626436	5.652701289
6.763750000	0.000000000	1.913077397
6.837981708	0.058851091	5.744390966
9.469250000	1.913077397	0.000000000
9.448406310	1.904561867	3.838938706
9.469250000	0.000000000	1.913077397
9.369528905	0.116291888	5.738470534

6.763750000	1.913077397	0.000000000
6.822085429	1.913957027	3.878226340
5.411000000	0.000000000	0.000000000
5.419885445	0.002796332	3.950037463
8.116500000	1.913077397	1.913077397
8.172107403	1.891320922	5.459677022
1.352750000	3.826154793	1.913077397
1.407385869	3.863072496	5.755438299
4.058250000	5.739232190	0.000000000
4.003998680	5.733593646	3.755727644
4.058250000	3.826154793	1.913077397
4.000505401	3.823001167	5.804616470
1.352750000	5.739232190	0.000000000
1.412742213	5.738900328	3.735639101
0.000000000	3.826154793	0.000000000
-0.011294411	3.827934394	3.939914453
2.705500000	5.739232190	1.913077397
2.701924371	5.736354085	5.603899320
6.763750000	3.826154793	1.913077397
6.842060130	3.789840397	5.735577820
9.469250000	5.739232190	0.000000000
9.466585938	5.739692937	3.928280415
9.469250000	3.826154793	1.913077397
9.364177038	3.702667491	5.728336180
6.763750000	5.739232190	0.000000000
6.759208752	5.743687428	3.903153915
5.411000000	3.826154793	0.000000000
5.420110414	3.828445429	3.939852448
8.116500000	5.739232190	1.913077397
8.088002227	5.740112168	5.689913145
8.111423450	2.881541685	8.953029057
6.538636528	4.712559372	9.308217940
7.595462075	1.801267730	8.111560607
6.851068274	3.426281096	9.048428934
6.227997033	2.330302960	8.200987806
6.273487159	3.522225034	10.072765160
5.662187117	1.529864571	8.688825753
5.772507629	2.700197695	7.267880335

CH_2COHNO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.399837	-0.039407	5.764762
3	O	4.058250	1.913077	0.000000
4	O	4.066838	1.920731	3.896136
5	O	4.058250	0.000000	1.913077
6	O	3.986849	-0.012240	5.798801
7	O	1.352750	1.913077	0.000000
8	O	1.348579	1.910656	3.886120
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.007777	-0.003046	3.932583
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.686802	1.910569	5.649791
13	O	6.763750	0.000000	1.913077
14	O	6.826342	0.048427	5.755565
15	O	9.469250	1.913077	0.000000
16	O	9.452503	1.904946	3.834433
17	O	9.469250	0.000000	1.913077

18	O	9.366998	0.116153	5.733741
19	O	6.763750	1.913077	0.000000
20	O	6.819490	1.917325	3.887740
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419010	0.004221	3.953206
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.167782	1.898073	5.467622
25	O	1.352750	3.826155	1.913077
26	O	1.404924	3.864500	5.760386
27	O	4.058250	5.739232	0.000000
28	O	4.004044	5.731609	3.762307
29	O	4.058250	3.826155	1.913077
30	O	3.997939	3.820864	5.837608
31	O	1.352750	5.739232	0.000000
32	O	1.411736	5.739225	3.734538
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.013648	3.822566	3.935427
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.693726	5.738386	5.594788
37	O	6.763750	3.826155	1.913077
38	O	6.823416	3.814485	5.739922
39	O	9.469250	5.739232	0.000000
40	O	9.469721	5.739207	3.917551
41	O	9.469250	3.826155	1.913077
42	O	9.362503	3.706533	5.720283
43	O	6.763750	5.739232	0.000000
44	O	6.760147	5.746806	3.889986
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.422779	3.830831	3.943663
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.094407	5.736799	5.669961
49	N	7.978297	3.020073	8.776960
50	O	6.197105	4.150647	9.818847
51	O	7.619660	1.864202	7.875546
52	C	6.716646	3.208346	9.015845
53	C	6.190284	2.143775	8.131189
54	H	5.220044	4.137447	9.721568
55	H	5.696749	1.270289	8.579320
56	H	5.683715	2.521228	7.228841

HCHO*+NCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.445269	-0.035450	5.755498
3	O	4.058250	1.913077	0.000000
4	O	4.077050	1.921324	3.873199
5	O	4.058250	0.000000	1.913077
6	O	4.027070	-0.022244	5.749906
7	O	1.352750	1.913077	0.000000
8	O	1.369284	1.917378	3.887704
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.022833	-0.005742	3.902909
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.708792	1.904288	5.651863
13	O	6.763750	0.000000	1.913077
14	O	6.872868	0.097465	5.684267
15	O	9.469250	1.913077	0.000000
16	O	9.472456	1.885253	3.837796

17	O	9.469250	0.000000	1.913077
18	O	9.422577	0.111025	5.734542
19	O	6.763750	1.913077	0.000000
20	O	6.832767	1.974574	3.879623
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.437567	-0.000366	3.927669
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.191709	1.852638	5.498840
25	O	1.352750	3.826155	1.913077
26	O	1.418944	3.860296	5.756010
27	O	4.058250	5.739232	0.000000
28	O	4.017793	5.729135	3.725000
29	O	4.058250	3.826155	1.913077
30	O	4.043184	3.839392	5.775293
31	O	1.352750	5.739232	0.000000
32	O	1.435022	5.736671	3.730454
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.030964	3.836266	3.937888
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.716558	5.735770	5.597885
37	O	6.763750	3.826155	1.913077
38	O	6.741093	3.619670	6.012069
39	O	9.469250	5.739232	0.000000
40	O	9.502452	5.776368	3.899003
41	O	9.469250	3.826155	1.913077
42	O	9.267895	3.747288	5.640775
43	O	6.763750	5.739232	0.000000
44	O	6.759848	5.682349	3.960146
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.397213	3.830405	3.859469
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.166523	5.854713	5.781068
49	N	7.797162	5.941011	8.184028
50	O	6.694028	4.447005	9.731488
51	O	8.225975	1.629873	7.855306
52	C	7.246925	5.179668	8.956850
53	C	7.424734	0.974855	8.521853
54	H	5.939856	3.580046	6.579688
55	H	7.612276	0.824330	9.600463
56	H	6.499473	0.570737	8.076968

NCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.445373	-0.034261	5.757096
3	O	4.058250	1.913077	0.000000
4	O	4.076965	1.921320	3.878723
5	O	4.058250	0.000000	1.913077
6	O	4.022915	-0.029512	5.741380
7	O	1.352750	1.913077	0.000000
8	O	1.364454	1.916388	3.892944
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.021741	-0.003857	3.917937
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.710119	1.904923	5.654183
13	O	6.763750	0.000000	1.913077
14	O	6.879766	0.113064	5.716789
15	O	9.469250	1.913077	0.000000

16	O	9.462544	1.880736	3.818695
17	O	9.469250	0.000000	1.913077
18	O	9.422801	0.173940	5.785461
19	O	6.763750	1.913077	0.000000
20	O	6.829765	1.964045	3.866099
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.440921	-0.009747	3.945463
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.187057	1.850688	5.451307
25	O	1.352750	3.826155	1.913077
26	O	1.437061	3.855470	5.759801
27	O	4.058250	5.739232	0.000000
28	O	4.013407	5.726807	3.728899
29	O	4.058250	3.826155	1.913077
30	O	4.065464	3.847151	5.783102
31	O	1.352750	5.739232	0.000000
32	O	1.430391	5.737201	3.739166
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.029465	3.839483	3.944662
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.720049	5.736942	5.601709
37	O	6.763750	3.826155	1.913077
38	O	6.770967	3.536468	6.067387
39	O	9.469250	5.739232	0.000000
40	O	9.504374	5.789316	3.935364
41	O	9.469250	3.826155	1.913077
42	O	9.281489	3.713073	5.642034
43	O	6.763750	5.739232	0.000000
44	O	6.748397	5.671631	3.993378
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.391419	3.831248	3.867562
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.170380	5.860695	5.836549
49	N	8.085974	5.781805	8.169839
50	O	7.902228	5.479112	10.555385
51	C	7.992240	5.630365	9.370215
52	H	5.941963	3.481712	6.594075

NCO*+NO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.430091	-0.037365	5.761246
3	O	4.058250	1.913077	0.000000
4	O	4.074126	1.918080	3.874404
5	O	4.058250	0.000000	1.913077
6	O	4.015738	-0.033220	5.742203
7	O	1.352750	1.913077	0.000000
8	O	1.359742	1.918318	3.891200
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.031841	0.000935	3.905281
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.707987	1.904024	5.657720
13	O	6.763750	0.000000	1.913077
14	O	6.871460	0.104511	5.723773
15	O	9.469250	1.913077	0.000000
16	O	9.458867	1.875283	3.836976
17	O	9.469250	0.000000	1.913077
18	O	9.401939	0.159780	5.827705

19	O	6.763750	1.913077	0.000000
20	O	6.823417	1.963757	3.871769
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.421314	-0.007953	3.928346
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.168360	1.855507	5.455307
25	O	1.352750	3.826155	1.913077
26	O	1.418820	3.863844	5.763767
27	O	4.058250	5.739232	0.000000
28	O	4.010778	5.724141	3.728269
29	O	4.058250	3.826155	1.913077
30	O	4.061532	3.834054	5.793417
31	O	1.352750	5.739232	0.000000
32	O	1.424324	5.739150	3.736683
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.029625	3.835293	3.941014
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.713444	5.735397	5.598930
37	O	6.763750	3.826155	1.913077
38	O	6.756631	3.509146	6.122026
39	O	9.469250	5.739232	0.000000
40	O	9.497816	5.797791	3.938286
41	O	9.469250	3.826155	1.913077
42	O	9.253714	3.730275	5.654047
43	O	6.763750	5.739232	0.000000
44	O	6.755371	5.668620	3.999455
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.387055	3.823861	3.855932
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.168427	5.881301	5.780072
49	N	7.926679	5.710983	8.334694
50	O	6.627302	4.406434	9.895810
51	C	7.254397	5.031658	9.096493
52	H	5.865817	3.430703	6.538277
53	N	9.186295	6.881896	9.494016
54	O	9.181944	6.597463	10.611522

TS4-5

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.431771106	-0.038377893	5.754712823
4.058250000	1.913077397	0.000000000
4.074336754	1.915418627	3.871799909
4.058250000	0.000000000	1.913077397
4.019654981	-0.035719240	5.738754828
1.352750000	1.913077397	0.000000000
1.358440375	1.918255576	3.888063997
0.000000000	0.000000000	0.000000000
0.034385985	0.001394002	3.900546107
2.705500000	1.913077397	1.913077397
2.706955079	1.903429608	5.653857251
6.763750000	0.000000000	1.913077397
6.875925615	0.102351843	5.732892242
9.469250000	1.913077397	0.000000000
9.459123013	1.876249776	3.836597678
9.469250000	0.000000000	1.913077397
9.404286113	0.159096391	5.821816992
6.763750000	1.913077397	0.000000000

6.825218314	1.965533863	3.881310119
5.411000000	0.000000000	0.000000000
5.418488615	-0.007597157	3.926014223
8.116500000	1.913077397	1.913077397
8.177236026	1.856995756	5.452554857
1.352750000	3.826154793	1.913077397
1.422788976	3.862071409	5.759809230
4.058250000	5.739232190	0.000000000
4.009933906	5.724154340	3.726474892
4.058250000	3.826154793	1.913077397
4.066512244	3.834679795	5.780857673
1.352750000	5.739232190	0.000000000
1.422155554	5.738244106	3.735262762
0.000000000	3.826154793	0.000000000
-0.024154943	3.835311698	3.933274494
2.705500000	5.739232190	1.913077397
2.711875853	5.735095250	5.596948530
6.763750000	3.826154793	1.913077397
6.778771645	3.543184085	6.127282782
9.469250000	5.739232190	0.000000000
9.494789203	5.798207041	3.930053724
9.469250000	3.826154793	1.913077397
9.262737768	3.735995882	5.649717030
6.763750000	5.739232190	0.000000000
6.757557312	5.674410015	3.995710173
5.411000000	3.826154793	0.000000000
5.381857691	3.824136905	3.854323916
8.116500000	5.739232190	1.913077397
8.168873714	5.881829627	5.750995617
7.883193313	5.721575108	8.499215995
6.132226236	4.343310775	9.474434769
7.025373404	5.035825602	9.179507412
5.910455087	3.467524242	6.583681911
8.608856857	6.351759455	9.491696939
8.134065583	5.955093136	10.601987132

$NNCO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.432978	-0.039127	5.750893
3	O	4.058250	1.913077	0.000000
4	O	4.075849	1.913203	3.869901
5	O	4.058250	0.000000	1.913077
6	O	4.020195	-0.036834	5.735235
7	O	1.352750	1.913077	0.000000
8	O	1.357914	1.917748	3.885675
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.029981	0.000700	3.897913
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.710283	1.904736	5.654146
13	O	6.763750	0.000000	1.913077
14	O	6.873684	0.101710	5.744322
15	O	9.469250	1.913077	0.000000
16	O	9.459907	1.874611	3.840957
17	O	9.469250	0.000000	1.913077
18	O	9.402995	0.160288	5.831187
19	O	6.763750	1.913077	0.000000
20	O	6.825869	1.966384	3.888248

21	Ce	5.411000	0.000000	0.000000
22	Ce	5.420180	-0.008605	3.925990
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.178184	1.860800	5.461509
25	O	1.352750	3.826155	1.913077
26	O	1.425694	3.861182	5.756758
27	O	4.058250	5.739232	0.000000
28	O	4.008852	5.723297	3.724860
29	O	4.058250	3.826155	1.913077
30	O	4.066099	3.832094	5.767714
31	O	1.352750	5.739232	0.000000
32	O	1.421952	5.738328	3.734520
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.026789	3.834370	3.931101
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.715369	5.733855	5.598541
37	O	6.763750	3.826155	1.913077
38	O	6.787560	3.556492	6.124582
39	O	9.469250	5.739232	0.000000
40	O	9.487827	5.800429	3.932221
41	O	9.469250	3.826155	1.913077
42	O	9.270229	3.737180	5.654706
43	O	6.763750	5.739232	0.000000
44	O	6.757805	5.677294	3.997130
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.387577	3.824456	3.857388
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.164361	5.885126	5.759965
49	N	7.788175	5.671671	8.453590
50	O	5.861364	4.313092	9.164729
51	C	6.823430	5.008424	9.299783
52	H	5.939272	3.489322	6.618521
53	N	8.375040	6.155893	9.498355
54	O	7.440449	5.513996	10.459119

TS4-6

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.432409903	-0.038736018	5.753973837
4.058250000	1.913077397	0.000000000
4.074356091	1.912906837	3.868733215
4.058250000	0.000000000	1.913077397
4.022026225	-0.037304147	5.738577039
1.352750000	1.913077397	0.000000000
1.359457086	1.918513027	3.886612765
0.000000000	0.000000000	0.000000000
0.039142254	0.003436711	3.899500068
2.705500000	1.913077397	1.913077397
2.709901963	1.903567227	5.653815183
6.763750000	0.000000000	1.913077397
6.877925019	0.097064033	5.748743470
9.469250000	1.913077397	0.000000000
9.459640192	1.876724307	3.837980794
9.469250000	0.000000000	1.913077397
9.405438260	0.159587331	5.827798915
6.763750000	1.913077397	0.000000000
6.826254683	1.964666485	3.887497602
5.411000000	0.000000000	0.000000000

5.415547124	-0.006538538	3.924586833
8.116500000	1.913077397	1.913077397
8.178720334	1.860008274	5.454407575
1.352750000	3.826154793	1.913077397
1.424729744	3.861124267	5.760265468
4.058250000	5.739232190	0.000000000
4.010472705	5.726329514	3.723804996
4.058250000	3.826154793	1.913077397
4.067674653	3.835903258	5.770121748
1.352750000	5.739232190	0.000000000
1.421817569	5.737649424	3.734226960
0.000000000	3.826154793	0.000000000
-0.018528966	3.834432000	3.931068917
2.705500000	5.739232190	1.913077397
2.715021171	5.733668323	5.596847181
6.763750000	3.826154793	1.913077397
6.793349660	3.558679546	6.137635816
9.469250000	5.739232190	0.000000000
9.492179728	5.798119593	3.928081433
9.469250000	3.826154793	1.913077397
9.269567478	3.737604176	5.656870308
6.763750000	5.739232190	0.000000000
6.756414588	5.678195995	3.988884673
5.411000000	3.826154793	0.000000000
5.376997176	3.823646430	3.853042043
8.116500000	5.739232190	1.913077397
8.169583355	5.878949632	5.724038253
7.882609902	5.672722157	8.482482261
5.866403468	4.362880924	9.178225834
6.831161535	5.020401618	9.416277440
5.929066754	3.485457712	6.604356143
8.509348427	6.134904410	9.411770016
7.310723658	5.454218795	10.568821496

N_2*+CO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.443161	-0.040456	5.774099
3	O	4.058250	1.913077	0.000000
4	O	4.076734	1.913569	3.872118
5	O	4.058250	0.000000	1.913077
6	O	4.036568	-0.035519	5.756494
7	O	1.352750	1.913077	0.000000
8	O	1.365932	1.919529	3.896428
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.042247	0.006951	3.911123
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.724342	1.902962	5.662120
13	O	6.763750	0.000000	1.913077
14	O	6.890802	0.078828	5.775705
15	O	9.469250	1.913077	0.000000
16	O	9.460921	1.880495	3.847739
17	O	9.469250	0.000000	1.913077
18	O	9.416433	0.160478	5.839228
19	O	6.763750	1.913077	0.000000
20	O	6.824394	1.971273	3.916897
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.424542	-0.004329	3.935162

23	Ce	8.116500	1.913077	1.913077
24	Zr	8.185103	1.859485	5.474150
25	O	1.352750	3.826155	1.913077
26	O	1.446467	3.863011	5.779122
27	O	4.058250	5.739232	0.000000
28	O	4.017263	5.729123	3.725740
29	O	4.058250	3.826155	1.913077
30	O	4.111416	3.837049	5.790664
31	O	1.352750	5.739232	0.000000
32	O	1.428966	5.737314	3.741315
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.009594	3.831037	3.937089
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.728175	5.736141	5.601219
37	O	6.763750	3.826155	1.913077
38	O	6.844456	3.556551	6.265790
39	O	9.469250	5.739232	0.000000
40	O	9.495451	5.793585	3.943778
41	O	9.469250	3.826155	1.913077
42	O	9.285222	3.735425	5.680213
43	O	6.763750	5.739232	0.000000
44	O	6.767295	5.671307	3.995288
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.373948	3.826017	3.835282
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.173400	5.857892	5.722390
49	N	9.582488	5.860246	8.465145
50	O	5.247613	4.354411	9.641045
51	C	6.075734	4.881312	10.287162
52	H	5.898370	3.487424	6.546049
53	N	10.246884	5.878477	9.350611
54	O	6.902268	5.411698	10.934083

$C_2H_5COONO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.415841	-0.025710	5.766640
3	O	4.058250	1.913077	0.000000
4	O	4.067453	1.911690	3.893687
5	O	4.058250	0.000000	1.913077
6	O	4.002740	-0.027857	5.777195
7	O	1.352750	1.913077	0.000000
8	O	1.351873	1.912422	3.886017
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.011388	-0.001460	3.942369
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.701424	1.915693	5.647747
13	O	6.763750	0.000000	1.913077
14	O	6.856278	0.082371	5.786740
15	O	9.469250	1.913077	0.000000
16	O	9.435854	1.907122	3.846846
17	O	9.469250	0.000000	1.913077
18	O	9.384207	0.084295	5.741937
19	O	6.763750	1.913077	0.000000
20	O	6.806666	1.900160	3.860565
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.424030	-0.001600	3.954615
23	Ce	8.116500	1.913077	1.913077

24	Zr	8.131314	1.921912	5.446252
25	O	1.352750	3.826155	1.913077
26	O	1.414305	3.854163	5.765509
27	O	4.058250	5.739232	0.000000
28	O	4.005264	5.735432	3.746567
29	O	4.058250	3.826155	1.913077
30	O	4.008073	3.850707	5.789959
31	O	1.352750	5.739232	0.000000
32	O	1.409231	5.739769	3.739643
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.007148	3.827919	3.932363
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.702031	5.737066	5.593837
37	O	6.763750	3.826155	1.913077
38	O	6.853604	3.717412	5.737104
39	O	9.469250	5.739232	0.000000
40	O	9.469723	5.745953	3.914408
41	O	9.469250	3.826155	1.913077
42	O	9.383847	3.729221	5.715648
43	O	6.763750	5.739232	0.000000
44	O	6.758219	5.748744	3.925696
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.418843	3.827577	3.940024
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.118183	5.744100	5.688995
49	N	7.737425	3.257903	8.689315
50	O	7.112283	3.065401	10.040194
51	O	7.995772	2.231331	8.083736
52	O	7.942754	4.419302	8.437119
53	C	5.253656	1.784695	8.905165
54	C	3.862437	1.240334	9.222289
55	H	5.214975	2.601342	8.162605
56	H	3.461340	0.716921	8.342348
57	H	3.169811	2.039334	9.527886
58	H	3.901618	0.510039	10.043942
59	C	5.944707	2.260469	10.154012
60	H	5.869521	1.000168	8.430985
61	O	5.597217	2.079500	11.292700

TS5-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.415806199	-0.031958173	5.753570214
4.058250000	1.913077397	0.000000000
4.056478673	1.909408265	3.899984766
4.058250000	0.000000000	1.913077397
3.995506223	-0.043250299	5.763122224
1.352750000	1.913077397	0.000000000
1.352048614	1.908820289	3.882335630
0.000000000	0.000000000	0.000000000
-0.007683292	-0.005391878	3.933761079
2.705500000	1.913077397	1.913077397
2.694504673	1.907146494	5.651277374
6.763750000	0.000000000	1.913077397
6.865809145	0.075260709	5.753184920
9.469250000	1.913077397	0.000000000
9.428944045	1.906066708	3.859500029
9.469250000	0.000000000	1.913077397

9.378555497	0.081285360	5.741563834
6.763750000	1.913077397	0.000000000
6.805175847	1.898479305	3.869472360
5.411000000	0.000000000	0.000000000
5.423973319	-0.008896739	3.950033748
8.116500000	1.913077397	1.913077397
8.135726262	1.895352133	5.476981100
1.352750000	3.826154793	1.913077397
1.415023117	3.840925530	5.750930440
4.058250000	5.739232190	0.000000000
4.003504197	5.733206334	3.740679054
4.058250000	3.826154793	1.913077397
3.992694961	3.848006216	5.768908040
1.352750000	5.739232190	0.000000000
1.411794469	5.734549552	3.728337618
0.000000000	3.826154793	0.000000000
-0.009116790	3.821591246	3.930554102
2.705500000	5.739232190	1.913077397
2.703117218	5.725910306	5.582849090
6.763750000	3.826154793	1.913077397
6.855541032	3.733628947	5.721241465
9.469250000	5.739232190	0.000000000
9.475202335	5.737222103	3.905665931
9.469250000	3.826154793	1.913077397
9.383787285	3.742801820	5.715756902
6.763750000	5.739232190	0.000000000
6.765466834	5.736125374	3.920806476
5.411000000	3.826154793	0.000000000
5.431989648	3.818458146	3.950717378
8.116500000	5.739232190	1.913077397
8.134066092	5.727836319	5.704231007
7.655026707	3.341107968	8.231584607
7.127922013	2.953814037	10.523057672
8.257484768	2.270614597	7.998405926
8.194651981	4.460711940	8.197965372
5.159252142	1.743543834	8.774220236
3.839535765	1.264485058	9.210595955
5.248813628	2.712869522	8.281847656
3.394661127	0.717594018	8.337659181
3.140950489	2.064587697	9.540392216
3.903084040	0.517371473	10.024675985
6.117028271	2.357827499	10.699854739
5.984727439	1.029933435	8.637232262
5.234360113	1.841460445	11.329776555

$CH_3CH_2NO_2$*+CO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.401002	-0.034337	5.759227
3	O	4.058250	1.913077	0.000000
4	O	4.062466	1.913963	3.894842
5	O	4.058250	0.000000	1.913077
6	O	3.991750	-0.012655	5.795869
7	O	1.352750	1.913077	0.000000
8	O	1.347390	1.911493	3.880783
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.010209	-0.001362	3.929468
11	Ce	2.705500	1.913077	1.913077

12	Ce	2.681174	1.912636	5.646020
13	O	6.763750	0.000000	1.913077
14	O	6.830569	0.062498	5.776205
15	O	9.469250	1.913077	0.000000
16	O	9.444743	1.911933	3.848310
17	O	9.469250	0.000000	1.913077
18	O	9.366657	0.098706	5.727257
19	O	6.763750	1.913077	0.000000
20	O	6.815449	1.915630	3.889388
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.416934	0.003898	3.950643
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.157499	1.902651	5.474782
25	O	1.352750	3.826155	1.913077
26	O	1.404551	3.857584	5.761699
27	O	4.058250	5.739232	0.000000
28	O	4.004836	5.739916	3.754775
29	O	4.058250	3.826155	1.913077
30	O	3.994099	3.840061	5.800139
31	O	1.352750	5.739232	0.000000
32	O	1.411077	5.739228	3.736532
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.011676	3.827182	3.930358
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.694640	5.739880	5.596591
37	O	6.763750	3.826155	1.913077
38	O	6.826354	3.786323	5.773915
39	O	9.469250	5.739232	0.000000
40	O	9.469896	5.739699	3.905848
41	O	9.469250	3.826155	1.913077
42	O	9.365101	3.735251	5.718607
43	O	6.763750	5.739232	0.000000
44	O	6.757278	5.742147	3.906230
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417222	3.827153	3.948042
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.106879	5.736331	5.668048
49	N	7.134724	2.070457	8.715490
50	O	7.511043	3.159705	13.200255
51	O	8.108727	1.986338	7.930788
52	O	7.277536	2.241839	9.922216
53	C	5.764833	1.960016	8.124405
54	C	4.676885	1.956224	9.173095
55	H	5.705763	2.812866	7.416754
56	H	3.706510	1.803644	8.675768
57	H	4.626995	2.905856	9.725523
58	H	4.805301	1.140982	9.900560
59	C	6.506367	2.577273	13.021630
60	H	5.794561	1.046019	7.500161
61	O	5.495999	1.997418	12.859921

$CH_3CH_2NO_2$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.401093	-0.034332	5.759286
3	O	4.058250	1.913077	0.000000
4	O	4.062477	1.913964	3.894833
5	O	4.058250	0.000000	1.913077

6	O	3.991838	-0.012676	5.795814
7	O	1.352750	1.913077	0.000000
8	O	1.347391	1.911492	3.880828
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.010204	-0.001365	3.929441
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.681197	1.912635	5.645994
13	O	6.763750	0.000000	1.913077
14	O	6.830549	0.062464	5.776029
15	O	9.469250	1.913077	0.000000
16	O	9.444775	1.911934	3.848271
17	O	9.469250	0.000000	1.913077
18	O	9.366725	0.098656	5.727068
19	O	6.763750	1.913077	0.000000
20	O	6.815377	1.915626	3.889388
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.416939	0.003890	3.950601
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.157331	1.902606	5.474718
25	O	1.352750	3.826155	1.913077
26	O	1.404512	3.857575	5.761560
27	O	4.058250	5.739232	0.000000
28	O	4.004873	5.739894	3.754811
29	O	4.058250	3.826155	1.913077
30	O	3.994131	3.840042	5.799965
31	O	1.352750	5.739232	0.000000
32	O	1.411090	5.739202	3.736513
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.011668	3.827177	3.930361
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.694669	5.739861	5.596542
37	O	6.763750	3.826155	1.913077
38	O	6.826337	3.786211	5.773752
39	O	9.469250	5.739232	0.000000
40	O	9.469894	5.739704	3.905850
41	O	9.469250	3.826155	1.913077
42	O	9.365123	3.735223	5.718536
43	O	6.763750	5.739232	0.000000
44	O	6.757267	5.742147	3.906164
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.417218	3.827145	3.948037
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.106889	5.736304	5.667956
49	N	7.138170	2.064609	8.718638
50	O	8.111106	1.983091	7.930367
51	O	7.278442	2.227355	9.925008
52	C	5.767259	1.960665	8.126616
53	C	4.680828	1.952592	9.177163
54	H	5.706811	2.817892	7.425384
55	H	3.708991	1.804911	8.681611
56	H	4.636648	2.899278	9.735133
57	H	4.812569	1.130385	9.896742
58	H	5.794695	1.051056	7.496163

CH_3CHNO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.309861	-0.048090	5.751567

3	O	4.058250	1.913077	0.000000
4	O	4.078144	1.919629	3.857037
5	O	4.058250	0.000000	1.913077
6	O	3.900741	0.048678	5.723100
7	O	1.352750	1.913077	0.000000
8	O	1.361450	1.914761	3.874346
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.043903	0.022780	3.930246
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.692278	1.929873	5.644710
13	O	6.763750	0.000000	1.913077
14	O	6.402308	-0.607827	6.151790
15	O	9.469250	1.913077	0.000000
16	O	9.486799	1.991493	3.840746
17	O	9.469250	0.000000	1.913077
18	O	9.103349	0.106704	5.624670
19	O	6.763750	1.913077	0.000000
20	O	6.820082	1.782957	4.036776
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.380415	-0.028240	3.903486
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.251059	2.124123	5.566598
25	O	1.352750	3.826155	1.913077
26	O	1.438697	3.883408	5.742378
27	O	4.058250	5.739232	0.000000
28	O	4.013208	5.739271	3.740926
29	O	4.058250	3.826155	1.913077
30	O	4.026616	3.843352	5.755411
31	O	1.352750	5.739232	0.000000
32	O	1.430642	5.753490	3.723280
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.040160	3.838872	3.877474
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.685511	5.752083	5.594404
37	O	6.763750	3.826155	1.913077
38	O	6.912795	3.818242	5.668718
39	O	9.469250	5.739232	0.000000
40	O	9.510685	5.710726	3.892161
41	O	9.469250	3.826155	1.913077
42	O	9.474292	3.743802	5.824362
43	O	6.763750	5.739232	0.000000
44	O	6.780723	5.767866	3.867823
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.423112	3.819131	3.924994
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.147736	5.685854	5.689022
49	N	7.223133	2.357915	8.659219
50	O	7.497242	1.583359	7.547727
51	O	7.951232	2.193854	9.665615
52	C	6.190693	3.189362	8.598661
53	C	5.842238	3.997507	9.793465
54	H	5.692106	3.279685	7.635802
55	H	5.664982	3.357332	10.676492
56	H	4.940622	4.594236	9.596361
57	H	6.660822	4.684845	10.078135
58	H	6.471058	0.094514	6.845814

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.314286171	-0.054842948	5.758404666
4.058250000	1.913077397	0.000000000
4.081824163	1.921744271	3.857802979
4.058250000	0.000000000	1.913077397
3.909483450	0.048769409	5.724870460
1.352750000	1.913077397	0.000000000
1.366592116	1.915395000	3.878267413
0.000000000	0.000000000	0.000000000
-0.032497583	0.014571245	3.919826392
2.705500000	1.913077397	1.913077397
2.693516624	1.931034411	5.641507140
6.763750000	0.000000000	1.913077397
6.409665269	-0.599593159	6.146375930
9.469250000	1.913077397	0.000000000
9.499644790	1.990298673	3.834260997
9.469250000	0.000000000	1.913077397
9.112675746	0.112862368	5.631227748
6.763750000	1.913077397	0.000000000
6.825727006	1.793799790	4.033214543
5.411000000	0.000000000	0.000000000
5.373475983	-0.030210453	3.889473732
8.116500000	1.913077397	1.913077397
8.269235690	2.127892888	5.526600657
1.352750000	3.826154793	1.913077397
1.443178885	3.883148919	5.749142775
4.058250000	5.739232190	0.000000000
4.016302376	5.737383384	3.738783317
4.058250000	3.826154793	1.913077397
4.038736649	3.841320974	5.768796571
1.352750000	5.739232190	0.000000000
1.432797002	5.750440611	3.722491565
0.000000000	3.826154793	0.000000000
0.048967112	3.845518305	3.874140651
2.705500000	5.739232190	1.913077397
2.687866559	5.755975499	5.593450835
6.763750000	3.826154793	1.913077397
6.913258595	3.817153095	5.707709739
9.469250000	5.739232190	0.000000000
9.516133016	5.711870864	3.893805625
9.469250000	3.826154793	1.913077397
9.480047763	3.745505309	5.827074082
6.763750000	5.739232190	0.000000000
6.783578000	5.769347551	3.867416366
5.411000000	3.826154793	0.000000000
5.421759458	3.820454994	3.923092568
8.116500000	5.739232190	1.913077397
8.158768607	5.694591894	5.672564733
7.194739732	2.313841888	8.651631221
7.572711578	1.629211114	7.558388162
6.573176842	1.621395296	9.686625332
6.208437945	3.229657150	8.551642420
5.941700091	4.254860558	9.595949346
5.594503230	3.178820829	7.638350875
5.728301570	3.843402036	10.610176842
5.108640757	4.899716230	9.296853772
6.861142491	4.852556440	9.695495363

6.451307765 0.092130062 6.842864905

CH_3CHONO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.310803	-0.055026	5.754483
3	O	4.058250	1.913077	0.000000
4	O	4.077389	1.921072	3.858041
5	O	4.058250	0.000000	1.913077
6	O	3.899196	0.046377	5.710585
7	O	1.352750	1.913077	0.000000
8	O	1.365718	1.914850	3.879291
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.041854	0.017817	3.926693
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.694407	1.931620	5.648978
13	O	6.763750	0.000000	1.913077
14	O	6.397243	-0.601672	6.131837
15	O	9.469250	1.913077	0.000000
16	O	9.491517	1.988137	3.837956
17	O	9.469250	0.000000	1.913077
18	O	9.111494	0.103535	5.625468
19	O	6.763750	1.913077	0.000000
20	O	6.820749	1.790782	4.032016
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.374363	-0.028627	3.897236
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.247251	2.126336	5.569965
25	O	1.352750	3.826155	1.913077
26	O	1.438487	3.881984	5.745823
27	O	4.058250	5.739232	0.000000
28	O	4.012795	5.739155	3.736732
29	O	4.058250	3.826155	1.913077
30	O	4.023649	3.846963	5.745095
31	O	1.352750	5.739232	0.000000
32	O	1.430348	5.749833	3.721738
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.038400	3.840355	3.879720
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.684297	5.753169	5.594970
37	O	6.763750	3.826155	1.913077
38	O	6.911825	3.825340	5.680207
39	O	9.469250	5.739232	0.000000
40	O	9.511206	5.711476	3.892821
41	O	9.469250	3.826155	1.913077
42	O	9.473283	3.745817	5.823457
43	O	6.763750	5.739232	0.000000
44	O	6.779340	5.773094	3.861506
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.423959	3.819652	3.929737
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.146220	5.694508	5.684189
49	N	7.243462	2.265315	8.669101
50	O	7.515011	1.581567	7.538053
51	O	5.844855	1.840558	9.217128
52	C	6.049275	3.101012	8.599281
53	C	6.023524	4.341615	9.458291
54	H	5.620739	3.197273	7.594944

55	H	5.879415	4.069698	10.515005
56	H	5.221536	5.028306	9.147724
57	H	6.979984	4.885408	9.382063
58	H	6.414848	0.083406	6.844275

CH_3CONO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.413685	-0.025174	5.773552
3	O	4.058250	1.913077	0.000000
4	O	4.082517	1.925574	3.870641
5	O	4.058250	0.000000	1.913077
6	O	4.012657	-0.072083	5.675108
7	O	1.352750	1.913077	0.000000
8	O	1.382909	1.909968	3.891361
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.015497	0.015582	3.910874
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.738107	1.899822	5.691723
13	O	6.763750	0.000000	1.913077
14	O	6.719734	0.119979	5.957227
15	O	9.469250	1.913077	0.000000
16	O	9.486402	1.913255	3.884631
17	O	9.469250	0.000000	1.913077
18	O	9.283183	0.068650	5.713503
19	O	6.763750	1.913077	0.000000
20	O	6.840540	1.924490	3.957620
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.375896	-0.002158	3.861860
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.169773	1.902826	5.588400
25	O	1.352750	3.826155	1.913077
26	O	1.430138	3.845972	5.763307
27	O	4.058250	5.739232	0.000000
28	O	4.014947	5.724585	3.693755
29	O	4.058250	3.826155	1.913077
30	O	4.065973	3.885891	5.755870
31	O	1.352750	5.739232	0.000000
32	O	1.423554	5.739201	3.730762
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.011311	3.809691	3.910612
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.706123	5.733542	5.586212
37	O	6.763750	3.826155	1.913077
38	O	6.730836	3.729410	5.997274
39	O	9.469250	5.739232	0.000000
40	O	9.505263	5.740164	3.917956
41	O	9.469250	3.826155	1.913077
42	O	9.264384	3.763971	5.714324
43	O	6.763750	5.739232	0.000000
44	O	6.783191	5.743192	3.977550
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.383602	3.832998	3.840597
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.205214	5.744779	5.711396
49	N	7.320183	2.311349	8.798540
50	O	8.034301	1.846353	7.799346
51	O	5.293551	1.648868	7.770494

52	C	5.946700	2.252158	8.674389
53	C	5.224164	2.953825	9.795187
54	H	5.860393	3.639728	6.455020
55	H	4.576465	2.240387	10.332701
56	H	4.566742	3.734207	9.376566
57	H	5.930093	3.408753	10.503293
58	H	6.099552	0.439860	6.670906

TS5-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.415188683	-0.028703221	5.774468122
4.058250000	1.913077397	0.000000000
4.097621504	1.923597061	3.885900204
4.058250000	0.000000000	1.913077397
3.980663178	-0.090586211	5.645320046
1.352750000	1.913077397	0.000000000
1.378549417	1.913073021	3.899818682
0.000000000	0.000000000	0.000000000
0.037700649	0.025400620	3.919843536
2.705500000	1.913077397	1.913077397
2.786083036	1.899337658	5.768493450
6.763750000	0.000000000	1.913077397
6.661832312	0.152062636	5.952791639
9.469250000	1.913077397	0.000000000
9.467806910	1.890466367	3.889072427
9.469250000	0.000000000	1.913077397
9.263785439	0.112105946	5.801221677
6.763750000	1.913077397	0.000000000
6.845384712	1.919925123	3.960008724
5.411000000	0.000000000	0.000000000
5.374830713	0.011273893	3.917737854
8.116500000	1.913077397	1.913077397
8.151124561	1.918788294	5.557033417
1.352750000	3.826154793	1.913077397
1.434684737	3.850430234	5.773517603
4.058250000	5.739232190	0.000000000
4.021366084	5.724171769	3.692091053
4.058250000	3.826154793	1.913077397
4.070115350	3.906204898	5.727073736
1.352750000	5.739232190	0.000000000
1.415733224	5.738448235	3.731105989
0.000000000	3.826154793	0.000000000
-0.001277260	3.799080056	3.955962599
2.705500000	5.739232190	1.913077397
2.701328115	5.732138796	5.588778246
6.763750000	3.826154793	1.913077397
6.743484275	3.758725711	5.958356694
9.469250000	5.739232190	0.000000000
9.494752545	5.771288520	3.959600609
9.469250000	3.826154793	1.913077397
9.254507540	3.740030419	5.733279887
6.763750000	5.739232190	0.000000000
6.788905748	5.762955074	3.991648498
5.411000000	3.826154793	0.000000000
5.375958345	3.843274179	3.850163848
8.116500000	5.739232190	1.913077397
8.165438051	5.823982795	5.727239192

6.439420078	2.473522556	8.619686990
7.056058681	1.566189174	7.768109641
4.284691705	1.779976718	7.861794875
5.091801205	2.462734171	8.606612989
4.451908447	3.442086849	9.601894110
5.983452616	3.680887159	6.575796142
3.796418978	2.893138787	10.305424398
3.800376210	4.140280380	9.051363636
5.184361872	4.021175352	10.181816272
6.471750279	0.775470203	6.975330396

CH_3CONOH*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.435406	-0.040535	5.753317
3	O	4.058250	1.913077	0.000000
4	O	4.072048	1.918470	3.886312
5	O	4.058250	0.000000	1.913077
6	O	4.044881	-0.085555	5.679551
7	O	1.352750	1.913077	0.000000
8	O	1.349317	1.915897	3.892409
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.021390	0.026096	3.935649
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.736303	1.911049	5.737683
13	O	6.763750	0.000000	1.913077
14	O	6.882514	-0.007416	5.681959
15	O	9.469250	1.913077	0.000000
16	O	9.435968	1.881801	3.870377
17	O	9.469250	0.000000	1.913077
18	O	9.396025	0.155728	5.838480
19	O	6.763750	1.913077	0.000000
20	O	6.824127	1.962769	3.921780
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.379581	-0.010271	3.886333
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.142350	1.841221	5.510114
25	O	1.352750	3.826155	1.913077
26	O	1.415734	3.868470	5.759540
27	O	4.058250	5.739232	0.000000
28	O	4.015942	5.735401	3.679678
29	O	4.058250	3.826155	1.913077
30	O	4.056153	3.926829	5.703855
31	O	1.352750	5.739232	0.000000
32	O	1.416565	5.738697	3.722658
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.004705	3.812398	3.943086
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.714483	5.739976	5.584561
37	O	6.763750	3.826155	1.913077
38	O	6.771343	3.748716	5.973871
39	O	9.469250	5.739232	0.000000
40	O	9.498294	5.781760	3.945981
41	O	9.469250	3.826155	1.913077
42	O	9.282931	3.727470	5.693227
43	O	6.763750	5.739232	0.000000
44	O	6.784597	5.672476	3.924719
45	Ce	5.411000	3.826155	0.000000

46	Ce	5.387818	3.853820	3.854578
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.171026	5.814306	5.696096
49	N	5.867905	2.673809	8.534913
50	O	6.408174	1.584258	7.785485
51	O	3.779936	1.861595	7.897807
52	C	4.545899	2.704143	8.528215
53	C	3.924778	3.802526	9.345857
54	H	6.122697	3.674748	6.710150
55	H	3.283781	3.363182	10.128187
56	H	3.274476	4.424103	8.710382
57	H	4.692330	4.432739	9.815983
58	H	5.641279	1.058701	7.414779

TS5-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.445303007	-0.037021544	5.758335231
4.058250000	1.913077397	0.000000000
4.078561838	1.917853856	3.873478696
4.058250000	0.000000000	1.913077397
4.041506652	-0.078959682	5.688503437
1.352750000	1.913077397	0.000000000
1.369839669	1.917682915	3.882085749
0.000000000	0.000000000	0.000000000
0.038118804	0.018028632	3.916415669
2.705500000	1.913077397	1.913077397
2.728858164	1.901972119	5.713686237
6.763750000	0.000000000	1.913077397
6.890390442	-0.005944289	5.662651301
9.469250000	1.913077397	0.000000000
9.461460179	1.880771513	3.865031646
9.469250000	0.000000000	1.913077397
9.414674318	0.080714248	5.773555050
6.763750000	1.913077397	0.000000000
6.833865492	1.954493338	3.927658551
5.411000000	0.000000000	0.000000000
5.421895609	-0.007368832	3.916750490
8.116500000	1.913077397	1.913077397
8.103276407	1.813925177	5.620699857
1.352750000	3.826154793	1.913077397
1.414286411	3.869466772	5.762230092
4.058250000	5.739232190	0.000000000
4.009241667	5.735855893	3.683003228
4.058250000	3.826154793	1.913077397
4.038469978	3.905312870	5.708904556
1.352750000	5.739232190	0.000000000
1.425374185	5.738278258	3.720948098
0.000000000	3.826154793	0.000000000
-0.005998547	3.808981298	3.939357762
2.705500000	5.739232190	1.913077397
2.712610471	5.740445791	5.585834490
6.763750000	3.826154793	1.913077397
6.732238285	3.737614467	5.932776339
9.469250000	5.739232190	0.000000000
9.489772675	5.771680635	3.889295344
9.469250000	3.826154793	1.913077397
9.274117319	3.771990460	5.659024085

6.763750000	5.739232190	0.000000000
6.782219043	5.670183239	3.906029466
5.411000000	3.826154793	0.000000000
5.371487214	3.816594448	3.876182691
8.116500000	5.739232190	1.913077397
8.174687671	5.811214035	5.665280653
5.504461852	3.055355862	8.596684965
7.570527565	1.768067221	7.700065962
3.447702990	1.892217028	7.991737253
4.311741503	2.593772525	8.648399317
3.801042596	3.122140118	10.084218193
6.134101314	3.637464256	6.698644800
3.491680223	2.224998598	10.642661430
2.926105049	3.768128771	9.891022436
4.586174238	3.663518400	10.636092720
6.678158747	1.390510268	7.898665633

CH_3NCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.424593	-0.034340	5.755053
3	O	4.058250	1.913077	0.000000
4	O	4.066280	1.921073	3.870456
5	O	4.058250	0.000000	1.913077
6	O	4.018683	-0.065737	5.689101
7	O	1.352750	1.913077	0.000000
8	O	1.362622	1.920191	3.874246
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.018821	0.021636	3.919058
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.725313	1.917256	5.745525
13	O	6.763750	0.000000	1.913077
14	O	6.863391	0.012552	5.667753
15	O	9.469250	1.913077	0.000000
16	O	9.468811	1.886697	3.877891
17	O	9.469250	0.000000	1.913077
18	O	9.412703	0.034951	5.748024
19	O	6.763750	1.913077	0.000000
20	O	6.805106	1.964031	3.900934
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.378779	-0.000482	3.884439
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.130871	1.806253	5.605463
25	O	1.352750	3.826155	1.913077
26	O	1.395919	3.879556	5.749442
27	O	4.058250	5.739232	0.000000
28	O	3.997540	5.739364	3.677577
29	O	4.058250	3.826155	1.913077
30	O	4.014364	3.913205	5.697074
31	O	1.352750	5.739232	0.000000
32	O	1.415885	5.741272	3.715280
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.015395	3.816560	3.945812
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.696490	5.737182	5.593177
37	O	6.763750	3.826155	1.913077
38	O	6.709683	3.721022	5.955872
39	O	9.469250	5.739232	0.000000

40	O	9.474870	5.777196	3.863294
41	O	9.469250	3.826155	1.913077
42	O	9.264459	3.836379	5.629724
43	O	6.763750	5.739232	0.000000
44	O	6.764406	5.681963	3.910317
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.384441	3.842105	3.856085
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.164223	5.814602	5.676521
49	N	5.275184	2.945543	8.391954
50	O	8.089486	1.843556	7.664183
51	O	3.200445	2.019537	8.073895
52	C	4.147046	2.489621	8.837903
53	C	3.902690	2.489316	10.332507
54	H	6.077531	3.628018	6.713207
55	H	3.759315	1.449889	10.669081
56	H	2.978071	3.048624	10.542405
57	H	4.741795	2.940017	10.880520
58	H	7.254490	2.172593	8.078402

CH_3COONO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.412869	-0.028734	5.769925
3	O	4.058250	1.913077	0.000000
4	O	4.065348	1.915984	3.895888
5	O	4.058250	0.000000	1.913077
6	O	4.002292	-0.026741	5.775649
7	O	1.352750	1.913077	0.000000
8	O	1.349600	1.914218	3.887270
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.007468	-0.000421	3.939362
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.694284	1.913380	5.650636
13	O	6.763750	0.000000	1.913077
14	O	6.857594	0.106363	5.788245
15	O	9.469250	1.913077	0.000000
16	O	9.438133	1.910214	3.847788
17	O	9.469250	0.000000	1.913077
18	O	9.382316	0.088996	5.743201
19	O	6.763750	1.913077	0.000000
20	O	6.807817	1.905043	3.862035
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419321	0.000254	3.953064
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.135851	1.929073	5.447172
25	O	1.352750	3.826155	1.913077
26	O	1.417546	3.855045	5.766323
27	O	4.058250	5.739232	0.000000
28	O	4.006980	5.734807	3.747567
29	O	4.058250	3.826155	1.913077
30	O	4.007021	3.846639	5.789317
31	O	1.352750	5.739232	0.000000
32	O	1.412497	5.740865	3.741035
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.005631	3.830261	3.932298
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.702197	5.738209	5.597707

37	O	6.763750	3.826155	1.913077
38	O	6.849884	3.721162	5.755226
39	O	9.469250	5.739232	0.000000
40	O	9.470813	5.748272	3.906275
41	O	9.469250	3.826155	1.913077
42	O	9.386070	3.749885	5.703878
43	O	6.763750	5.739232	0.000000
44	O	6.760422	5.743723	3.932754
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.418715	3.825156	3.946414
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.131110	5.748330	5.685924
49	N	7.710267	3.156471	8.671275
50	O	6.913659	2.885621	9.892357
51	O	8.054615	2.164242	8.045479
52	O	7.946099	4.326823	8.504863
53	C	5.789541	1.997094	9.788130
54	C	5.259813	1.676520	8.428714
55	O	5.345312	1.661149	10.853139
56	H	4.268013	1.227674	8.572827
57	H	5.883998	0.943268	7.888899
58	H	5.198786	2.572309	7.786255

TS6-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.423499195	-0.022600349	5.765500758
4.058250000	1.913077397	0.000000000
4.065244779	1.913969311	3.907310869
4.058250000	0.000000000	1.913077397
4.003866657	-0.036550172	5.757344669
1.352750000	1.913077397	0.000000000
1.361599464	1.913774812	3.898433170
0.000000000	0.000000000	0.000000000
-0.001418211	0.005643462	3.941801691
2.705500000	1.913077397	1.913077397
2.714190203	1.911515472	5.669271917
6.763750000	0.000000000	1.913077397
6.863805342	0.076403784	5.744922301
9.469250000	1.913077397	0.000000000
9.434914830	1.914567794	3.863217341
9.469250000	0.000000000	1.913077397
9.379875138	0.092648824	5.745846840
6.763750000	1.913077397	0.000000000
6.810153724	1.912523309	3.868476825
5.411000000	0.000000000	0.000000000
5.422866649	-0.001680289	3.937654134
8.116500000	1.913077397	1.913077397
8.144874668	1.904892041	5.467912972
1.352750000	3.826154793	1.913077397
1.423681144	3.851911045	5.763525507
4.058250000	5.739232190	0.000000000
4.006180884	5.738963520	3.743120203
4.058250000	3.826154793	1.913077397
4.005308583	3.862920267	5.766935061
1.352750000	5.739232190	0.000000000
1.415574806	5.740578722	3.739571418
0.000000000	3.826154793	0.000000000

-0.002740403	3.827752726	3.941184721
2.705500000	5.739232190	1.913077397
2.701781750	5.738435614	5.595383448
6.763750000	3.826154793	1.913077397
6.862855807	3.741448503	5.736501697
9.469250000	5.739232190	0.000000000
9.475298846	5.746066370	3.914826377
9.469250000	3.826154793	1.913077397
9.381384802	3.749566400	5.729710268
6.763750000	5.739232190	0.000000000
6.765147014	5.742061902	3.918707219
5.411000000	3.826154793	0.000000000
5.429844119	3.828821721	3.946244814
8.116500000	5.739232190	1.913077397
8.129557427	5.741910310	5.695802201
7.645690161	3.174011814	8.294907994
6.925644909	2.622296765	10.481609796
8.305172387	2.149603980	8.030048380
8.103789747	4.310948272	8.437082179
5.901120745	2.006147849	10.353988634
5.186127815	1.688048517	8.361159387
4.964860783	1.417016788	10.862311774
4.227878892	1.315760440	8.729132639
5.947117470	0.958045737	8.071584616
5.234503150	2.679989133	7.907981417

CH_3NO_2*+CO_2*

	ATOM	X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407771	-0.045543	5.761852
3	O	4.058250	1.913077	0.000000
4	O	4.062391	1.921582	3.897354
5	O	4.058250	0.000000	1.913077
6	O	3.998510	-0.003761	5.801074
7	O	1.352750	1.913077	0.000000
8	O	1.356875	1.909280	3.885710
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000383	-0.006285	3.926306
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.683881	1.912512	5.653198
13	O	6.763750	0.000000	1.913077
14	O	6.833195	0.055772	5.768236
15	O	9.469250	1.913077	0.000000
16	O	9.455441	1.907056	3.840023
17	O	9.469250	0.000000	1.913077
18	O	9.369112	0.099353	5.721844
19	O	6.763750	1.913077	0.000000
20	O	6.819118	1.919909	3.888684
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419792	0.006396	3.946802
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.168920	1.901734	5.469064
25	O	1.352750	3.826155	1.913077
26	O	1.407324	3.855092	5.757586
27	O	4.058250	5.739232	0.000000
28	O	4.008082	5.742216	3.757496
29	O	4.058250	3.826155	1.913077
30	O	3.998221	3.844522	5.802112

31	O	1.352750	5.739232	0.000000
32	O	1.418124	5.736381	3.734350
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004673	3.823393	3.930461
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.701353	5.737581	5.600825
37	O	6.763750	3.826155	1.913077
38	O	6.828949	3.793520	5.772040
39	O	9.469250	5.739232	0.000000
40	O	9.477675	5.739976	3.911682
41	O	9.469250	3.826155	1.913077
42	O	9.367564	3.721334	5.718112
43	O	6.763750	5.739232	0.000000
44	O	6.755709	5.744232	3.903293
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.416584	3.828336	3.945555
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.103995	5.738112	5.668061
49	N	7.094072	1.956191	8.693875
50	O	7.440497	2.329120	13.245742
51	O	8.087560	1.923258	7.929780
52	O	7.202867	2.009469	9.915439
53	C	6.490111	1.664383	13.059983
54	C	5.750692	1.931155	8.072376
55	O	5.535232	0.999184	12.891361
56	H	5.011463	1.929461	8.880047
57	H	5.702584	1.031223	7.431718
58	H	5.681852	2.821583	7.419193

CH_3NO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.407773	-0.045474	5.761824
3	O	4.058250	1.913077	0.000000
4	O	4.062385	1.921567	3.897308
5	O	4.058250	0.000000	1.913077
6	O	3.998500	-0.003775	5.800967
7	O	1.352750	1.913077	0.000000
8	O	1.356873	1.909276	3.885741
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000381	-0.006281	3.926333
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.683890	1.912511	5.653181
13	O	6.763750	0.000000	1.913077
14	O	6.833041	0.055793	5.768205
15	O	9.469250	1.913077	0.000000
16	O	9.455355	1.907152	3.840140
17	O	9.469250	0.000000	1.913077
18	O	9.369162	0.099480	5.721875
19	O	6.763750	1.913077	0.000000
20	O	6.819152	1.919901	3.888694
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.419791	0.006400	3.946788
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.168917	1.902092	5.469020
25	O	1.352750	3.826155	1.913077
26	O	1.407386	3.855118	5.757757
27	O	4.058250	5.739232	0.000000

28	O	4.008068	5.742248	3.757470
29	O	4.058250	3.826155	1.913077
30	O	3.998211	3.844485	5.802182
31	O	1.352750	5.739232	0.000000
32	O	1.418140	5.736369	3.734438
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.004693	3.823402	3.930468
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.701367	5.737608	5.600783
37	O	6.763750	3.826155	1.913077
38	O	6.829038	3.793489	5.771943
39	O	9.469250	5.739232	0.000000
40	O	9.477673	5.739969	3.911578
41	O	9.469250	3.826155	1.913077
42	O	9.367642	3.721393	5.718034
43	O	6.763750	5.739232	0.000000
44	O	6.755743	5.744228	3.903209
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.416608	3.828338	3.945559
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.104029	5.738085	5.667897
49	N	7.093361	1.957612	8.693536
50	O	8.088270	1.923693	7.929092
51	O	7.199432	2.009464	9.913585
52	C	5.750184	1.936618	8.070833
53	H	5.011176	1.936863	8.878478
54	H	5.699375	1.037480	7.429487
55	H	5.683317	2.827736	7.418487

CH_2NO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.434879	-0.031973	5.760847
3	O	4.058250	1.913077	0.000000
4	O	4.070733	1.929412	3.872921
5	O	4.058250	0.000000	1.913077
6	O	4.013331	-0.018763	5.752970
7	O	1.352750	1.913077	0.000000
8	O	1.366299	1.906775	3.877513
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.000561	-0.001667	3.908306
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.694091	1.910305	5.653114
13	O	6.763750	0.000000	1.913077
14	O	6.865813	0.058990	5.762852
15	O	9.469250	1.913077	0.000000
16	O	9.453189	1.862165	3.866524
17	O	9.469250	0.000000	1.913077
18	O	9.405464	0.093927	5.799179
19	O	6.763750	1.913077	0.000000
20	O	6.824412	1.941098	3.911867
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.435756	0.005616	3.960208
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.179093	1.822294	5.563624
25	O	1.352750	3.826155	1.913077
26	O	1.401661	3.855955	5.749228
27	O	4.058250	5.739232	0.000000

28	O	4.019996	5.726201	3.742092
29	O	4.058250	3.826155	1.913077
30	O	4.016787	3.843486	5.810839
31	O	1.352750	5.739232	0.000000
32	O	1.435193	5.738734	3.730167
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.007579	3.834167	3.923590
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.710307	5.737834	5.596866
37	O	6.763750	3.826155	1.913077
38	O	6.659155	3.682580	5.906844
39	O	9.469250	5.739232	0.000000
40	O	9.495933	5.804917	3.887378
41	O	9.469250	3.826155	1.913077
42	O	9.220149	3.793834	5.497630
43	O	6.763750	5.739232	0.000000
44	O	6.769359	5.696023	3.940369
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.401631	3.821681	3.825874
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.164108	5.779472	5.752428
49	N	7.835301	3.445291	8.336832
50	O	8.345885	2.372179	7.746450
51	O	8.244354	4.640738	8.021651
52	C	6.936345	3.271229	9.279444
53	H	6.560589	4.155954	9.786670
54	H	6.661174	2.252412	9.534527
55	H	5.836501	3.657322	6.452063

TS6-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.441530957	-0.031900968	5.762358546
4.058250000	1.913077397	0.000000000
4.075016641	1.924517965	3.875495757
4.058250000	0.000000000	1.913077397
4.020076848	-0.024738761	5.749053095
1.352750000	1.913077397	0.000000000
1.367392793	1.913718826	3.882435832
0.000000000	0.000000000	0.000000000
0.014226606	0.000421724	3.911680834
2.705500000	1.913077397	1.913077397
2.702651555	1.907105274	5.646607174
6.763750000	0.000000000	1.913077397
6.878494165	0.079738984	5.749593989
9.469250000	1.913077397	0.000000000
9.464355287	1.865270930	3.848868376
9.469250000	0.000000000	1.913077397
9.421042446	0.117099407	5.793155156
6.763750000	1.913077397	0.000000000
6.830304864	1.944992823	3.890119306
5.411000000	0.000000000	0.000000000
5.443440475	-0.001111485	3.949043376
8.116500000	1.913077397	1.913077397
8.185633690	1.824911172	5.526364464
1.352750000	3.826154793	1.913077397
1.409456453	3.856075293	5.752749177
4.058250000	5.739232190	0.000000000

4.017755668	5.726095671	3.732656015
4.058250000	3.826154793	1.913077397
4.030699267	3.844696212	5.806322273
1.352750000	5.739232190	0.000000000
1.434108620	5.738473427	3.732561580
0.000000000	3.826154793	0.000000000
-0.028054910	3.833707475	3.917870995
2.705500000	5.739232190	1.913077397
2.713601199	5.738317082	5.590997614
6.763750000	3.826154793	1.913077397
6.689351757	3.646013503	5.925080892
9.469250000	5.739232190	0.000000000
9.502463349	5.795831897	3.898074999
9.469250000	3.826154793	1.913077397
9.240926557	3.770617501	5.558634154
6.763750000	5.739232190	0.000000000
6.764599739	5.690192172	3.953049662
5.411000000	3.826154793	0.000000000
5.397313544	3.826786991	3.852142323
8.116500000	5.739232190	1.913077397
8.166016796	5.803410941	5.768256172
8.394142198	3.435585303	8.468341029
8.195922604	2.381647235	7.795091477
8.104922222	5.067771933	7.979348791
7.499155578	3.820866776	9.375543121
7.786252476	4.503585333	10.131378523
6.623955063	3.162558327	9.495686160
5.884617061	3.606107585	6.491085764

H_2CONO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.439622	-0.028955	5.760430
3	O	4.058250	1.913077	0.000000
4	O	4.074513	1.923917	3.875446
5	O	4.058250	0.000000	1.913077
6	O	4.017402	-0.029338	5.740885
7	O	1.352750	1.913077	0.000000
8	O	1.362793	1.915242	3.883137
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.015461	-0.001809	3.910709
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.700200	1.909145	5.648419
13	O	6.763750	0.000000	1.913077
14	O	6.877132	0.103199	5.739335
15	O	9.469250	1.913077	0.000000
16	O	9.460383	1.866984	3.835207
17	O	9.469250	0.000000	1.913077
18	O	9.425636	0.140981	5.794754
19	O	6.763750	1.913077	0.000000
20	O	6.828985	1.951237	3.878405
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.440361	-0.004555	3.945233
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.184805	1.819133	5.491209
25	O	1.352750	3.826155	1.913077
26	O	1.413823	3.857840	5.750837
27	O	4.058250	5.739232	0.000000

28	O	4.011927	5.726227	3.727107
29	O	4.058250	3.826155	1.913077
30	O	4.036391	3.849170	5.792828
31	O	1.352750	5.739232	0.000000
32	O	1.428261	5.740551	3.731369
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.036598	3.838399	3.927692
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.709978	5.738072	5.592916
37	O	6.763750	3.826155	1.913077
38	O	6.717847	3.607113	5.969360
39	O	9.469250	5.739232	0.000000
40	O	9.500156	5.796080	3.911739
41	O	9.469250	3.826155	1.913077
42	O	9.250421	3.753983	5.585262
43	O	6.763750	5.739232	0.000000
44	O	6.753404	5.687206	3.969372
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.393139	3.831093	3.859575
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.175534	5.831444	5.812591
49	N	8.814592	3.341906	8.343574
50	O	8.018418	2.487715	7.950119
51	O	8.136253	5.436138	8.075676
52	C	8.120483	4.482844	9.058625
53	H	8.744775	4.751410	9.935673
54	H	7.104993	4.165059	9.371226
55	H	5.921490	3.555903	6.544081

TS6-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.442256085	-0.033409170	5.759436211
4.058250000	1.913077397	0.000000000
4.075060471	1.922917085	3.873963145
4.058250000	0.000000000	1.913077397
4.024991799	-0.029308604	5.735349557
1.352750000	1.913077397	0.000000000
1.368472827	1.914253027	3.884065172
0.000000000	0.000000000	0.000000000
0.024815254	0.002507477	3.908202867
2.705500000	1.913077397	1.913077397
2.705973417	1.907645371	5.653230024
6.763750000	0.000000000	1.913077397
6.890786665	0.055157940	5.749433132
9.469250000	1.913077397	0.000000000
9.465646899	1.859494918	3.867170422
9.469250000	0.000000000	1.913077397
9.424191868	0.094198278	5.796232105
6.763750000	1.913077397	0.000000000
6.826994929	1.954478692	3.919659271
5.411000000	0.000000000	0.000000000
5.439210168	0.003645991	3.938037646
8.116500000	1.913077397	1.913077397
8.201119385	1.813588250	5.557257285
1.352750000	3.826154793	1.913077397
1.413850954	3.856984714	5.752502232
4.058250000	5.739232190	0.000000000

4.019290160	5.725173678	3.728776914
4.058250000	3.826154793	1.913077397
4.038386838	3.842036968	5.795753026
1.352750000	5.739232190	0.000000000
1.428225924	5.739389766	3.732715993
0.000000000	3.826154793	0.000000000
-0.029067622	3.829785000	3.923678589
2.705500000	5.739232190	1.913077397
2.711611815	5.734688785	5.593568581
6.763750000	3.826154793	1.913077397
6.720315070	3.705327290	5.982192622
9.469250000	5.739232190	0.000000000
9.491240883	5.800817832	3.904343753
9.469250000	3.826154793	1.913077397
9.243936087	3.780833049	5.546540152
6.763750000	5.739232190	0.000000000
6.773505127	5.695380431	3.952319023
5.411000000	3.826154793	0.000000000
5.396209987	3.824450723	3.856494209
8.116500000	5.739232190	1.913077397
8.172796595	5.827053693	5.740340163
8.574608877	3.391949794	8.172906221
8.277502501	2.156208543	7.906996500
7.804871797	5.178277730	9.539441783
8.190186018	3.816601142	9.412472709
9.077317818	4.502034357	9.814222467
7.717798631	3.068896420	10.111978446
5.904329018	3.654770336	6.530913359

HOCHNO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.440973	7.618619	5.761596
3	O	4.058250	1.913077	0.000000
4	O	4.070859	1.922023	3.872281
5	O	4.058250	0.000000	1.913077
6	O	4.025371	7.624034	5.736314
7	O	1.352750	1.913077	0.000000
8	O	1.370965	1.911697	3.880894
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.022246	7.651976	3.899898
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.704523	1.904456	5.653316
13	O	6.763750	0.000000	1.913077
14	O	6.883841	0.027415	5.746335
15	O	9.469250	1.913077	0.000000
16	O	9.470293	1.870106	3.873466
17	O	9.469250	0.000000	1.913077
18	O	9.423506	0.062017	5.775291
19	O	6.763750	1.913077	0.000000
20	O	6.814389	1.963394	3.930414
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.436421	0.007949	3.930600
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.194127	1.806642	5.589441
25	O	1.352750	3.826155	1.913077
26	O	1.410167	3.853945	5.754681
27	O	4.058250	5.739232	0.000000

28	O	4.016317	5.725590	3.728409
29	O	4.058250	3.826155	1.913077
30	O	4.030258	3.839287	5.801425
31	O	1.352750	5.739232	0.000000
32	O	1.427753	5.739724	3.730720
33	Ce	0.000000	3.826155	0.000000
34	Ce	10.788837	3.819932	3.928321
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.710556	5.732019	5.586761
37	O	6.763750	3.826155	1.913077
38	O	6.694990	3.784447	5.947756
39	O	9.469250	5.739232	0.000000
40	O	9.488927	5.783241	3.882947
41	O	9.469250	3.826155	1.913077
42	O	9.248076	3.800164	5.589736
43	O	6.763750	5.739232	0.000000
44	O	6.772171	5.701565	3.916056
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.397669	3.820207	3.853648
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.161493	5.816935	5.688371
49	N	8.282949	3.231628	8.393045
50	O	8.264858	2.040665	7.723421
51	O	8.548850	4.191952	10.471738
52	C	8.508228	3.104666	9.653821
53	H	8.383641	4.976143	9.893491
54	H	8.676708	2.157376	10.176232
55	H	5.901008	3.736295	6.528358

TS6-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.439409568	-0.035151690	5.758752107
4.058250000	1.913077397	0.000000000
4.076479751	1.922932989	3.870565204
4.058250000	0.000000000	1.913077397
4.028928345	-0.031623789	5.735501597
1.352750000	1.913077397	0.000000000
1.364930200	1.915278164	3.880902099
0.000000000	0.000000000	0.000000000
0.039495000	0.000271877	3.885640618
2.705500000	1.913077397	1.913077397
2.705289994	1.903571248	5.649779670
6.763750000	0.000000000	1.913077397
6.902344190	0.061131226	5.749736163
9.469250000	1.913077397	0.000000000
9.448578045	1.867809598	3.896545106
9.469250000	0.000000000	1.913077397
9.429819730	0.090937532	5.786660941
6.763750000	1.913077397	0.000000000
6.843855319	1.962268248	3.951739257
5.411000000	0.000000000	0.000000000
5.423669309	0.002287405	3.926837869
8.116500000	1.913077397	1.913077397
8.188423272	1.824036389	5.553125765
1.352750000	3.826154793	1.913077397
1.402792805	3.860791376	5.757074887
4.058250000	5.739232190	0.000000000

4.019624377	5.723618221	3.728127838
4.058250000	3.826154793	1.913077397
4.041139020	3.834546982	5.807642735
1.352750000	5.739232190	0.000000000
1.428087070	5.738296066	3.730313152
0.000000000	3.826154793	0.000000000
-0.025551249	3.831245486	3.917480503
2.705500000	5.739232190	1.913077397
2.711795528	5.735096236	5.584139988
6.763750000	3.826154793	1.913077397
6.697925378	3.690068036	6.090132979
9.469250000	5.739232190	0.000000000
9.495151391	5.793644487	3.884631241
9.469250000	3.826154793	1.913077397
9.221842180	3.819592483	5.555137589
6.763750000	5.739232190	0.000000000
6.774334574	5.688123316	3.953710817
5.411000000	3.826154793	0.000000000
5.389955737	3.826212721	3.849962956
8.116500000	5.739232190	1.913077397
8.175610150	5.818878589	5.669663275
8.759616916	2.814956751	7.955873787
7.909547752	1.734663897	8.401959303
8.182142897	4.436020892	9.569476717
8.727964097	3.269465691	9.202773267
7.535897111	4.669187634	8.844435615
9.263538913	2.756980891	10.029689471
5.789553707	3.621063253	6.483205685

COCHON*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.444607	-0.035359	5.754245
3	O	4.058250	1.913077	0.000000
4	O	4.072444	1.921888	3.868822
5	O	4.058250	0.000000	1.913077
6	O	4.027515	-0.033776	5.733022
7	O	1.352750	1.913077	0.000000
8	O	1.364210	1.920933	3.882522
9	Ce	0.000000	0.000000	0.000000
10	Ce	0.034893	0.001424	3.886254
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.700168	1.901651	5.656078
13	O	6.763750	0.000000	1.913077
14	O	6.898189	0.072403	5.764620
15	O	9.469250	1.913077	0.000000
16	O	9.467391	1.872884	3.878319
17	O	9.469250	0.000000	1.913077
18	O	9.440019	0.060147	5.769222
19	O	6.763750	1.913077	0.000000
20	O	6.815978	1.970681	3.925428
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.427129	0.005104	3.933155
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.194466	1.786997	5.553583
25	O	1.352750	3.826155	1.913077
26	O	1.398801	3.867109	5.755409
27	O	4.058250	5.739232	0.000000

28	O	4.017413	5.722200	3.726319
29	O	4.058250	3.826155	1.913077
30	O	4.045506	3.825849	5.803638
31	O	1.352750	5.739232	0.000000
32	O	1.429988	5.737644	3.729985
33	Ce	0.000000	3.826155	0.000000
34	Ce	-0.032635	3.831615	3.921959
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.710397	5.736776	5.593484
37	O	6.763750	3.826155	1.913077
38	O	6.639748	3.580749	6.187722
39	O	9.469250	5.739232	0.000000
40	O	9.498949	5.792248	3.884495
41	O	9.469250	3.826155	1.913077
42	O	9.179391	3.806057	5.594366
43	O	6.763750	5.739232	0.000000
44	O	6.763913	5.675238	3.982049
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.386813	3.821994	3.826536
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.193960	5.852677	5.719882
49	N	8.782826	2.221832	7.793842
50	O	7.981656	2.118938	9.004087
51	O	7.830384	4.401751	8.243224
52	C	8.632921	3.360071	8.605186
53	H	7.209963	4.003441	7.469984
54	H	9.452371	3.671763	9.262618
55	H	5.667426	3.519068	6.407602

TS6-5

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.435328081	-0.031226471	5.753305774
4.058250000	1.913077397	0.000000000
4.066265624	1.922624348	3.877625726
4.058250000	0.000000000	1.913077397
4.010773972	-0.029762988	5.738346886
1.352750000	1.913077397	0.000000000
1.354026758	1.920143586	3.886162223
0.000000000	0.000000000	0.000000000
-0.010906001	-0.005747588	3.918008517
2.705500000	1.913077397	1.913077397
2.696767936	1.902828514	5.642981694
6.763750000	0.000000000	1.913077397
6.883446448	0.093527991	5.783762191
9.469250000	1.913077397	0.000000000
9.445160684	1.895391525	3.887972066
9.469250000	0.000000000	1.913077397
9.410888394	0.038180066	5.757464621
6.763750000	1.913077397	0.000000000
6.802350792	1.965694128	3.889981971
5.411000000	0.000000000	0.000000000
5.455355602	-0.003567509	3.956300979
8.116500000	1.913077397	1.913077397
8.149830195	1.770698773	5.526776418
1.352750000	3.826154793	1.913077397
1.410345665	3.864326248	5.760362511
4.058250000	5.739232190	0.000000000

4.009337855	5.725990226	3.729550119
4.058250000	3.826154793	1.913077397
4.036569074	3.836967728	5.803414349
1.352750000	5.739232190	0.000000000
1.424050902	5.738539590	3.734887113
0.000000000	3.826154793	0.000000000
-0.027110678	3.836365738	3.919855127
2.705500000	5.739232190	1.913077397
2.713808235	5.743058940	5.583698620
6.763750000	3.826154793	1.913077397
6.662006925	3.582163024	6.031562255
9.469250000	5.739232190	0.000000000
9.486513165	5.767058408	3.901182933
9.469250000	3.826154793	1.913077397
9.258778458	3.781180756	5.621939523
6.763750000	5.739232190	0.000000000
6.759365012	5.674837367	3.994308062
5.411000000	3.826154793	0.000000000
5.406951513	3.825522408	3.865316104
8.116500000	5.739232190	1.913077397
8.192466946	5.799067522	5.868955064
9.019697264	2.413854252	7.512035738
8.365674469	2.307439453	9.230664980
8.106215858	4.898147988	8.173683833
9.045405191	3.215710938	8.555472206
7.221418029	4.499181198	8.050334717
9.849655970	3.823921374	9.004666078
5.777599536	3.501363273	6.468038150

NCHO*+OH*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.415621	-0.028420	5.713884
3	O	4.058250	1.913077	0.000000
4	O	4.057470	1.930202	3.869138
5	O	4.058250	0.000000	1.913077
6	O	3.998369	-0.018280	5.737656
7	O	1.352750	1.913077	0.000000
8	O	1.347545	1.922279	3.867863
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.003746	0.003505	3.892171
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.698107	1.911318	5.651657
13	O	6.763750	0.000000	1.913077
14	O	6.802438	0.166713	5.813295
15	O	9.469250	1.913077	0.000000
16	O	9.433680	1.963154	3.925793
17	O	9.469250	0.000000	1.913077
18	O	9.378968	0.074864	5.727966
19	O	6.763750	1.913077	0.000000
20	O	6.789928	1.931840	3.856346
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.412134	0.014843	3.921689
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.102216	1.700722	5.522893
25	O	1.352750	3.826155	1.913077
26	O	1.444541	3.849592	5.728223
27	O	4.058250	5.739232	0.000000

28	O	3.995644	5.737415	3.724545
29	O	4.058250	3.826155	1.913077
30	O	4.067357	3.870633	5.774885
31	O	1.352750	5.739232	0.000000
32	O	1.417873	5.736846	3.719019
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.023705	3.851618	3.891584
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.713599	5.749950	5.591853
37	O	6.763750	3.826155	1.913077
38	O	6.837597	3.601579	5.961471
39	O	9.469250	5.739232	0.000000
40	O	9.495634	5.711310	3.936245
41	O	9.469250	3.826155	1.913077
42	O	9.523807	3.972300	6.018125
43	O	6.763750	5.739232	0.000000
44	O	6.721854	5.725220	3.967600
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.388518	3.833053	3.866894
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.096508	5.893769	5.865757
49	N	9.404850	2.916611	6.898391
50	O	10.036817	2.210199	8.977312
51	O	7.983893	5.878751	8.016182
52	C	10.027593	3.084563	8.104672
53	H	8.095878	6.677778	8.577041
54	H	10.519906	4.076039	8.212460
55	H	6.113185	3.596845	6.624077

TS6-6

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.408868507	-0.033007290	5.736366247
4.058250000	1.913077397	0.000000000
4.049647089	1.920554798	3.868595387
4.058250000	0.000000000	1.913077397
3.999471321	-0.029431588	5.733933603
1.352750000	1.913077397	0.000000000
1.341910504	1.917292841	3.874346317
0.000000000	0.000000000	0.000000000
0.007754614	-0.016292290	3.910453919
2.705500000	1.913077397	1.913077397
2.703721615	1.908437548	5.652532743
6.763750000	0.000000000	1.913077397
6.796981345	0.137729758	5.792089161
9.469250000	1.913077397	0.000000000
9.421950053	1.982729199	3.930029772
9.469250000	0.000000000	1.913077397
9.379916447	0.063486359	5.721413278
6.763750000	1.913077397	0.000000000
6.771618641	1.921580713	3.831944251
5.411000000	0.000000000	0.000000000
5.393874055	-0.012064094	3.881231352
8.116500000	1.913077397	1.913077397
8.075926013	1.690807701	5.480463651
1.352750000	3.826154793	1.913077397
1.456890140	3.858648568	5.739219166
4.058250000	5.739232190	0.000000000

3.989038455	5.736220094	3.716438290
4.058250000	3.826154793	1.913077397
4.066864568	3.867276285	5.773838574
1.352750000	5.739232190	0.000000000
1.415075466	5.735334876	3.728896225
0.000000000	3.826154793	0.000000000
0.046702207	3.845524341	3.876954451
2.705500000	5.739232190	1.913077397
2.721815956	5.741094536	5.608763638
6.763750000	3.826154793	1.913077397
6.822668498	3.613713333	5.895309493
9.469250000	5.739232190	0.000000000
9.496252672	5.682270425	3.957046331
9.469250000	3.826154793	1.913077397
9.647865355	3.938636906	6.298992760
6.763750000	5.739232190	0.000000000
6.725529134	5.719394400	3.970281876
5.411000000	3.826154793	0.000000000
5.380362275	3.841292260	3.847209412
8.116500000	5.739232190	1.913077397
8.127422599	5.864250496	5.872066314
8.951068989	2.581721003	7.293188474
9.857950592	2.423346911	9.489402762
7.969612890	5.893995839	8.022146984
9.678192057	2.818157663	8.341362137
8.012816492	6.723662583	8.549174152
10.194655350	3.794895167	7.525819299
6.168337588	3.614088992	6.632091675

NCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.415321	-0.025658	5.735536
3	O	4.058250	1.913077	0.000000
4	O	4.052662	1.919780	3.868007
5	O	4.058250	0.000000	1.913077
6	O	3.989969	-0.026203	5.735104
7	O	1.352750	1.913077	0.000000
8	O	1.356034	1.921450	3.867761
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.011126	-0.000708	3.905768
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.703095	1.901149	5.649699
13	O	6.763750	0.000000	1.913077
14	O	6.826583	0.093750	5.699423
15	O	9.469250	1.913077	0.000000
16	O	9.436912	1.948283	3.887021
17	O	9.469250	0.000000	1.913077
18	O	9.411523	0.090343	5.714680
19	O	6.763750	1.913077	0.000000
20	O	6.792284	1.951582	3.882827
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.420298	-0.000111	3.902170
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.115864	1.739941	5.594742
25	O	1.352750	3.826155	1.913077
26	O	1.387652	3.852285	5.766377
27	O	4.058250	5.739232	0.000000

28	O	3.991216	5.732963	3.721768
29	O	4.058250	3.826155	1.913077
30	O	4.012211	3.854129	5.758816
31	O	1.352750	5.739232	0.000000
32	O	1.415582	5.731399	3.723303
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.019034	3.831276	3.862282
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.703532	5.741828	5.595747
37	O	6.763750	3.826155	1.913077
38	O	6.795186	3.686830	5.891380
39	O	9.469250	5.739232	0.000000
40	O	9.495212	5.706997	3.920552
41	O	9.469250	3.826155	1.913077
42	O	9.452324	3.694916	5.898320
43	O	6.763750	5.739232	0.000000
44	O	6.733249	5.704041	3.926314
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.389134	3.830248	3.868521
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.115756	5.881929	5.828851
49	N	8.072224	1.840212	7.784004
50	O	8.535611	2.169029	10.122766
51	O	8.008191	5.924514	7.962226
52	C	8.309258	2.017937	8.955324
53	H	7.962657	6.821328	8.371086
54	H	10.065836	3.647726	6.660977
55	H	6.265207	3.641260	6.714075

TS6-7

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.352750000	0.000000000	1.913077397
1.398301261	-0.022233949	5.741379292
4.058250000	1.913077397	0.000000000
4.051328183	1.915411796	3.881945006
4.058250000	0.000000000	1.913077397
3.979906836	-0.025412825	5.738561074
1.352750000	1.913077397	0.000000000
1.351095055	1.918752129	3.871435824
0.000000000	0.000000000	0.000000000
-0.016689992	0.022210123	3.918083812
2.705500000	1.913077397	1.913077397
2.703791323	1.904968447	5.656809453
6.763750000	0.000000000	1.913077397
6.808440452	0.099165886	5.720096863
9.469250000	1.913077397	0.000000000
9.414194030	1.945858042	3.900898254
9.469250000	0.000000000	1.913077397
9.387256985	0.093106573	5.738950558
6.763750000	1.913077397	0.000000000
6.764862337	1.997697962	3.954496694
5.411000000	0.000000000	0.000000000
5.399981105	0.016188429	3.922886945
8.116500000	1.913077397	1.913077397
8.062872917	1.864822150	5.630407279
1.352750000	3.826154793	1.913077397
1.400910140	3.850119532	5.780485026
4.058250000	5.739232190	0.000000000

3.996885517	5.739906906	3.734754565
4.058250000	3.826154793	1.913077397
4.000901234	3.854698981	5.744117963
1.352750000	5.739232190	0.000000000
1.410285254	5.733343700	3.725980709
0.000000000	3.826154793	0.000000000
0.029322353	3.814034472	3.860890349
2.705500000	5.739232190	1.913077397
2.695193953	5.742164262	5.587563189
6.763750000	3.826154793	1.913077397
6.952938044	3.834683905	6.022203687
9.469250000	5.739232190	0.000000000
9.495538760	5.715067217	3.895287323
9.469250000	3.826154793	1.913077397
9.544896899	3.679592493	5.868496572
6.763750000	5.739232190	0.000000000
6.733407507	5.719315843	3.918281958
5.411000000	3.826154793	0.000000000
5.418871090	3.835436783	3.970530112
8.116500000	5.739232190	1.913077397
8.127252507	5.912238383	5.696680214
8.087865706	1.911857547	7.805928387
8.106480433	0.965252557	10.025011683
7.936907710	5.074815631	7.882022167
8.056048612	1.417515419	8.904004635
7.628223052	5.598298800	8.648030095
10.152150928	3.650803917	6.636918427
7.254858946	4.368749277	7.302218953

$NCO^*+HO_2^*$

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.352750	0.000000	1.913077
2	O	1.389310	-0.026145	5.736863
3	O	4.058250	1.913077	0.000000
4	O	4.040862	1.916842	3.879959
5	O	4.058250	0.000000	1.913077
6	O	3.969267	-0.025708	5.757591
7	O	1.352750	1.913077	0.000000
8	O	1.339225	1.922089	3.872311
9	Ce	0.000000	0.000000	0.000000
10	Ce	-0.026918	0.003266	3.936206
11	Ce	2.705500	1.913077	1.913077
12	Ce	2.707965	1.909738	5.652123
13	O	6.763750	0.000000	1.913077
14	O	6.808839	0.075285	5.765872
15	O	9.469250	1.913077	0.000000
16	O	9.410143	1.954142	3.906532
17	O	9.469250	0.000000	1.913077
18	O	9.347282	0.053877	5.729209
19	O	6.763750	1.913077	0.000000
20	O	6.763395	1.869461	3.866417
21	Ce	5.411000	0.000000	0.000000
22	Ce	5.390796	0.004198	3.904089
23	Ce	8.116500	1.913077	1.913077
24	Zr	8.044688	1.824075	5.566438
25	O	1.352750	3.826155	1.913077
26	O	1.384773	3.846103	5.787901
27	O	4.058250	5.739232	0.000000

28	O	3.980444	5.739688	3.730973
29	O	4.058250	3.826155	1.913077
30	O	4.002415	3.856075	5.753302
31	O	1.352750	5.739232	0.000000
32	O	1.395408	5.727487	3.727527
33	Ce	0.000000	3.826155	0.000000
34	Ce	0.018569	3.822973	3.861704
35	Zr	2.705500	5.739232	1.913077
36	Ce	2.701078	5.736487	5.590880
37	O	6.763750	3.826155	1.913077
38	O	6.983859	3.790813	5.576643
39	O	9.469250	5.739232	0.000000
40	O	9.469028	5.692736	3.932750
41	O	9.469250	3.826155	1.913077
42	O	9.519555	3.683067	5.937854
43	O	6.763750	5.739232	0.000000
44	O	6.734017	5.789758	3.878486
45	Ce	5.411000	3.826155	0.000000
46	Ce	5.442842	3.828951	3.924027
47	Ce	8.116500	5.739232	1.913077
48	Ce	8.060794	5.828103	5.722330
49	N	7.955194	2.039571	7.845819
50	O	7.682232	0.234966	9.427719
51	O	8.038801	4.992633	8.129826
52	C	7.816021	1.127278	8.635070
53	H	7.809070	5.416187	8.984080
54	H	10.257198	3.640147	6.584523
55	H	7.938930	3.995239	8.190706

$ONOCH_2CHCO$*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.481076	-0.031451	5.761938
3	O	4.135936	1.910185	-0.008043
4	O	4.137835	1.914982	3.892886
5	O	4.135936	-0.002892	1.905034
6	O	4.070101	-0.017259	5.786640
7	O	1.430436	1.910185	-0.008043
8	O	1.426648	1.907587	3.883158
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.066482	-0.000228	3.933077
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.768973	1.907791	5.654560
13	O	6.841436	-0.002892	1.905034
14	O	6.910182	0.039433	5.741049
15	O	9.546936	1.910185	-0.008043
16	O	9.518978	1.911631	3.843089
17	O	9.546936	-0.002892	1.905034
18	O	9.445163	0.100815	5.724324
19	O	6.841436	1.910185	-0.008043
20	O	6.889805	1.906487	3.872559
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.494962	0.000359	3.933668
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.222624	1.913221	5.466756
25	O	1.430436	3.823263	1.905034
26	O	1.487406	3.849116	5.755576
27	O	4.135936	5.736340	-0.008043

28	O	4.076480	5.740226	3.741053
29	O	4.135936	3.823263	1.905034
30	O	4.082294	3.860427	5.791498
31	O	1.430436	5.736340	-0.008043
32	O	1.484836	5.737102	3.732099
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.069807	3.819396	3.933755
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.774865	5.741940	5.587179
37	O	6.841436	3.823263	1.905034
38	O	6.907734	3.781734	5.714921
39	O	9.546936	5.736340	-0.008043
40	O	9.550634	5.733248	3.905467
41	O	9.546936	3.823263	1.905034
42	O	9.442031	3.717826	5.736429
43	O	6.841436	5.736340	-0.008043
44	O	6.834222	5.740973	3.880837
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.494797	3.826445	3.926551
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.177631	5.736210	5.651085
49	N	8.813338	2.469394	8.963242
50	O	8.347247	2.587989	10.031284
51	O	7.797568	1.894770	7.922967
52	C	5.605957	2.888454	8.455148
53	C	6.453724	1.649239	8.428845
54	H	5.300981	3.349905	7.497386
55	H	6.540293	1.187000	9.425078
56	H	6.062489	0.908909	7.714252
57	C	5.278454	3.528511	9.561862
58	O	4.954334	4.109492	10.534255

TS7-1

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.430436238	-0.002892170	1.905034240
1.491626307	-0.033968812	5.759490405
4.135936238	1.910185227	-0.008043157
4.142683771	1.921076933	3.895133439
4.135936238	-0.002892170	1.905034240
4.079344779	-0.007681863	5.792439760
1.430436238	1.910185227	-0.008043157
1.435404094	1.909317558	3.882036750
0.077686238	-0.002892170	-0.008043157
0.069848199	0.000266130	3.930227630
2.783186238	1.910185227	1.905034240
2.770942636	1.910837740	5.649056179
6.841436238	-0.002892170	1.905034240
6.924079262	0.061078871	5.766448196
9.546936238	1.910185227	-0.008043157
9.528275467	1.909925786	3.838807250
9.546936238	-0.002892170	1.905034240
9.457091808	0.104585074	5.728719410
6.841436238	1.910185227	-0.008043157
6.899289725	1.896735431	3.867989899
5.488686238	-0.002892170	-0.008043157
5.506234045	0.005335036	3.944184449
8.194186238	1.910185227	1.905034240
8.230838797	1.913349252	5.491358505

1.430436238	3.823262623	1.905034240
1.494262957	3.854565452	5.752215419
4.135936238	5.736340020	-0.008043157
4.084174868	5.737452914	3.748622403
4.135936238	3.823262623	1.905034240
4.086618138	3.858002369	5.829141627
1.430436238	5.736340020	-0.008043157
1.493734405	5.737614687	3.730786464
0.077686238	3.823262623	-0.008043157
0.069933698	3.820482010	3.928061309
2.783186238	5.736340020	1.905034240
2.778956516	5.743659280	5.588829533
6.841436238	3.823262623	1.905034240
6.911393225	3.775976012	5.684974058
9.546936238	5.736340020	-0.008043157
9.552653766	5.738107975	3.913396799
9.546936238	3.823262623	1.905034240
9.452081968	3.718736010	5.721263396
6.841436238	5.736340020	-0.008043157
6.843315069	5.755337305	3.896188729
5.488686238	3.823262623	-0.008043157
5.505182799	3.826749595	3.928337674
8.194186238	5.736340020	1.905034240
8.191521998	5.734720150	5.672498188
7.697414088	3.709904019	8.604087601
7.806873477	3.630052137	9.830913751
7.821582031	2.041461503	7.983490832
5.948182649	3.321740526	8.487939544
6.458477231	1.865776909	8.324985800
5.204900559	3.718249310	7.739827448
6.334931987	1.286377866	9.255314708
5.939252043	1.337424203	7.522849527
5.816281205	3.736169734	9.827482005
5.328142619	4.160390666	10.800767674

OCH_2CNHCO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.486222	-0.037505	5.752338
3	O	4.135936	1.910185	-0.008043
4	O	4.140958	1.919991	3.895632
5	O	4.135936	-0.002892	1.905034
6	O	4.077479	-0.004981	5.797150
7	O	1.430436	1.910185	-0.008043
8	O	1.427699	1.908024	3.878642
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.073195	-0.006411	3.923830
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.764712	1.910826	5.647796
13	O	6.841436	-0.002892	1.905034
14	O	6.925104	0.071365	5.784493
15	O	9.546936	1.910185	-0.008043
16	O	9.527271	1.907360	3.835074
17	O	9.546936	-0.002892	1.905034
18	O	9.453006	0.108901	5.735539
19	O	6.841436	1.910185	-0.008043
20	O	6.897548	1.891922	3.862952
21	Ce	5.488686	-0.002892	-0.008043

22	Ce	5.500595	0.002982	3.944811
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.242008	1.906397	5.447216
25	O	1.430436	3.823263	1.905034
26	O	1.485064	3.854511	5.744710
27	O	4.135936	5.736340	-0.008043
28	O	4.082622	5.738430	3.751547
29	O	4.135936	3.823263	1.905034
30	O	4.077927	3.856277	5.835001
31	O	1.430436	5.736340	-0.008043
32	O	1.489630	5.736855	3.728216
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.071161	3.822389	3.925173
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.775132	5.741074	5.591338
37	O	6.841436	3.823263	1.905034
38	O	6.898990	3.761994	5.674745
39	O	9.546936	5.736340	-0.008043
40	O	9.551746	5.736492	3.915722
41	O	9.546936	3.823263	1.905034
42	O	9.442143	3.710629	5.725034
43	O	6.841436	5.736340	-0.008043
44	O	6.840343	5.757576	3.900995
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.497210	3.827519	3.927052
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.187726	5.730035	5.675852
49	N	7.444333	3.756149	8.229336
50	O	7.553950	4.038937	9.753128
51	O	7.746894	2.332982	8.039781
52	C	5.985139	3.417252	8.481746
53	C	6.344076	1.937854	8.310026
54	H	5.243132	3.848990	7.794224
55	H	6.276316	1.307585	9.208778
56	H	5.919456	1.424457	7.438233
57	C	6.181019	3.895793	9.895876
58	O	5.519106	4.117226	10.872791

TS7-2

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.430436238	-0.002892170	1.905034240
1.477375405	-0.034218941	5.789094340
4.135936238	1.910185227	-0.008043157
4.133295572	1.973994379	3.951535623
4.135936238	-0.002892170	1.905034240
4.051680576	-0.011748135	5.790366023
1.430436238	1.910185227	-0.008043157
1.429012183	1.892577374	3.890384302
0.077686238	-0.002892170	-0.008043157
0.051311740	0.001042810	3.928100620
2.783186238	1.910185227	1.905034240
2.764308598	1.882222548	5.699088149
6.841436238	-0.002892170	1.905034240
6.898467275	0.047296012	5.745210778
9.546936238	1.910185227	-0.008043157
9.517883934	1.910200839	3.856265495
9.546936238	-0.002892170	1.905034240
9.436888263	0.081399850	5.729805148

6.841436238	1.910185227	-0.008043157
6.889974014	1.893555786	3.877885703
5.488686238	-0.002892170	-0.008043157
5.513247695	0.006549937	3.953018847
8.194186238	1.910185227	1.905034240
8.206740279	1.905854236	5.542405960
1.430436238	3.823262623	1.905034240
1.579527018	3.844109134	5.712478870
4.135936238	5.736340020	-0.008043157
4.079827463	5.692740328	3.795542081
4.135936238	3.823262623	1.905034240
4.271055958	3.876497636	6.311670023
1.430436238	5.736340020	-0.008043157
1.491317244	5.750249485	3.739544727
0.077686238	3.823262623	-0.008043157
0.067102825	3.817624187	3.923116152
2.783186238	5.736340020	1.905034240
2.784823263	5.756125543	5.639494220
6.841436238	3.823262623	1.905034240
6.915402445	3.792334951	5.632242126
9.546936238	5.736340020	-0.008043157
9.545227320	5.737187005	3.898966383
9.546936238	3.823262623	1.905034240
9.463750563	3.747191609	5.706522288
6.841436238	5.736340020	-0.008043157
6.837955200	5.756182925	3.879652590
5.488686238	3.823262623	-0.008043157
5.541270137	3.830043773	3.930919234
8.194186238	5.736340020	1.905034240
8.195390220	5.715348440	5.690904113
7.491938232	4.121572836	8.306183452
7.584525681	4.548197468	9.611141546
7.866015781	2.135446749	7.793386154
6.157616617	3.523985742	8.448886124
6.558581843	2.025445488	8.322215737
5.183040706	3.824619109	7.391219578
6.547007266	1.495384175	9.309620214
5.919032480	1.432461796	7.642138722
6.185516297	4.020527548	9.877731319
5.655031268	4.171394468	10.918689014

OCH_2CNCO_2*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.437636	-0.038777	5.809128
3	O	4.135936	1.910185	-0.008043
4	O	4.120110	1.962009	3.937857
5	O	4.135936	-0.002892	1.905034
6	O	4.007104	-0.025820	5.769675
7	O	1.430436	1.910185	-0.008043
8	O	1.423125	1.879439	3.885730
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.025605	-0.004732	3.903648
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.717955	1.843140	5.672230
13	O	6.841436	-0.002892	1.905034
14	O	6.854381	0.025948	5.696162
15	O	9.546936	1.910185	-0.008043
16	O	9.527105	1.900757	3.855721

17	O	9.546936	-0.002892	1.905034
18	O	9.408785	0.039732	5.687497
19	O	6.841436	1.910185	-0.008043
20	O	6.877241	1.914637	3.867174
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.501654	0.003852	3.926543
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.184271	1.815112	5.564568
25	O	1.430436	3.823263	1.905034
26	O	1.562137	3.846978	5.706653
27	O	4.135936	5.736340	-0.008043
28	O	4.067106	5.689989	3.781809
29	O	4.135936	3.823263	1.905034
30	O	4.140750	3.838867	6.180877
31	O	1.430436	5.736340	-0.008043
32	O	1.485189	5.760753	3.735719
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.035926	3.820395	3.911564
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.724012	5.786857	5.605825
37	O	6.841436	3.823263	1.905034
38	O	6.735342	3.823553	5.732158
39	O	9.546936	5.736340	-0.008043
40	O	9.543947	5.739429	3.855231
41	O	9.546936	3.823263	1.905034
42	O	9.376003	3.800907	5.628751
43	O	6.841436	5.736340	-0.008043
44	O	6.822939	5.732355	3.842215
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.533834	3.824552	3.840701
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.157419	5.711677	5.683814
49	N	7.816475	4.909822	8.369269
50	O	7.294794	5.841305	9.511308
51	O	8.183936	1.997104	7.625660
52	C	7.368698	3.854049	8.964911
53	C	7.368228	2.401967	8.636814
54	H	5.120252	3.832693	6.403813
55	H	7.619281	1.886584	9.595588
56	H	6.286768	2.152101	8.473612
57	C	6.828717	4.686432	10.114877
58	O	6.238985	4.567806	11.148822

TS7-3

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.430436238	-0.002892170	1.905034240
1.440115917	-0.038152222	5.806363984
4.135936238	1.910185227	-0.008043157
4.122183775	1.963745994	3.936726066
4.135936238	-0.002892170	1.905034240
4.010203238	-0.025562658	5.763845965
1.430436238	1.910185227	-0.008043157
1.423350418	1.879732159	3.885907480
0.077686238	-0.002892170	-0.008043157
0.028238767	-0.004944412	3.900370305
2.783186238	1.910185227	1.905034240
2.721385073	1.840859408	5.677725515
6.841436238	-0.002892170	1.905034240

6.861032054	0.032898667	5.684852421
9.546936238	1.910185227	-0.008043157
9.527090144	1.901123636	3.851913581
9.546936238	-0.002892170	1.905034240
9.411961843	0.041609027	5.680926795
6.841436238	1.910185227	-0.008043157
6.877477284	1.918094796	3.864661693
5.488686238	-0.002892170	-0.008043157
5.500526965	0.003118494	3.922860453
8.194186238	1.910185227	1.905034240
8.187675734	1.817776666	5.549492467
1.430436238	3.823262623	1.905034240
1.565684042	3.845636559	5.705009646
4.135936238	5.736340020	-0.008043157
4.067314810	5.690290374	3.782671980
4.135936238	3.823262623	1.905034240
4.146158740	3.840138098	6.174306413
1.430436238	5.736340020	-0.008043157
1.483991076	5.759810431	3.735071302
0.077686238	3.823262623	-0.008043157
0.043181003	3.819788091	3.912769072
2.783186238	5.736340020	1.905034240
2.729550895	5.786909739	5.611165017
6.841436238	3.823262623	1.905034240
6.745720775	3.821451883	5.730962231
9.546936238	5.736340020	-0.008043157
9.544830641	5.739376965	3.854841064
9.546936238	3.823262623	1.905034240
9.377114862	3.797857836	5.638578833
6.841436238	5.736340020	-0.008043157
6.824871345	5.732255510	3.841927881
5.488686238	3.823262623	-0.008043157
5.536303925	3.825538580	3.844072178
8.194186238	5.736340020	1.905034240
8.158134560	5.723223548	5.690875562
7.913910753	4.886245714	8.327032717
6.735795570	6.110586250	9.655356736
8.200433859	1.977381333	7.630208173
7.393668684	3.949554589	8.929617741
7.414997609	2.415886174	8.633332897
5.122819517	3.835978757	6.406418833
7.687286544	1.954625201	9.605137650
6.333635224	2.216974508	8.488303160
6.578211783	4.916668972	10.106563645
6.003514635	4.499626075	11.096209262

$OCH_2CN^*+CO_2^*$

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.441892	-0.035753	5.808269
3	O	4.135936	1.910185	-0.008043
4	O	4.122443	1.970283	3.936070
5	O	4.135936	-0.002892	1.905034
6	O	4.011986	-0.024219	5.750218
7	O	1.430436	1.910185	-0.008043
8	O	1.424005	1.880606	3.886552
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.026035	-0.003054	3.900874

11	Ce	2.783186	1.910185	1.905034
12	Ce	2.723242	1.842939	5.673528
13	O	6.841436	-0.002892	1.905034
14	O	6.860574	0.030727	5.666811
15	O	9.546936	1.910185	-0.008043
16	O	9.526408	1.899817	3.847287
17	O	9.546936	-0.002892	1.905034
18	O	9.412850	0.047530	5.682621
19	O	6.841436	1.910185	-0.008043
20	O	6.874208	1.928611	3.864425
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.501575	0.005731	3.916795
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.191755	1.818817	5.562347
25	O	1.430436	3.823263	1.905034
26	O	1.570833	3.846679	5.710171
27	O	4.135936	5.736340	-0.008043
28	O	4.065533	5.687851	3.781142
29	O	4.135936	3.823263	1.905034
30	O	4.152343	3.847338	6.181913
31	O	1.430436	5.736340	-0.008043
32	O	1.484121	5.760956	3.735748
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.035750	3.819782	3.918998
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.729781	5.790513	5.604786
37	O	6.841436	3.823263	1.905034
38	O	6.753210	3.822060	5.750325
39	O	9.546936	5.736340	-0.008043
40	O	9.544892	5.741350	3.856870
41	O	9.546936	3.823263	1.905034
42	O	9.379844	3.791917	5.634794
43	O	6.841436	5.736340	-0.008043
44	O	6.822926	5.728773	3.839061
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.539190	3.826544	3.845289
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.160727	5.726961	5.685295
49	N	8.064516	5.204512	8.384214
50	O	4.769838	6.754799	9.212385
51	O	8.185181	1.917563	7.642741
52	C	7.798991	4.075058	8.523459
53	C	7.507611	2.622413	8.605524
54	H	5.132394	3.837623	6.405100
55	H	7.793441	2.294872	9.628610
56	H	6.401633	2.523612	8.539872
57	C	4.977459	5.803124	9.867990
58	O	5.168054	4.849279	10.530066

OCH_2CN*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.442091	-0.037347	5.808810
3	O	4.135936	1.910185	-0.008043
4	O	4.122110	1.968871	3.935584
5	O	4.135936	-0.002892	1.905034
6	O	4.017767	-0.026275	5.764244
7	O	1.430436	1.910185	-0.008043

8	O	1.423753	1.880071	3.886420
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.025594	-0.002764	3.900526
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.723276	1.840705	5.672331
13	O	6.841436	-0.002892	1.905034
14	O	6.858399	0.029136	5.669408
15	O	9.546936	1.910185	-0.008043
16	O	9.524164	1.899457	3.850129
17	O	9.546936	-0.002892	1.905034
18	O	9.411842	0.049691	5.681043
19	O	6.841436	1.910185	-0.008043
20	O	6.874168	1.926052	3.861948
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.501106	0.004579	3.917386
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.186645	1.820255	5.562970
25	O	1.430436	3.823263	1.905034
26	O	1.572593	3.844423	5.706672
27	O	4.135936	5.736340	-0.008043
28	O	4.066905	5.687021	3.779564
29	O	4.135936	3.823263	1.905034
30	O	4.149028	3.845204	6.178352
31	O	1.430436	5.736340	-0.008043
32	O	1.481724	5.760782	3.734265
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.035213	3.818989	3.918773
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.729663	5.789014	5.602102
37	O	6.841436	3.823263	1.905034
38	O	6.756415	3.817839	5.747182
39	O	9.546936	5.736340	-0.008043
40	O	9.545087	5.742120	3.856453
41	O	9.546936	3.823263	1.905034
42	O	9.380235	3.790336	5.633123
43	O	6.841436	5.736340	-0.008043
44	O	6.823346	5.728217	3.840093
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.540418	3.825072	3.845662
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.162555	5.727404	5.685988
49	N	8.086020	5.214989	8.385814
50	O	8.157194	1.930979	7.642657
51	C	7.792582	4.095403	8.523492
52	C	7.470133	2.649503	8.588269
53	H	5.125565	3.838773	6.418652
54	H	7.716951	2.304883	9.615826
55	H	6.363646	2.580111	8.484658

HCHO*+NCO*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.490407	-0.056752	5.786738
3	O	4.135936	1.910185	-0.008043
4	O	4.127453	1.942067	3.891829
5	O	4.135936	-0.002892	1.905034
6	O	4.084346	-0.038183	5.757307
7	O	1.430436	1.910185	-0.008043

8	O	1.426864	1.897716	3.874256
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.112082	-0.016883	3.833786
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.733371	1.824682	5.660612
13	O	6.841436	-0.002892	1.905034
14	O	7.002516	0.098933	5.770995
15	O	9.546936	1.910185	-0.008043
16	O	9.550691	1.864415	3.874336
17	O	9.546936	-0.002892	1.905034
18	O	9.573592	0.088085	5.797039
19	O	6.841436	1.910185	-0.008043
20	O	6.897622	2.049017	4.032839
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.503754	0.007587	3.943721
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.347017	1.750872	5.560398
25	O	1.430436	3.823263	1.905034
26	O	1.543006	3.858427	5.734561
27	O	4.135936	5.736340	-0.008043
28	O	4.074604	5.700023	3.747176
29	O	4.135936	3.823263	1.905034
30	O	4.327118	3.809736	6.021549
31	O	1.430436	5.736340	-0.008043
32	O	1.503829	5.734682	3.721893
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.061401	3.829085	3.885651
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.757439	5.783362	5.606157
37	O	6.841436	3.823263	1.905034
38	O	6.732096	2.806857	7.323087
39	O	9.546936	5.736340	-0.008043
40	O	9.594918	5.777282	3.905296
41	O	9.546936	3.823263	1.905034
42	O	8.997697	3.760208	5.686806
43	O	6.841436	5.736340	-0.008043
44	O	6.817355	5.643118	4.056868
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.464149	3.829485	3.726235
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.291758	5.927329	5.768864
49	N	7.429462	5.015220	8.070107
50	O	9.426581	1.823060	7.872723
51	C	7.097381	3.920157	7.721153
52	C	8.973534	1.620739	8.987035
53	H	5.035829	3.543041	6.648972
54	H	9.635873	1.679694	9.878852
55	H	7.902545	1.383112	9.149071

TS7-4

X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1.430436238	-0.002892170	1.905034240
1.439382523	-0.034815453	5.809615051
4.135936238	1.910185227	-0.008043157
4.115867134	1.964724432	3.933704481
4.135936238	-0.002892170	1.905034240
4.011996885	-0.014515931	5.768401539
1.430436238	1.910185227	-0.008043157

1.412770127	1.877508691	3.890144839
0.077686238	-0.002892170	-0.008043157
0.022304728	-0.012552402	3.907004608
2.783186238	1.910185227	1.905034240
2.715781155	1.838804487	5.669073396
6.841436238	-0.002892170	1.905034240
6.873678799	0.097591076	5.656147331
9.546936238	1.910185227	-0.008043157
9.508189851	1.908227750	3.844406734
9.546936238	-0.002892170	1.905034240
9.415325764	0.066582400	5.681862077
6.841436238	1.910185227	-0.008043157
6.877501558	1.920255094	3.825497973
5.488686238	-0.002892170	-0.008043157
5.500643545	0.003746621	3.914450222
8.194186238	1.910185227	1.905034240
8.181462047	1.887567488	5.445343892
1.430436238	3.823262623	1.905034240
1.574390398	3.846566166	5.702257293
4.135936238	5.736340020	-0.008043157
4.060007804	5.698316685	3.779600747
4.135936238	3.823262623	1.905034240
4.164697539	3.873234248	6.110449282
1.430436238	5.736340020	-0.008043157
1.477295140	5.761624415	3.740597690
0.077686238	3.823262623	-0.008043157
0.048520898	3.826270402	3.922880930
2.783186238	5.736340020	1.905034240
2.726211335	5.798150982	5.606009682
6.841436238	3.823262623	1.905034240
6.840543756	3.733032489	5.680316736
9.546936238	5.736340020	-0.008043157
9.546748622	5.732914059	3.865566618
9.546936238	3.823262623	1.905034240
9.424013373	3.757456274	5.674079980
6.841436238	5.736340020	-0.008043157
6.816664218	5.733909535	3.864012912
5.488686238	3.823262623	-0.008043157
5.537604171	3.828012628	3.866568451
8.194186238	5.736340020	1.905034240
8.164798083	5.725667176	5.738458223
7.583111753	5.560085991	8.225749086
8.174669262	1.864940632	7.763485697
6.770188529	4.745243155	8.509768902
7.248145298	1.724556510	8.559064944
5.011506643	3.964393399	6.602364218
7.489934237	1.643903053	9.620762167
6.218040725	1.580834693	8.246186408

HCHO*+CN*

ATOM		X (Angstroms)	Y (Angstroms)	Z (Angstroms)
1	O	1.430436	-0.002892	1.905034
2	O	1.438432	-0.033171	5.818553
3	O	4.135936	1.910185	-0.008043
4	O	4.109567	1.963901	3.932605
5	O	4.135936	-0.002892	1.905034
6	O	4.011782	0.000878	5.776153
7	O	1.430436	1.910185	-0.008043

8	O	1.406353	1.875780	3.900376
9	Ce	0.077686	-0.002892	-0.008043
10	Ce	0.013553	-0.016069	3.925043
11	Ce	2.783186	1.910185	1.905034
12	Ce	2.718692	1.841689	5.672488
13	O	6.841436	-0.002892	1.905034
14	O	6.872173	0.135484	5.627431
15	O	9.546936	1.910185	-0.008043
16	O	9.503037	1.913241	3.841572
17	O	9.546936	-0.002892	1.905034
18	O	9.410031	0.056789	5.702750
19	O	6.841436	1.910185	-0.008043
20	O	6.867663	1.923161	3.790024
21	Ce	5.488686	-0.002892	-0.008043
22	Ce	5.501756	0.007038	3.907303
23	Ce	8.194186	1.910185	1.905034
24	Zr	8.170760	1.923618	5.450441
25	O	1.430436	3.823263	1.905034
26	O	1.581244	3.849017	5.709505
27	O	4.135936	5.736340	-0.008043
28	O	4.053282	5.704322	3.778478
29	O	4.135936	3.823263	1.905034
30	O	4.189133	3.878754	6.068137
31	O	1.430436	5.736340	-0.008043
32	O	1.471424	5.761679	3.748446
33	Ce	0.077686	3.823263	-0.008043
34	Ce	0.053776	3.827437	3.936018
35	Zr	2.783186	5.736340	1.905034
36	Ce	2.738681	5.804229	5.618911
37	O	6.841436	3.823263	1.905034
38	O	6.894048	3.693021	5.656065
39	O	9.546936	5.736340	-0.008043
40	O	9.542690	5.724436	3.888685
41	O	9.546936	3.823263	1.905034
42	O	9.451047	3.745656	5.721680
43	O	6.841436	5.736340	-0.008043
44	O	6.813599	5.732798	3.890916
45	Ce	5.488686	3.823263	-0.008043
46	Ce	5.536235	3.824906	3.873915
47	Ce	8.194186	5.736340	1.905034
48	Ce	8.156245	5.731276	5.736832
49	N	7.039595	5.837058	8.037495
50	O	8.041117	1.696364	7.821593
51	C	5.972738	5.320455	8.117034
52	C	7.118466	1.120183	8.393725
53	H	4.883831	4.070430	6.755623
54	H	7.177547	0.967858	9.489169
55	H	6.236208	0.751556	7.843963